

**Supporting Information (S.I.)**

Hydride-mediated chemoselective C-H bond formation during benzoic acid

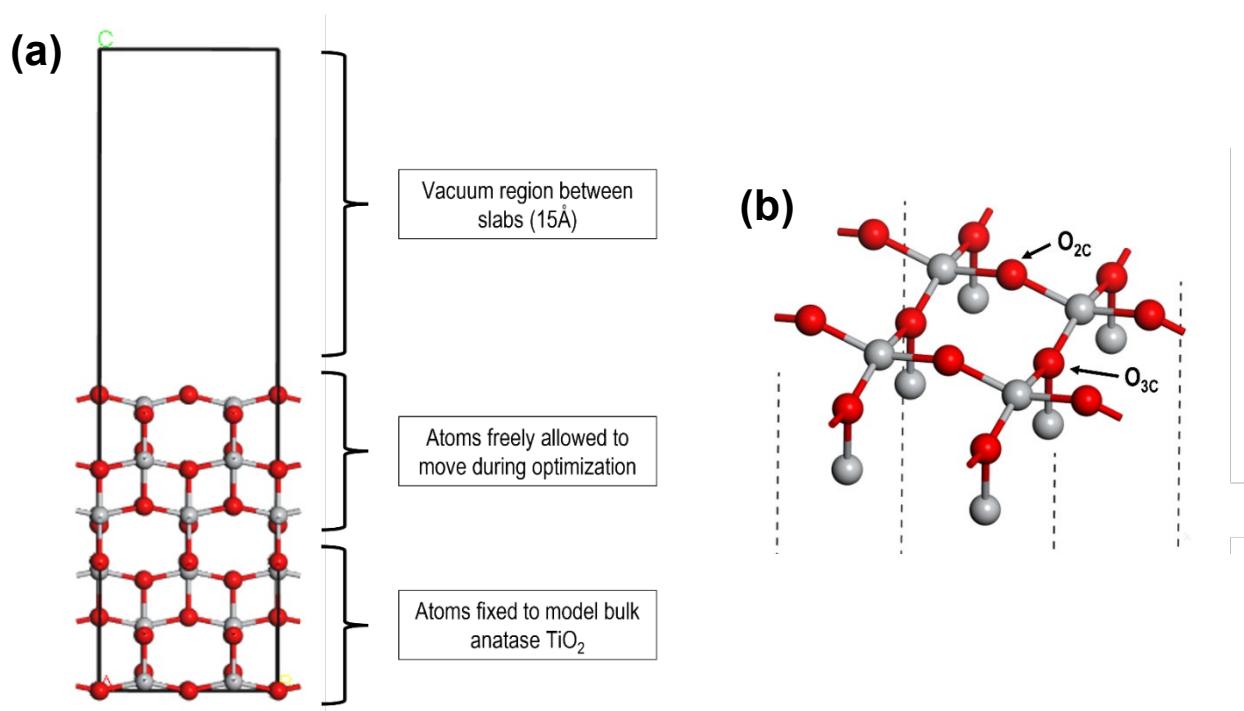
hydrodeoxygenation on anatase TiO<sub>2</sub>

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**Figure S1.** (a) Model slab for anatase TiO<sub>2</sub> depicting atomic layers frozen and relaxed during DFT geometric optimization calculations, and (b) top view of model slab. Ti is depicted in gray, and O is depicted in red.

### Adjustment of gas-phase DFT for thermodynamic consistency

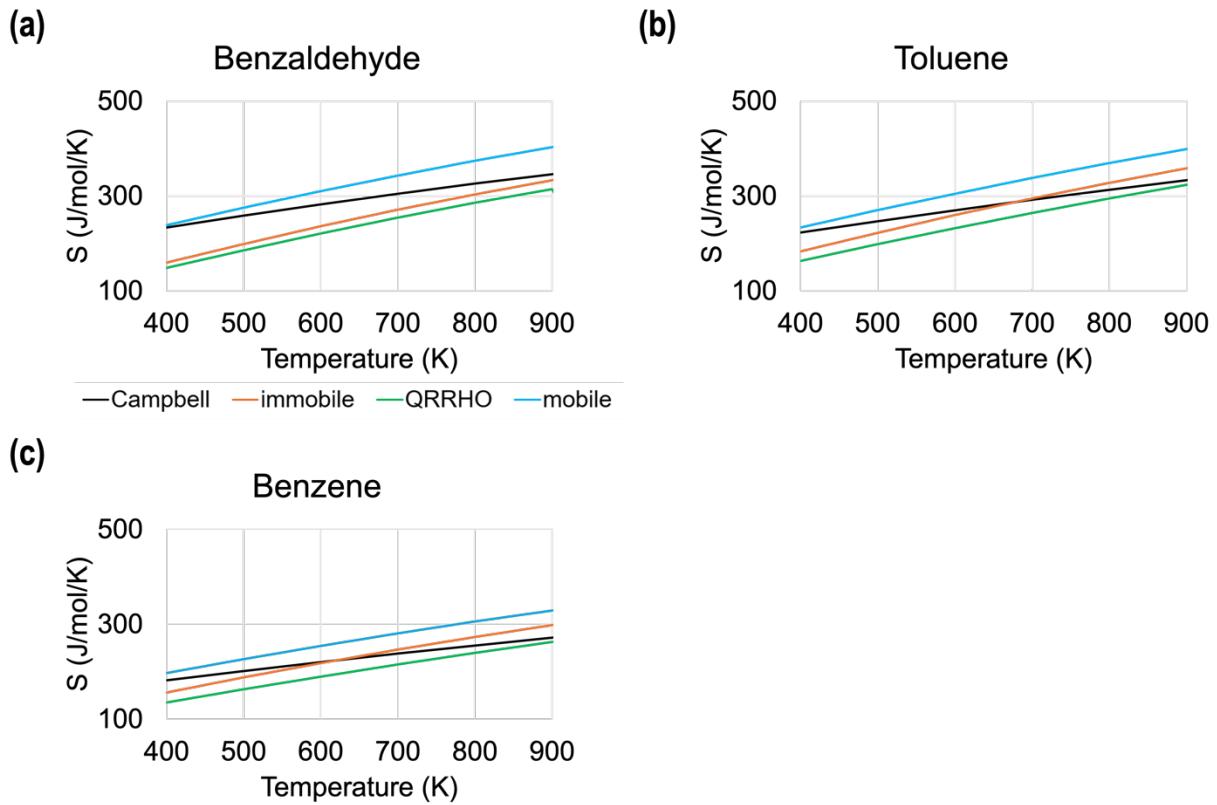
Following the method of Vorotnikov et al.<sup>1</sup>, a reference adjustment is made for DFT-calculated gas-phase energies by minimizing the errors between DFT-calculated gas phase energies and their experimentally determined heats of formation<sup>2</sup> (Eqn. S1).

$$\text{Correction} = H_{f,\text{DFT}}^i - H_{f,\text{exp}}^i + n^i (A^T A)^{-1} (A^T h) \quad (\text{Eqn. S1})$$

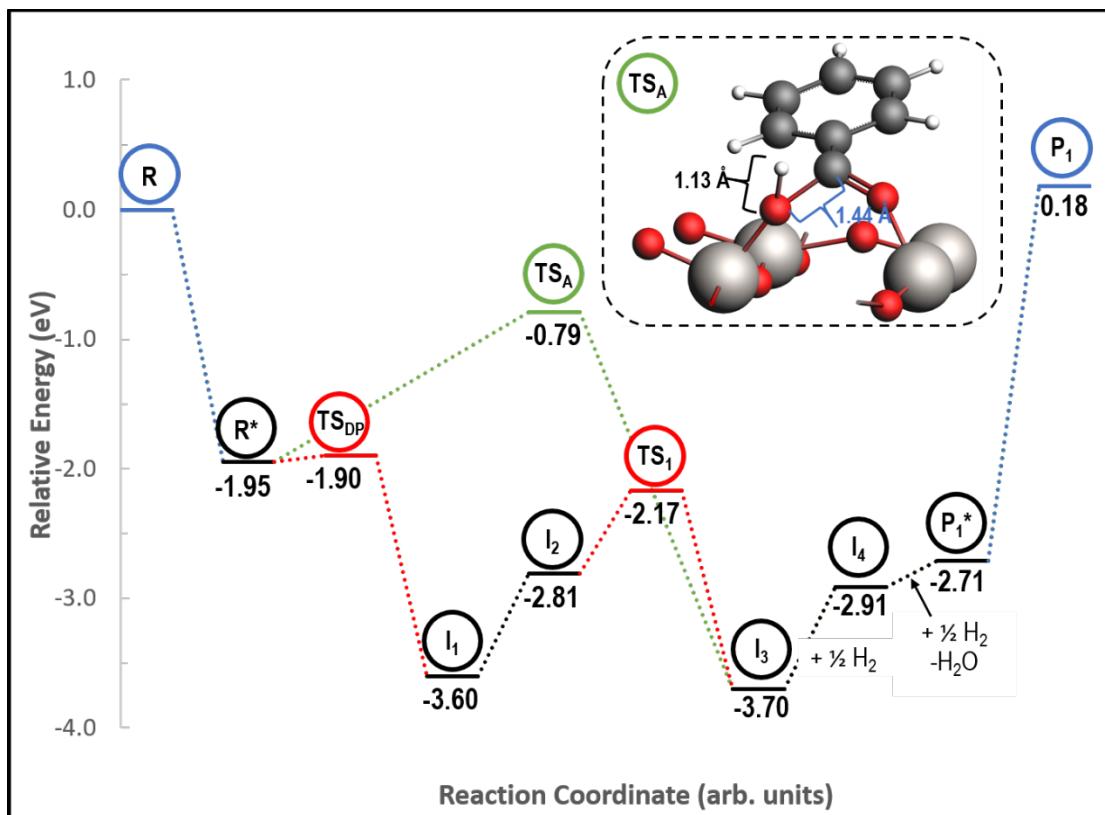
where  $H_{f,\text{DFT}}^i$  is the heat of formation of species  $i$  computed using DFT,  $H_{f,\text{exp}}^i$  is the heat of formation of species  $i$  from NIST database, vector  $n^i$  contains the number of each constituent atom of species  $i$ , matrix  $A$  contains the atomic composition of each reference compound, and vector  $h$  contains energy difference between DFT and NIST heats of formation.

**Table S1.** Matrices and vectors corresponding to Eqn. S1, and calculated corrections for gas-phase DFT thermodynamic values.

Species	C	H	O	$H_{f,\text{exp}}$ (kJ/mol)	$H_{f,\text{DFT}}$ (kJ/mol)	$H_{f,\text{exp}} - H_{f,\text{DFT}}$ (kJ/mol)	Correction (kJ/mol)
BZA	7	6	2	-294.10	-9284.79	8990.69	-10.27
BAld	7	6	1	-36.80	-8577.88	8541.08	-14.75
BnOH	7	8	1	-94.60	-9246.96	9152.36	-2.85
Tol	7	8	0	50.17	-8627.27	8677.44	17.97
Benz	6	6	0	82.88	-7097.73	7180.61	5.52
$H_2$	0	2	0	0.00	-627.40	627.40	-4.22
$H_2O$	0	2	1	-241.83	-1316.88	1075.05	2.22
CO	1	0	1	-110.53	-1414.36	1303.83	36.36
$CO_2$	1	0	2	-393.52	-2188.03	1794.51	-0.22



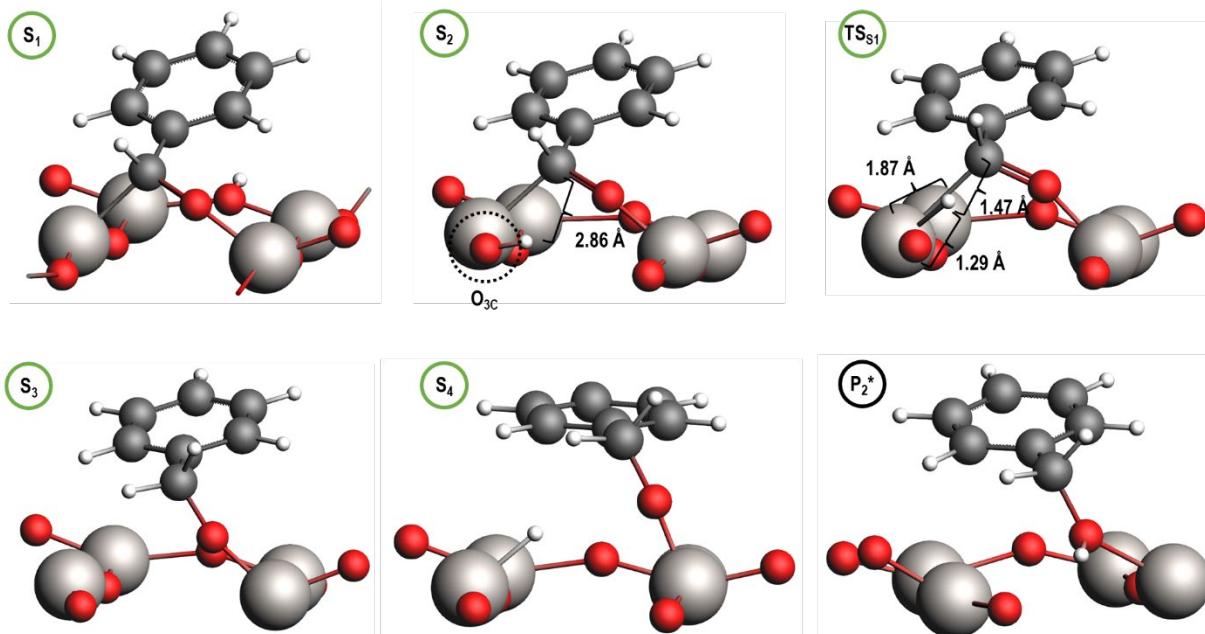
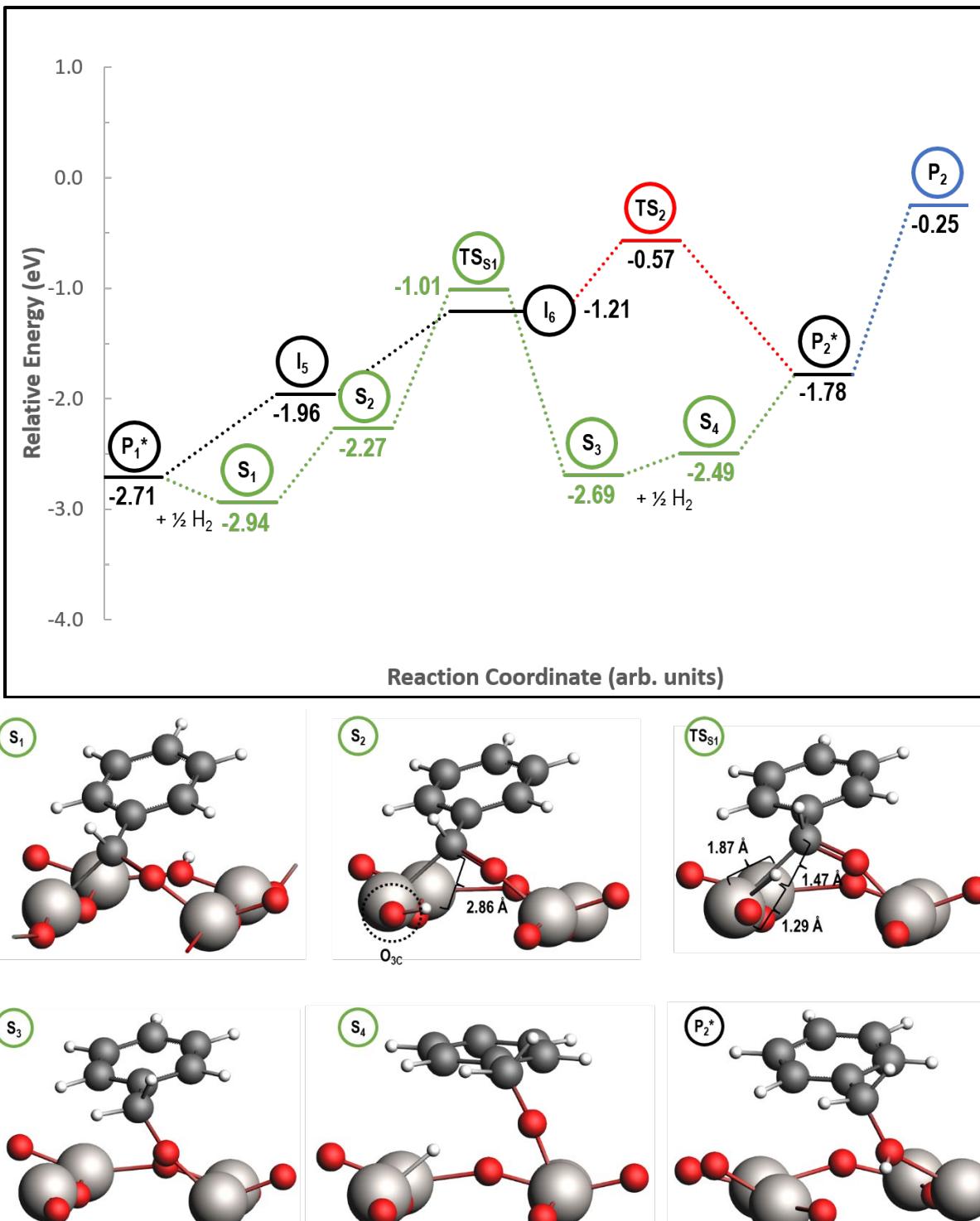
**Figure S2.** Comparison of adsorbed species entropies using Campbell and Sellers' method (black), immobile (orange) and mobile approximations<sup>3</sup> (blue), and Quasi Rigid Rotor Harmonic Oscillator approximation (QRRHO)<sup>4</sup> (green) for (a) benzaldehyde, (b) toluene, and (c) benzene. In the mobile approach, harmonic frequencies associated with rotational and translational motions of adsorbates were examined based on visual inspection of frequencies lower than  $125\text{ cm}^{-1}$ . 2-dimensional motion with 700 pm translational freedom at each direction on the surface and 1-dimensional rotational motion with the axis perpendicular to the aromatic ring were identified for these aromatic products. At low temperatures, entropies using Campbell-Sellers' method are close to the entropies from mobile approximation, but as the temperature increases, they get closer to the values from the quasi-harmonic approximation. Entropies using Campbell-Sellers' method fall well within the limits set by reasonable assumptions for the adsorbed state in the investigated temperature range for hydrogenation reactions.



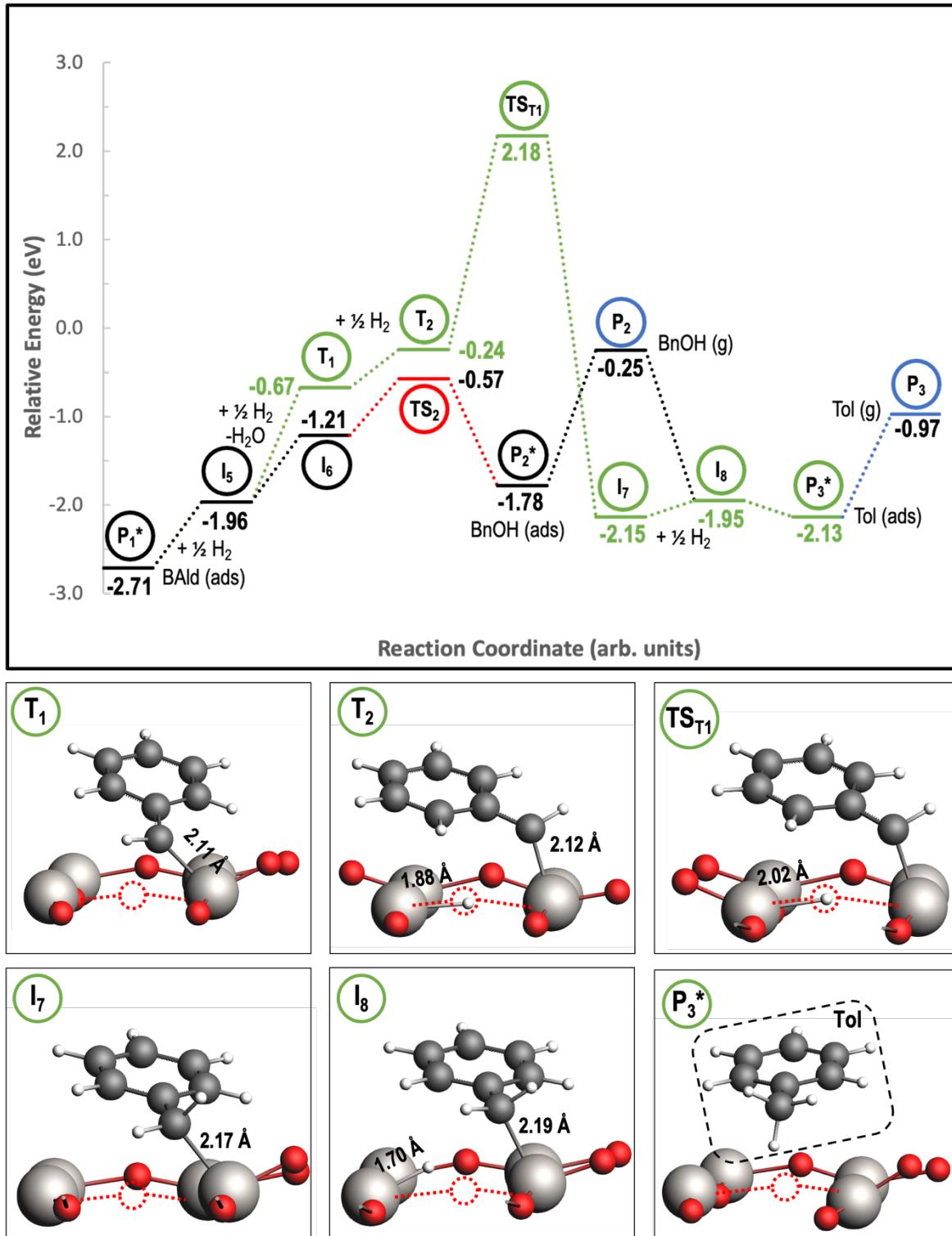
**Figure S3.** The alternate mechanism is shown in green for the first C-H bond formation to form benzaldehyde from benzoic acid, where the H migrates directly from the O on benzoic acid to the C. Ti is depicted in gray, O in red, C in black, and H in white.

Comparisons between the time scale ( $\tau$ ) of the mechanisms given an activation barrier of  $E_a$  were made using the Eyring equation and an attempt frequency of  $\frac{k_B T}{h}$  from transition state theory<sup>5,6</sup> (Eqn. S2):

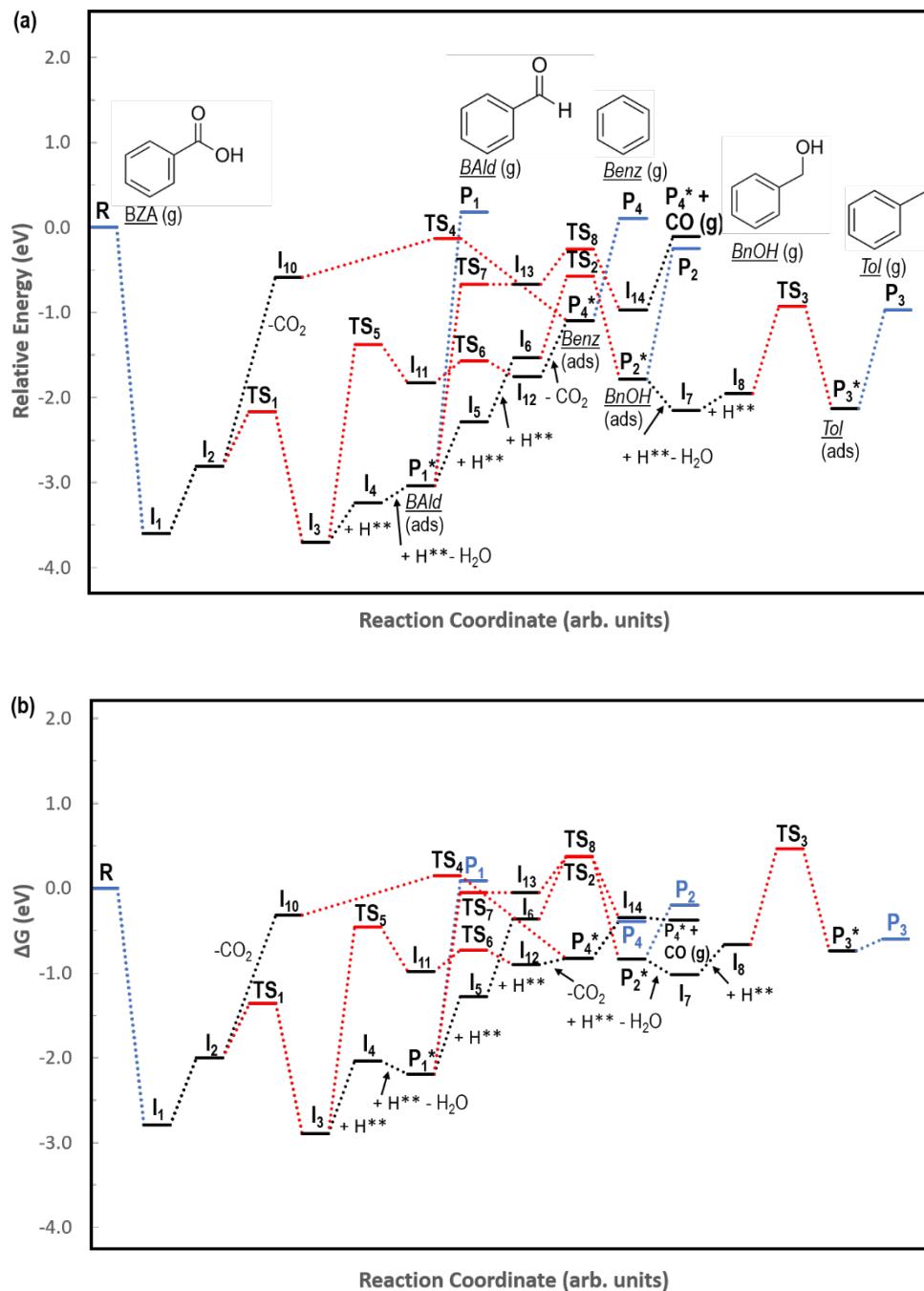
$$\tau = k^{-1} = \left( \frac{k_B T}{h} \exp\left(-\frac{E_a}{RT}\right) \right)^{-1} \quad (\text{Eqn. S2})$$



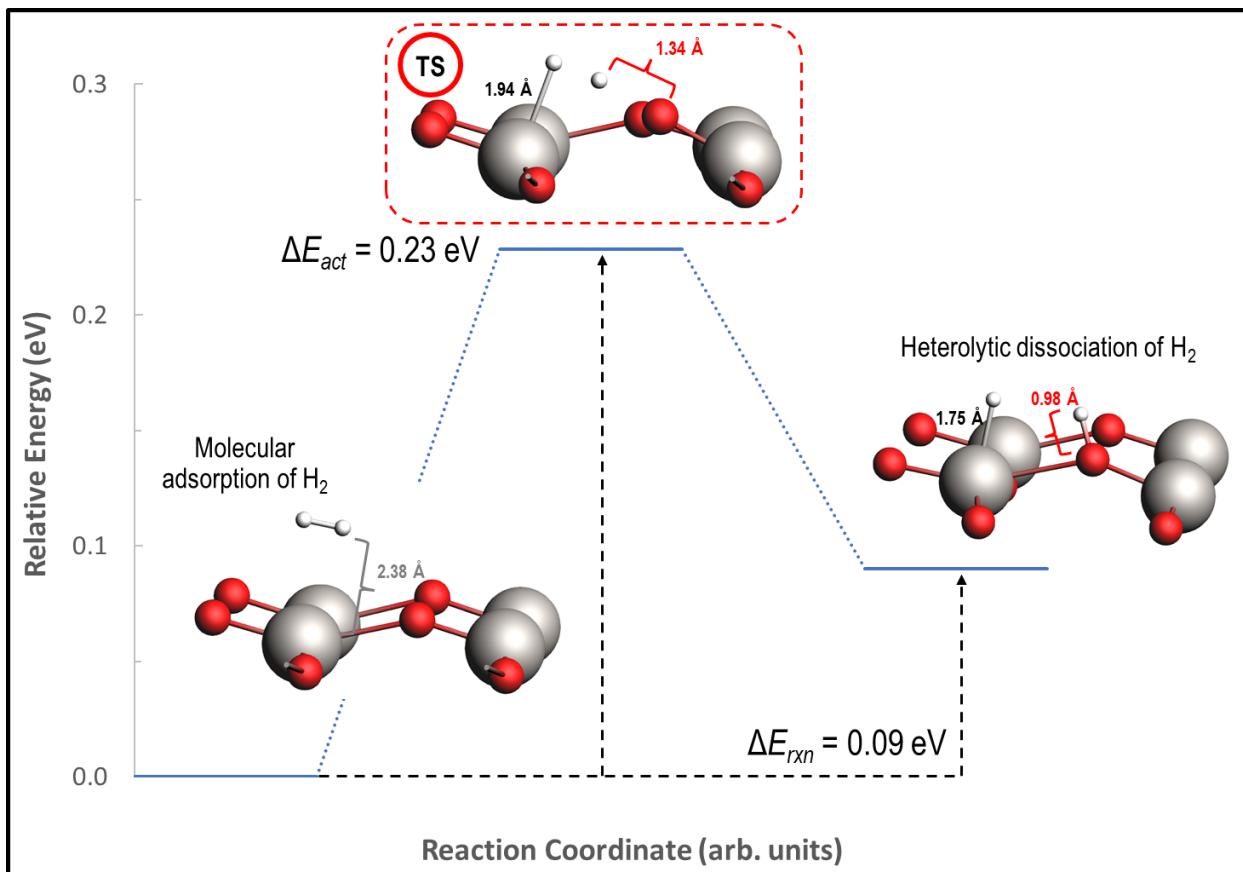
**Figure S4.** Alternate mechanism of benzyl alcohol formation from benzaldehyde is shown in green, where the first H atom is added to C via H migration from O<sub>3C</sub> (i.e., not the hydride). Ti is depicted in gray, O in red, C in black, and H in white.



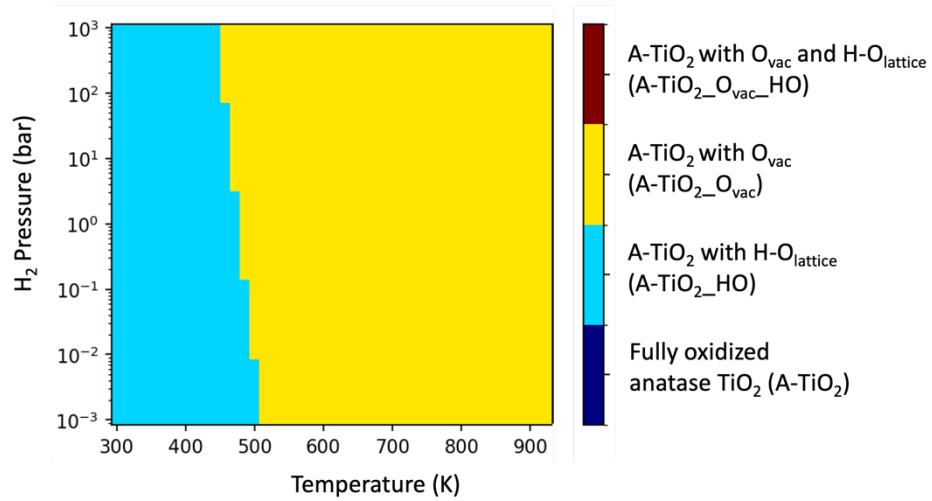
**Figure S5.** Alternative mechanism of toluene formation directly from benzaldehyde and bypassing benzyl alcohol is shown in green. Ti is depicted in gray, O in red, C in black, and H in white.



**Figure S6.** (a) Overall reaction energy diagram using DFT-calculated  $\Delta E$  for benzoic acid hydrogenation to benzaldehyde (P<sub>1</sub>), benzyl alcohol (P<sub>2</sub>), toluene (P<sub>3</sub>), and benzene (P<sub>4</sub>) with hydrogen provided from adsorbed hydrogen on lattice O sites (H<sup>\*\*</sup>); (b) Gibbs free energy diagram along the reaction coordinate at 540 K. The names of intermediates are consistent with the structures shown throughout the publication. Black dotted lines show reaction energies, red lines are kinetic activation barriers, and blue dotted lines correspond to desorption of products into the gas phase.



**Figure S7.** Reaction energy diagram of the heterolytic dissociation of  $\text{H}_2$  on anatase  $\text{TiO}_2$  (001) following  $\text{H}_2$  molecular adsorption. Ti is depicted in gray, O in red, C in black, and H in white. The coordination of adsorbed H species ( $\text{H}^{**}$ ) considered in the MKM is provided in the Appendix. Hydrogen spillover on anatase titania can involve activation barriers of 1.10 eV on the (001) surface.<sup>7</sup> Using a PEI analysis, we confirmed that this step is at equilibrium even when its barrier is increased from 0.23 to 1.10 eV. In addition, Karim et al. showed that iron oxide particles adsorbed on anatase  $\text{TiO}_2$  can be reduced regardless of the distance between the metal sites that activate and spillover hydrogen, suggesting that hydrogen diffusion and addition to O atoms of adsorbates on anatase  $\text{TiO}_2$  is kinetically favorable.<sup>8</sup> It is also worth noting that once H spillovers to the support, hydride species can readily be formed in the presence of oxygen vacancies at temperatures as low as 423 K, as shown in a recent NMR study regarding the evolution of multiple spillover hydrogen species on anatase  $\text{TiO}_2$ .<sup>9</sup> Hence, H diffusion and addition to O atoms and vacancies is expected to be as facile as H spillover on the titania surface, which is not found to be rate-determining in the current work.



**Figure S8.** Phase diagram of anatase  $\text{TiO}_2$  surface under dry conditions (water pressure was fixed at  $10^{-20}$  bar).

**Kinetic Model Differential Equations:**

(Eqns. S3)

$$\begin{aligned}
r_0 &= k_0 \theta_{**}^2 P_{H2} - k_{-0} \theta_{H**}^2 \\
r_1 &= k_1 \theta_* P_{BZA} - k_{-1} \theta_1 \\
r_2 &= k_2 \theta_1 - k_{-2} \theta_2 \\
r_3 &= k_3 \theta_2 - k_{-3} \theta_3 \\
r_4 &= k_4 \theta_3 \theta_{H**} - k_{-4} \theta_4 \theta_{**} \\
r_5 &= k_5 \theta_4 \theta_{H**} - k_{-5} \theta_{P1} \theta_{**} P_{H2O} \\
r_6 &= k_6 \theta_{P1} - k_{-6} \theta_* P_{BAld} \\
r_7 &= k_7 \theta_{P1} \theta_{H**} - k_{-7} \theta_5 \theta_{**} \\
r_8 &= k_8 \theta_5 \theta_{H**} - k_{-8} \theta_6 \theta_{**} \\
r_9 &= k_9 \theta_6 - k_{-9} \theta_{P2} \\
r_{10} &= k_{10} \theta_{P2} - k_{-10} \theta_* P_{BnOH} \\
r_{11} &= k_{11} \theta_{P2} \theta_{H**} - k_{-11} \theta_7 \theta_{**} P_{H2O} \\
r_{12} &= k_{12} \theta_7 \theta_{H**} - k_{-12} \theta_8 \theta_{**} \\
r_{13} &= k_{13} \theta_8 - k_{-13} \theta_{P3} \\
r_{14} &= k_{14} \theta_{P3} - k_{-14} \theta_* P_{Tol} \\
r_{15} &= k_{15} \theta_2 - k_{-15} \theta_{10} P_{CO_2} \\
r_{16} &= k_{16} \theta_{10} - k_{-16} \theta_{P4} \\
r_{17} &= k_{17} \theta_3 - k_{-17} \theta_{11} \\
r_{18} &= k_{18} \theta_{11} - k_{-18} \theta_{12} \\
r_{19} &= k_{19} \theta_{12} - k_{-19} \theta_{P4} P_{CO_2} \\
r_{20} &= k_{20} \theta_{P1} - k_{-20} \theta_{13} \\
r_{21} &= k_{21} \theta_{13} - k_{-21} \theta_{14} \\
r_{22} &= k_{22} \theta_{14} - k_{-22} \theta_{P4} P_{CO} \\
r_{23} &= k_{23} \theta_{P4} - k_{-23} \theta_* P_{Benz}
\end{aligned}$$

$$\begin{aligned}
\frac{d\theta_{**}}{dt} &= -2r_0 + r_4 + r_5 + r_7 + r_8 + r_{11} + r_{12} \\
\frac{d\theta_*}{dt} &= -r_1 + r_6 + r_{10} + r_{14} + r_{23} \\
\frac{d\theta_{H**}}{dt} &= 2r_0 - r_4 - r_5 - r_7 - r_8 - r_{11} - r_{12} \\
\frac{d\theta_1}{dt} &= r_1 - r_2 \\
\frac{d\theta_2}{dt} &= r_2 - r_3 - r_{15} \\
\frac{d\theta_3}{dt} &= r_3 - r_4 - r_{17} \\
\frac{d\theta_4}{dt} &= r_4 - r_5 \\
\frac{d\theta_{P1}}{dt} &= r_5 - r_6 - r_7 - r_{20} \\
\frac{d\theta_5}{dt} &= r_7 - r_8 \\
\frac{d\theta_6}{dt} &= r_8 - r_9 \\
\frac{d\theta_{P2}}{dt} &= r_9 - r_{10} - r_{11} \\
\frac{d\theta_7}{dt} &= r_{11} - r_{12} \\
\frac{d\theta_8}{dt} &= r_{12} - r_{13} \\
\frac{d\theta_{P3}}{dt} &= r_{13} - r_{14} \\
\frac{d\theta_{10}}{dt} &= r_{15} - r_{16} \\
\frac{d\theta_{11}}{dt} &= r_{17} - r_{18} \\
\frac{d\theta_{12}}{dt} &= r_{18} - r_{19} \\
\frac{d\theta_{13}}{dt} &= r_{20} - r_{21}
\end{aligned}$$

$$\frac{d\theta_{14}}{dt} = r_{21} - r_{22}$$

$$\frac{d\theta_{P4}}{dt} = r_{16} + r_{19} + r_{22} - r_{23}$$

Initial value constraint (site balance):

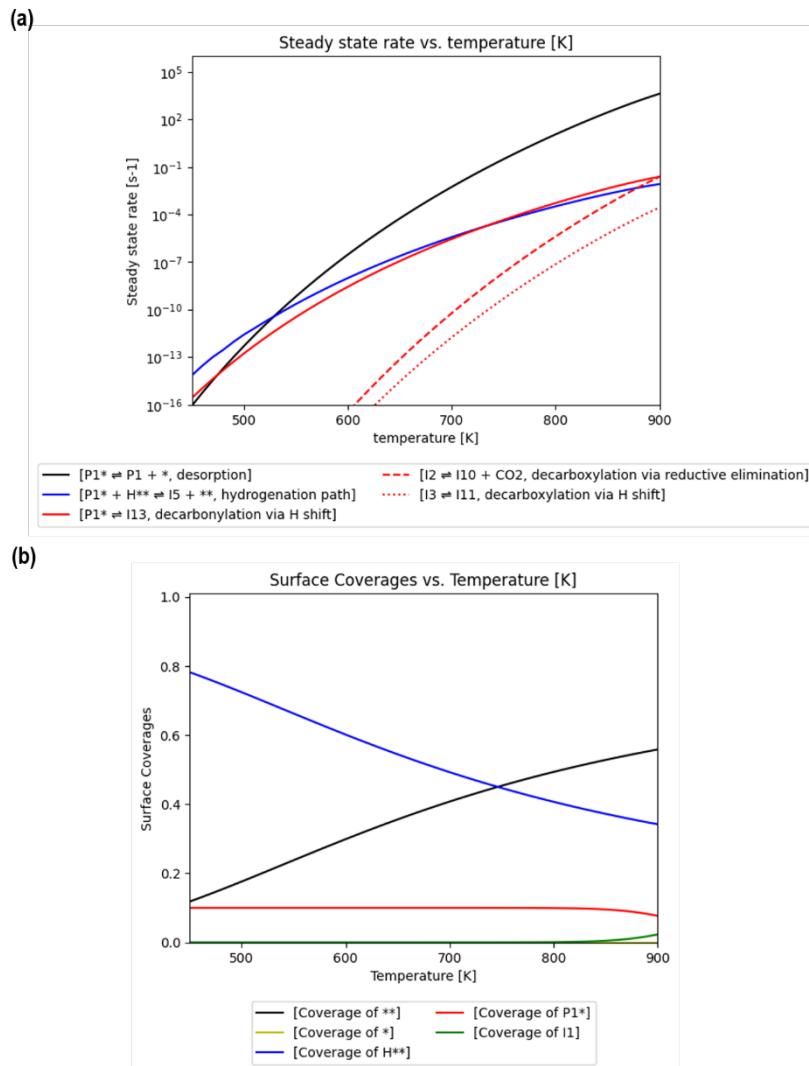
At t = 0,  $\theta_{**} = 0.9$ ,  $\theta_* = 0.1$ , with all others = 0 such that:

$$\theta_{**} + \theta_* + \theta_{H**} + \theta_R + \theta_{P1} + \theta_{P2} + \theta_{P3} + \theta_{P4} + \sum_{i=1}^{n=14} \theta_i = (\theta_{**} + \theta_*)|_{t=0}$$

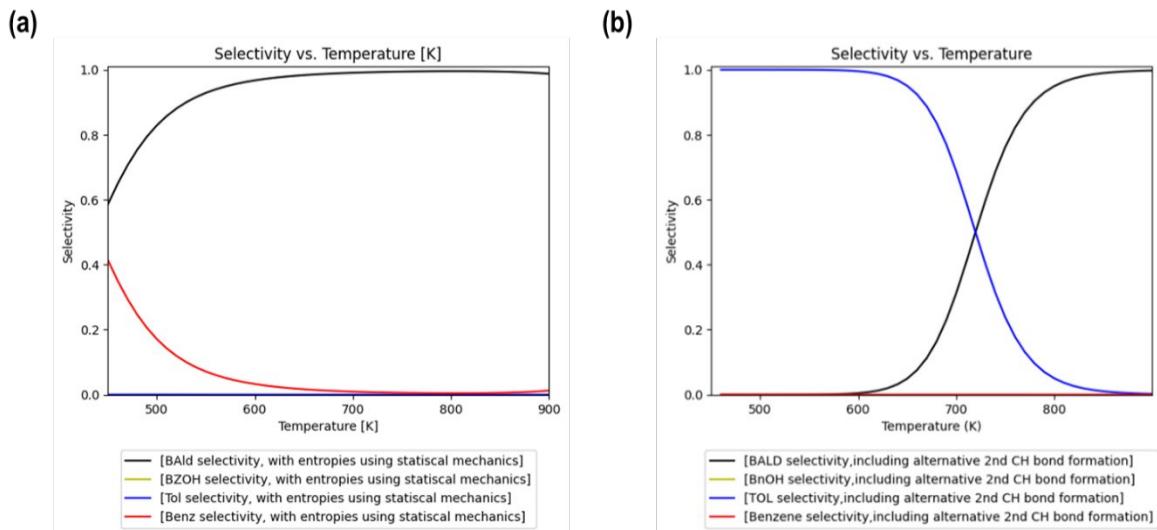
### Kinetic Model Parameters:

$$P_{BZA} = P_{H2} = 1.0 \text{ bar}$$

$$P_{H2O} = P_{BAld} = P_{BnOH} = P_{Tol} = P_{Benz} = P_{CO} = P_{CO2} = 0$$



**Figure S9.** (a) Steady-state rates of reaction of adsorbed benzaldehyde (P1\*) including desorption, hydrogenation and decarbonylation, and steady-state rate of decarboxylation; (b) steady-state surface coverages in the temperature range of T = 450-900 K.



**Figure S10.** (a) Selectivity of products from the MKM results with entropies of surface species and transition states calculated with statistical mechanics (as described in Eqns. S4, including a desorption transition state where 1-dimensional translational degree of freedom is lost relative to gas phase). Enthalpies are calculated as in the main text. Instead of assuming no entropy difference between surface intermediates, the statistical mechanics calculation (using Eqns. S4 at 540 K) results in an activation entropy for benzaldehyde decarbonylation that is  $7 \text{ J mol}^{-1} \text{ K}^{-1}$  higher than its hydrogenation. Even though this difference is below the uncertainty in the entropy treatment (e.g., see Figure S2), it is enough to tilt the balance between benzaldehyde hydrogenation and decarbonylation, favoring benzene over toluene formation. Nevertheless, this difference in selectivity occurs only at low temperatures where the rates are too low to be observed experimentally. Meanwhile, the trend of increasing benzaldehyde selectivity at higher temperatures remains consistent across different entropy approximations. (b) Selectivity of products from the MKM results including the alternative second C-H bond formation pathway depicted in Figure S4. Entropies are calculated as in the main text. Lower barriers for further hydrogenation of benzaldehyde makes this step more competitive compared to decarbonylation or desorption of benzaldehyde, resulting in higher selectivity of toluene at low temperatures and a shift of temperature where benzaldehyde becomes dominant to higher temperatures. Once again though, the trend of increasing benzaldehyde selectivity with rising temperatures remains consistent. Since the focus of the present work is on the C-H bond formation mechanism that occurs between hydrides and monoanionic adsorbates on the same  $\text{O}_{\text{vac}}$ , this alternative mechanism without hydride (i.e.,  $\text{S}_2$  to  $\text{S}_3$  in Figure S4) is not considered in the main text.

## Descriptions for Calculation of Entropy Using Statistical Mechanics:

(Eqns. S4)

$$S = k_B \ln Q + k_B T \left( \frac{\partial \ln Q}{\partial T} \right)_{N,V}$$

where S is entropy,  $k_B$  is Boltzmann constant, Q is partition function, T is temperature, and N is total number of particles.

$$Q = q_{el} q_{vib} q_{trans} q_{rot}$$

$$q_{el} = e^{-\frac{E_{elec}}{k_B T}}$$

$$q_{vib} = \prod_{i=1}^{3N-6} \left( \frac{1}{1 - e^{-h\omega_i/k_B T}} \right)$$

where h is Planck's constant and  $\omega$  is vibrational frequency. To reduce errors in the entropy calculations from low-lying frequencies ( $< 50 \text{ cm}^{-1}$ ) associated with the frustrated motions of the surface bound specie, the immobile adsorbate approach was used by replacing low-lying frequencies with normal modes of 50  $\text{cm}^{-1}$ .<sup>3</sup>

$$q_{trans} = \left( \frac{2\pi M k_B T}{h^2} \right)^{\frac{3}{2}} V$$

where M is molecular mass and V is volume calculated by ideal gas law.

$$q_{rot} = \frac{\sqrt{\pi I_A I_B I_C}}{\sigma} \left( \frac{8\pi k_B T}{h^2} \right)^{\frac{3}{2}}$$

where  $I_A$ ,  $I_B$  and  $I_C$  are the principal moments of inertia, and  $\sigma$  is a symmetry number.

*Equations for 1-translational degree of freedom:*

$$S_{1D-trans} = k_B \ln Q_{1D-trans} + k_B T \left( \frac{\partial \ln Q_{1D-trans}}{\partial T} \right)_{N,V}$$

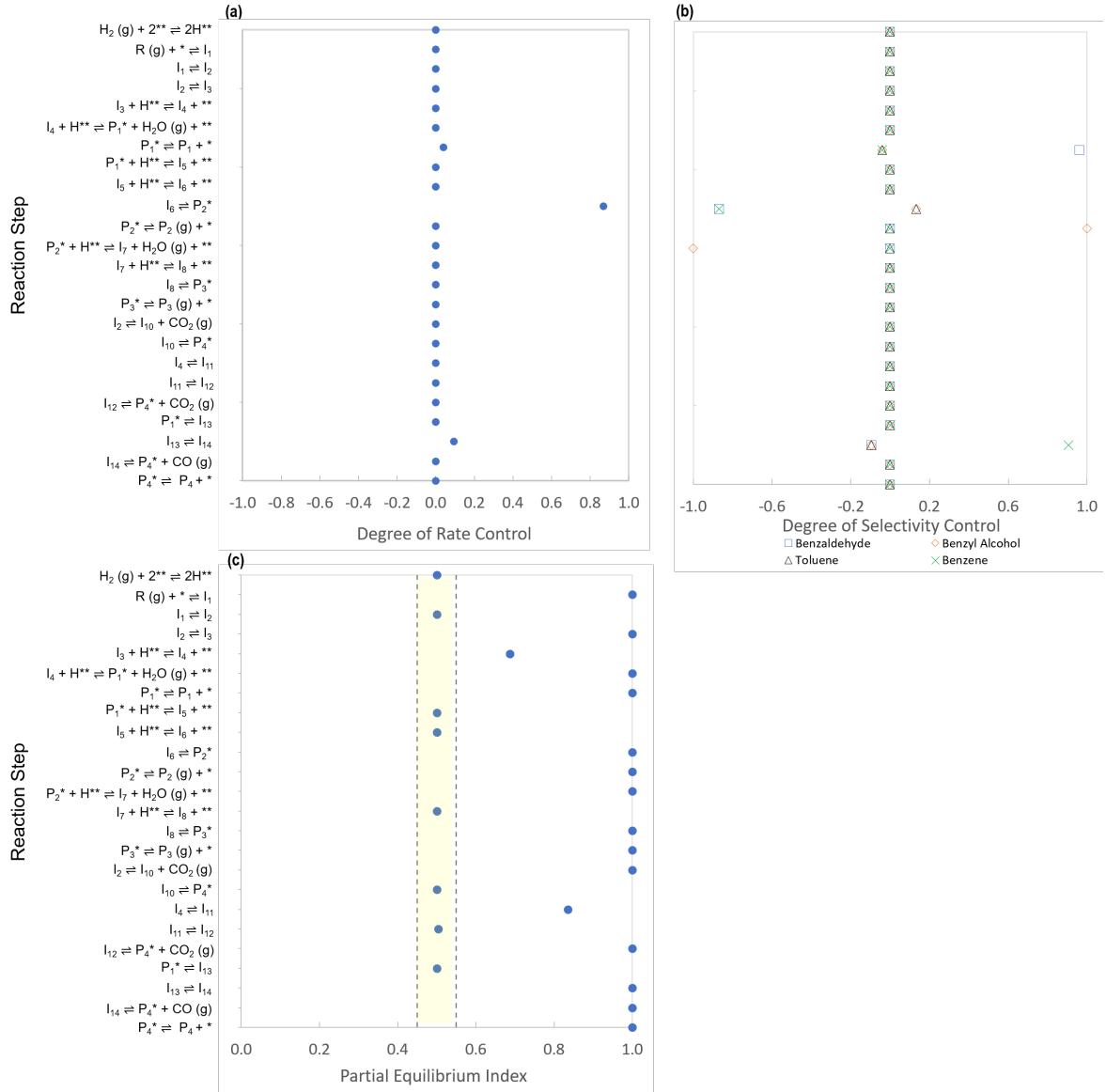
$$Q_{1D-trans} = q_{1D-trans}$$

$$q_{1D-trans} = \left( \frac{2\pi M k_B T}{h^2} \right)^{\frac{1}{2}} V^{\frac{1}{3}}$$

## Degree of selectivity control (DSC<sub>i</sub>)

$$DSC_i = DRC_{i,P} - DRC_{i,R}$$

$$DSC_i = \left( \frac{\partial \ln(r_{i,P})}{\partial \ln(k_i)} \right)_{k_j \neq i, K_i} - \left( \frac{\partial \ln(r_{i,R})}{\partial \ln(k_i)} \right)_{k_j \neq i, K_i}$$



**Figure S11.** (a) Partial equilibrium index; (b) Degree of Rate control (DRC); and (c) Degree of selectivity control (DSC) respect to benzaldehyde, benzyl alcohol, toluene, and benzene formation, calculated for each reaction step in the kinetic model corresponding to Table 1 at 540 K. A reaction step with a PEI in the yellow region (having a PEI between 0.45 and 0.55) is generally considered near equilibrium.

## Appendix. Coordinates for all intermediates in Figure S6

I1

Ti O C H

1.0000000000000000

7.7404954086981297 0.0000004499309580 0.0000000000000000

0.0000000000000000 7.7404983529264300 0.0000000000000000

0.0000000000000000 0.0000000000000000 27.7849839816825011

Ti O C H

24 49 7 6

Selective dynamics

Cartesian

1.9351236277001749 1.9351235473800663 2.7933008483844719 F F F

1.7875108258928447 1.7535990283650846 12.2954018587652349 T T T

7.6632458250249433 0.0028848754867596 7.5327780938804532 T T T

1.8582687225526759 0.0001935079910965 5.1606135970544758 T T T

7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F

7.6414358665784103 1.9438779686953329 9.8803813268453453 T T T

5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F

5.6931944901037257 1.8199366591220225 12.1611519784964841 T T T

3.7884448638923272 0.0030161486654632 7.5343940711971724 T T T

5.7276765882069087 -0.0000610374502840 5.1631521390766926 T T T

3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F

3.7076517013052248 1.9413482191618165 9.8882820607816395 T T T

1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F

1.7857379255353045 6.0438776738561311 12.3103298213245544 T T T

7.6587186198468453 3.8777603001058631 7.5232563558249010 T T T

1.8589050658072139 3.8702243063107931 5.1595388043479735 T T T

7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F

7.6497220432237034 5.8022449504414757 9.8896876292192726 T T T

5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F  
 5.6948269555288027 5.9486104846174017 12.1512965555784387 T T T  
 3.7936857096670722 3.8778145581853765 7.5277556267404435 T T T  
 5.7270815193575446 3.8703856234824814 5.1575491778363496 T T T  
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 1.8627749303755650 1.9354547317094650 4.7893175558964796 T T T  
 0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F  
 7.6782595997342442 0.0051882902717923 9.5552780779799349 T T T  
 1.8543144187863223 0.0062252772749215 7.1661268183289568 T T T  
 7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F  
 7.6051471410305247 2.0139739715272587 11.9528311953335429 T T T  
 7.6575098121987644 1.9405428100438382 7.9288954347769787 T T T  
 1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F  
 1.8085545833626770 0.0437677043749572 12.8861824424805853 T T T  
 7.6643196837722494 -0.0000547289850014 5.5589894110702156 T T T  
 1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F  
 1.8035567745097039 1.9684291880454385 10.3401777914040593 T T T  
 5.7342333660186942 1.9350616924126671 4.7903720021321794 T T T  
 3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F  
 3.6918888781107397 0.0055705749970448 9.5521069841580957 T T T  
 5.7257115808297518 0.0025324879467589 7.1797486197327656 T T T  
 3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F  
 3.7320222426076390 2.0032265297488419 11.9351847848785031 T T T  
 3.7789624802796147 1.9410421821732426 7.9299495267053199 T T T  
 5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F  
 5.6747820528996149 0.0160848793288176 12.7177229291135028 T T T  
 3.7962238962583004 0.0011605273513479 5.5583123688624463 T T T  
 5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F

5.6801134410739058 1.8580784636538406 10.2898299405161886 T T T  
 1.8629896181341734 5.8060440020870434 4.7890389732033736 T T T  
 0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F  
 7.5993863246104940 3.8751080622471701 9.5415549943205349 T T T  
 1.8545974948749511 3.8737071037704012 7.1712697215719468 T T T  
 7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F  
 7.6006899583484042 5.7399139595493329 11.9624852804331283 T T T  
 7.6624213180930054 5.8095414374486447 7.9312057508357876 T T T  
 1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F  
 7.6653419603148558 3.8725103542709336 5.5523768060609919 T T T  
 1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F  
 1.8049353551121365 5.7817477698980957 10.3386425058077762 T T T  
 5.7341724726018706 5.8064060364254928 4.7891732805014655 T T T  
 3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F  
 3.7715306711807686 3.8760386682360277 9.5466052214815473 T T T  
 5.7255849307678117 3.8774552444519332 7.1680865089224302 T T T  
 3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F  
 3.7435443605887921 5.7713708361949809 11.9330217437253037 T T T  
 3.7779221391600659 5.8096997245402378 7.9291200214534703 T T T  
 5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F  
 5.5466723325309681 3.8835136208159819 12.6327566502928921 T T T  
 3.7954745405238932 3.8720855814814348 5.5530703093915541 T T T  
 5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F  
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 6.1094511228315822 1.5667511642230081 15.9247018472304749 T T T  
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 3.9099536684329248 5.9853193195259804 15.2368740371305318 T T T  
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I2

Ti O C H

1.0000000000000000

7.7404954086981297 0.0000004499309580 0.0000000000000000  
 0.0000000000000000 7.7404983529264300 0.0000000000000000  
 0.0000000000000000 0.0000000000000000 27.7849839816825011

Ti O C H

24 49 7 6

Selective dynamics

Cartesian

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 1.8502781076096335 1.7447157488895140 12.2698271779084855 T T T  
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 1.8984584805014246 7.7363241320836087 5.1786048523982986 T T T  
 7.7404950271152559 1.9351240312453248 0.3938262668217468 F F F  
 7.6658295711820292 1.8480033269008842 9.9329300505432254 T T T  
 5.8053713350726186 1.9351237743724437 2.7933008378649218 F F F

5.7209919656136998 1.9352551491018826 12.2494706189922233 T T T  
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 3.8702473227661907 1.9351238062798457 0.3938262668217468 F F F  
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 1.9351236307235535 5.8053727258701802 2.7933008378649218 F F F  
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 7.7404950271152559 5.8053732077085396 0.3938262668217468 F F F  
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 3.8702478969348064 3.8702480463223226 0.0000000000000000 F F F  
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 5.7646792985935003 3.8086509975212923 7.1765965998459196 T T T  
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3.7488639566527331 5.5988237239979135 11.9458857832341803 T T T  
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TS1

Ti O C H

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0.0000000000000000	0.0000000000000000	27.7849839816825011

Ti O C H

24 49 7 6

Selective dynamics

Cartesian

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1.9181003667782417 7.7374303106476292 5.1825666648342077 T T T  
7.7404950271152559 1.9351240312453248 0.3938262668217468 F F F  
7.7817944292804198 1.8949933058302852 9.9619143589847354 T T T  
5.8053713350726186 1.9351237743724437 2.7933008378649218 F F F  
5.8239344245970184 1.9932375281481038 12.2708252450759794 T T T  
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0.0000001925857419 7.7404969978200588 0.0000000000000000 F F F

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 1.9351241436230258 1.9351235318700586 0.7876614242995419 F F F  
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I3

Ti O C H

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0.0000000000000000 0.0000000000000000 27.7849839816825011

Ti O C H

24 49 7 6

Selective dynamics

Cartesian

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1.8482438659314575 0.0027289889348033 5.1760476388711663 T T T  
7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F  
-0.1716988703605772 1.9677450472550087 9.9384560958289399 T T T  
5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F  
5.6229250912208038 2.1131969649889379 12.2662680089582121 T T T  
3.7784232612505377 0.0365691668114255 7.5636249719076565 T T T  
5.7164485294935572 0.0025888932343847 5.1753277149031325 T T T  
3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F  
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1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F  
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 7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F  
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 3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F  
 3.6927918371492883 0.0427553562715686 9.5580176422516434 T T T  
 5.7124269374846426 0.0323394442763136 7.1731596061734493 T T T  
 3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F  
 3.6698385540161440 1.9704370307707668 11.9294869794834462 T T T  
 3.7732786279310266 1.9727243728557520 7.9496038575848065 T T T  
 5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F

5.6136552137070428 7.6937769712348967 12.7900430382873402 T T T  
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 5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F  
 5.6280227059510057 2.0219085260394141 10.3261081923880358 T T T  
 1.8559329377130713 5.8087325580833840 4.7848259542475153 T T T  
 0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F  
 -0.1546775644015269 3.9123797197381323 9.5575376798119933 T T T  
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14

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Ti O C H

24 49 7 7

Selective dynamics

Cartesian

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Ti O C H

24 48 7 6

Selective dynamics

Cartesian

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Ti O C H

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Ti O C H

24 47 6 6

Selective dynamics

Cartesian

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3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F  
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 5.8304625286416982 5.8046525443915922 4.7810923173211082 T T T  
 3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F  
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TS4

Ti O C H

1.0000000000000000

7.7404954086981297	0.0000004499309580	0.0000000000000000
0.0000000000000000	7.7404983529264300	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.7849839816825011

Ti O C H

24 47 6 6

Selective dynamics

Cartesian

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 1.9846535228800242 1.6896030354778793 12.1946997769213148 T T T  
 0.0258507815269826 -0.0176309283644988 7.4981965870299438 T T T

1.9621501734265807 0.0000920022444007 5.1509233913650361 T T T  
 7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F  
 0.0479480772105787 1.9265604238378509 9.8547182861361069 T T T  
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 5.8540792962053771 2.0337922084293836 12.2216975255655012 T T T  
 3.8983458467248138 -0.0179044891370598 7.4976698991270210 T T T  
 5.8325807295872005 -0.0003860731026270 5.1497820099238485 T T T  
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 3.1919016335786408 4.8987116432984941 15.0577115321019104 T T T  
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P4\*

Ti O C H

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0.0000000000000000 0.0000000000000000 27.7849839816825011

Ti O C H

24 47 6 6

Selective dynamics

Cartesian

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1.9617804266026719 0.0035356869051410 5.1803724112067133 T T T  
7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F  
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5.8320271862932573 0.0021421701607864 5.1787767956190844 T T T  
3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F  
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1.9620534393620435 3.8712773654693731 5.1756780895839976 T T T  
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5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F  
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 3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F  
 3.8676534322203220 1.8795116450919707 11.9616382362828304 T T T  
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 5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F  
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 0.0838927893479185 3.9267278379492252 9.5764357584378637 T T T  
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TS5

Ti O C H

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0.0000000000000000 7.7404983529264300 0.0000000000000000

0.0000000000000000 0.0000000000000000 27.7849839816825011

Ti O C H

24 49 7 6

Selective dynamics

Cartesian

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1.9072992843048069 7.7399667565011407 5.1752800918197863 T T T

7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F

7.6452704446614401 1.9245272339257242 9.9366714274099319 T T T

5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F

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5.7764876969889718 7.7400752594069067 5.1743175568451205 T T T

3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F

3.7764005707911958 1.9299074519231012 9.9367758739538985 T T T

1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F

1.8287485388223095 5.9802070264136455 12.2979034482604597 T T T

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 5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F  
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|11

Ti O C H

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Ti O C H

24 49 7 6

Selective dynamics

Cartesian

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TS6

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Ti O C H

24 49 7 6

Selective dynamics

Cartesian

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I12

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Ti O C H

24 49 7 6

Selective dynamics

Cartesian

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15

Ti O C H

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Ti O C H

24 48 7 7

Selective dynamics

Cartesian

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Ti O C H

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Ti O C H

24 48 7 8

Selective dynamics

Cartesian

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 2.3435070928460480 4.3432205246228435 15.2166851057764525 T T T  
 1.0131325364046528 2.6739061858754369 14.6024889885408093 T T T  
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TS2

Ti O C H

1.0000000000000000

7.7404954086981297 0.0000004499309580 0.0000000000000000  
 0.0000000000000000 7.7404983529264300 0.0000000000000000  
 0.0000000000000000 0.0000000000000000 27.7849839816825011

Ti O C H

24 48 7 8

Selective dynamics

Cartesian

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 0.0121139775579139 0.0245977817255033 7.5550925145515277 T T T  
 1.9479251178676509 0.0015632122228950 5.1722369737618310 T T T  
 7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F  
 7.6989653071407300 1.9486229493664262 9.9557753186285538 T T T  
 5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F

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 3.8855301125293455 0.0322245341911074 7.5491547995760646 T T T  
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 3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F  
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 1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F  
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 0.0147554882299331 3.8804198813896296 7.5462478615083945 T T T  
 1.9478728591467771 3.8709008320477012 5.1670847600731094 T T T  
 7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F  
 0.0250447266492533 5.8095465220385556 9.9039830767236605 T T T  
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 5.8312630384349005 6.0004830654165513 12.2350065287384364 T T T  
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P2\*

Ti O C H

1.0000000000000000

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 0.0000000000000000 7.7404983529264300 0.0000000000000000  
 0.0000000000000000 0.0000000000000000 27.7849839816825011

Ti O C H

24 48 7 8

Selective dynamics

Cartesian

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2.0063561053574914 0.0001392723197526 5.1754936835647936 T T T  
7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F  
0.1296744322116102 1.9308001728074853 9.9386832847362303 T T T  
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5.9105807274069297 2.0823705553203320 12.2206990734102874 T T T  
3.9467365239400198 0.0342142095011928 7.5584571455420644 T T T  
5.8747178177171007 0.0014776754228335 5.1712165534052552 T T T  
3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F  
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1.9997333660100027 1.9371380045169997 4.7841579193115900 T T T

0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F  
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 0.0653792009566562 1.8309249884739998 11.8904375373548330 T T T  
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 1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F  
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 1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F  
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 3.5961791168566646 2.5070358692745063 15.2552241315236241 T T T  
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TS7

Ti O C H

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 0.0000000000000000 7.7404983529264300 0.0000000000000000  
 0.0000000000000000 0.0000000000000000 27.7849839816825011

Ti O C H

24 48 7 6

Selective dynamics

Cartesian

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 7.7404950294138555 1.9351240318977576 0.3938262801202625 F F F  
 7.6990111524146609 1.9173399713436361 9.9061508035512897 T T T  
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 5.7781669739105910 0.0002893807823457 5.1725168846979637 T T T  
 3.8702473250647897 1.9351238069322787 0.3938262801202625 F F F  
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 3.8702474876151935 1.9351240081852452 2.3994608702671258 F F F  
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 5.7666100969050929 1.9923879304644478 10.2717899398317183 T T T  
 1.9084419542544933 5.8049580405741104 4.7826381561768994 T T T  
 0.0000001927383357 3.8702478218760143 0.0000000000000000 F F F  
 7.7322804364018696 3.8670693415418840 9.5529670643202014 T T T  
 1.9041754009257144 3.8825865655923111 7.1652069787224573 T T T  
 7.7404951919642579 5.8053734096139396 2.3994608702671258 F F F  
 7.7304552508059849 5.7931649015156541 11.9960384674654250 T T T  
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|13

Ti O C H

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Ti O C H

24 48 7 6

Selective dynamics

Cartesian

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TS8

Ti O C H

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Ti O C H

24 48 7 6

Selective dynamics

Cartesian

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|14

Ti O C H

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Ti O C H

24 48 7 6

Selective dynamics

Cartesian

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17

Ti O C H

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Ti O C H

24 47 7 7

Selective dynamics

Cartesian

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Ti O C H

24 47 7 8

Selective dynamics

Cartesian

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TS3

Ti O C H

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Ti O C H

24 47 7 8

Selective dynamics

Cartesian

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Ti O C H

24 47 7 8

Selective dynamics

Cartesian

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Ti O H

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Selective dynamics

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