

Supporting Information (S.I.)

Hydride-mediated chemoselective C-H bond formation during benzoic acid
hydrodeoxygenation on anatase TiO₂

Mikyung Hwang¹, Jeremy Hu¹, Michael J. Janik, and Konstantinos Alexopoulos*

*Department of Chemical Engineering, The Pennsylvania State University, University Park,
Pennsylvania, 16801, United States*

¹Denotes equal authorship

*Corresponding author: kxa5325@psu.edu

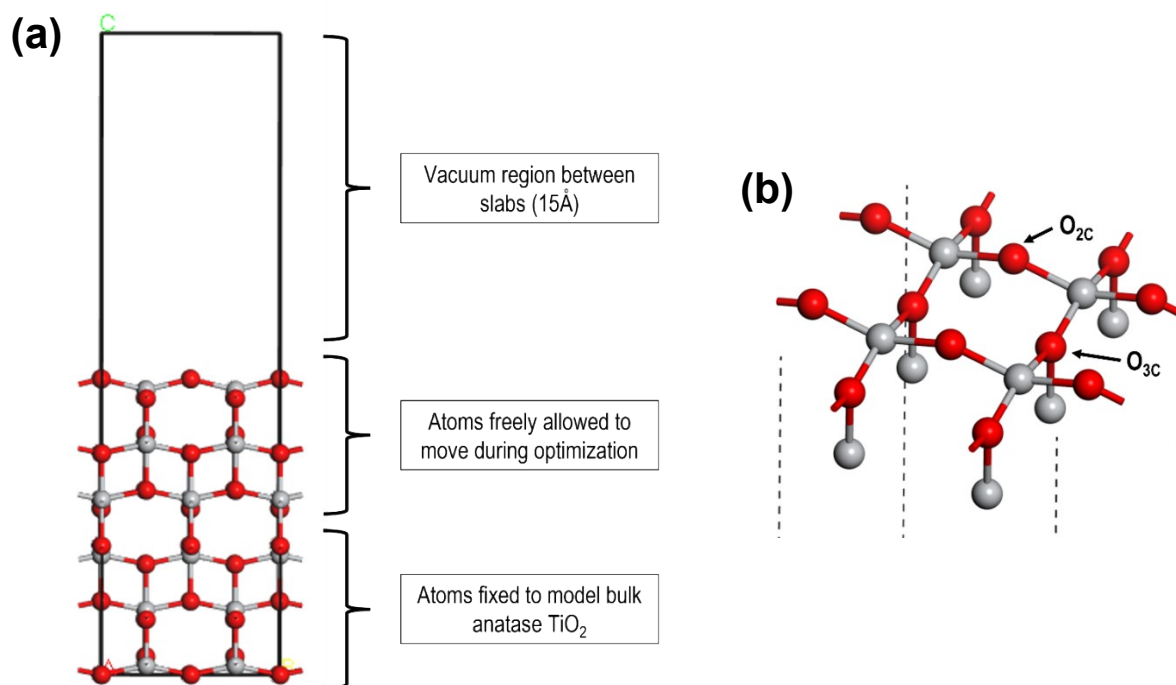


Figure S1. (a) Model slab for anatase TiO₂ depicting atomic layers frozen and relaxed during DFT geometric optimization calculations, and (b) top view of model slab. Ti is depicted in gray, and O is depicted in red.

Adjustment of gas-phase DFT for thermodynamic consistency

Following the method of Vorotnikov et al.¹, 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 formation² (Eqn. S1).

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

where $H_{f,DFT}^i$ is the heat of formation of species i computed using DFT, $H_{f,exp}^i$ 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	$H_{f,exp}$ (kJ/mol)	$H_{f,DFT}$ (kJ/mol)	$H_{f,exp} - H_{f,DFT}$ (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 ₂ O	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

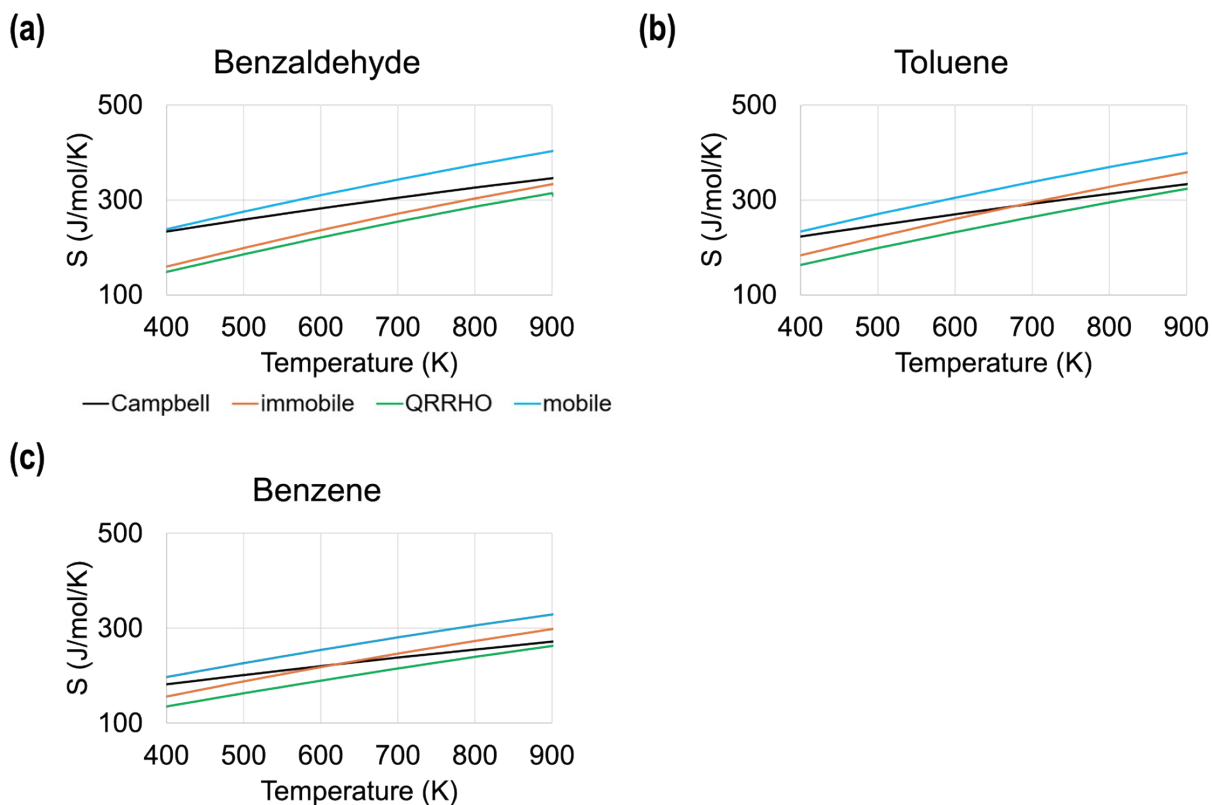


Figure S2. Comparison of adsorbed species entropies using Campbell and Sellers' method (black), immobile (orange) and mobile approximations³ (blue), and Quasi Rigid Rotor Harmonic Oscillator approximation (QRRHO)⁴ (green) for (a) benzaldehyde, (b) toluene, and (c) benzene. In the mobile approach, harmonic frequencies associated with rotational and translational motions of adsorbates were examined based on visual inspection of frequencies lower than 125 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.

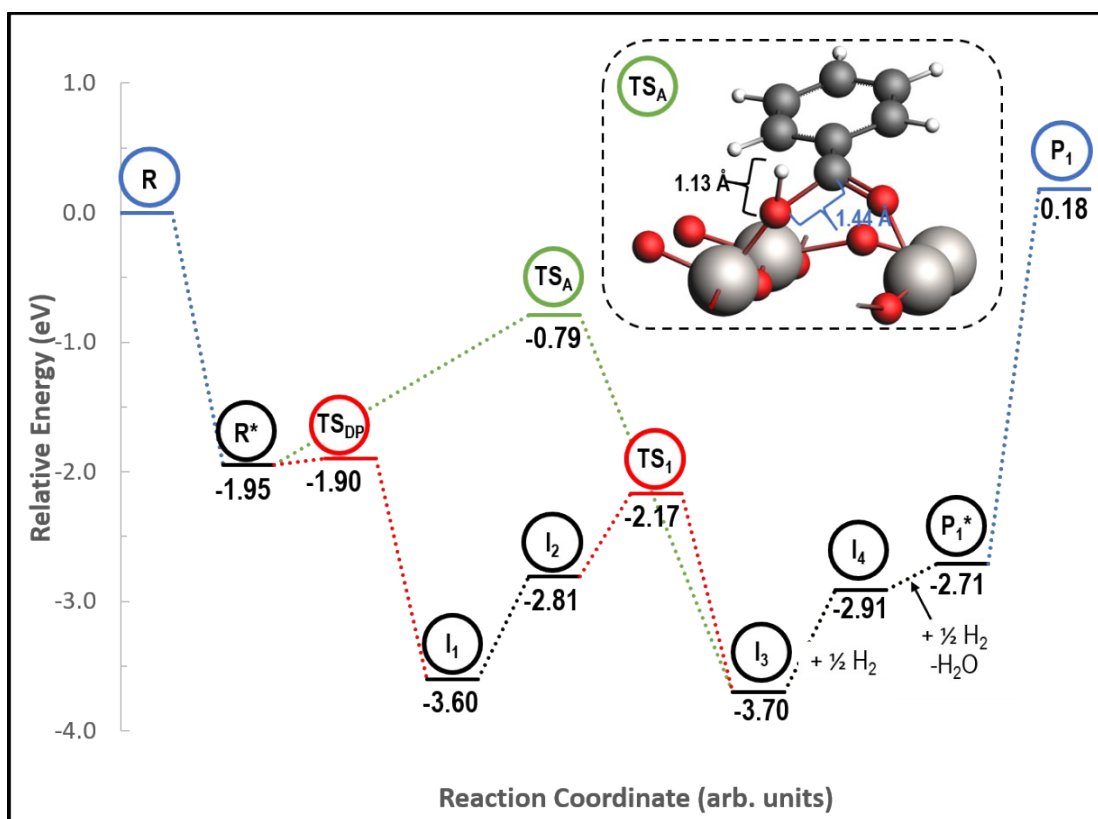


Figure S3. The alternate mechanism is shown in green for the first C-H bond formation to form benzaldehyde from benzoic acid, where the H migrates directly from the O on benzoic acid to the C. Ti is depicted in gray, O in red, C in black, and H in white.

Comparisons between the time scale (τ) 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^{5,6} (Eqn. S2):

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

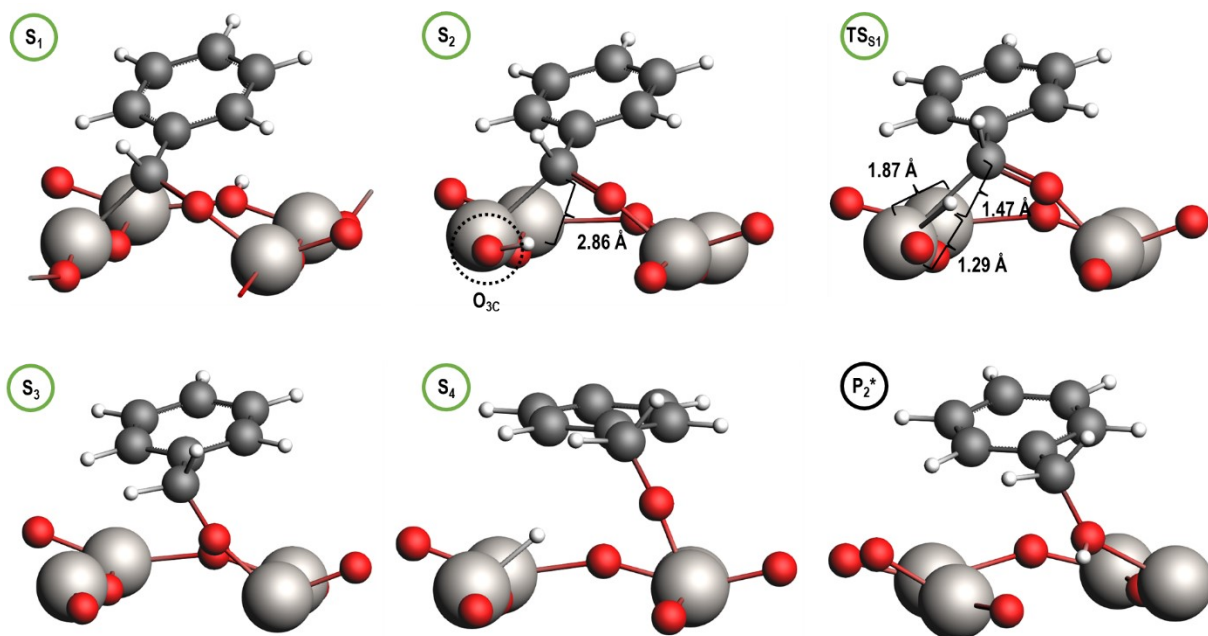
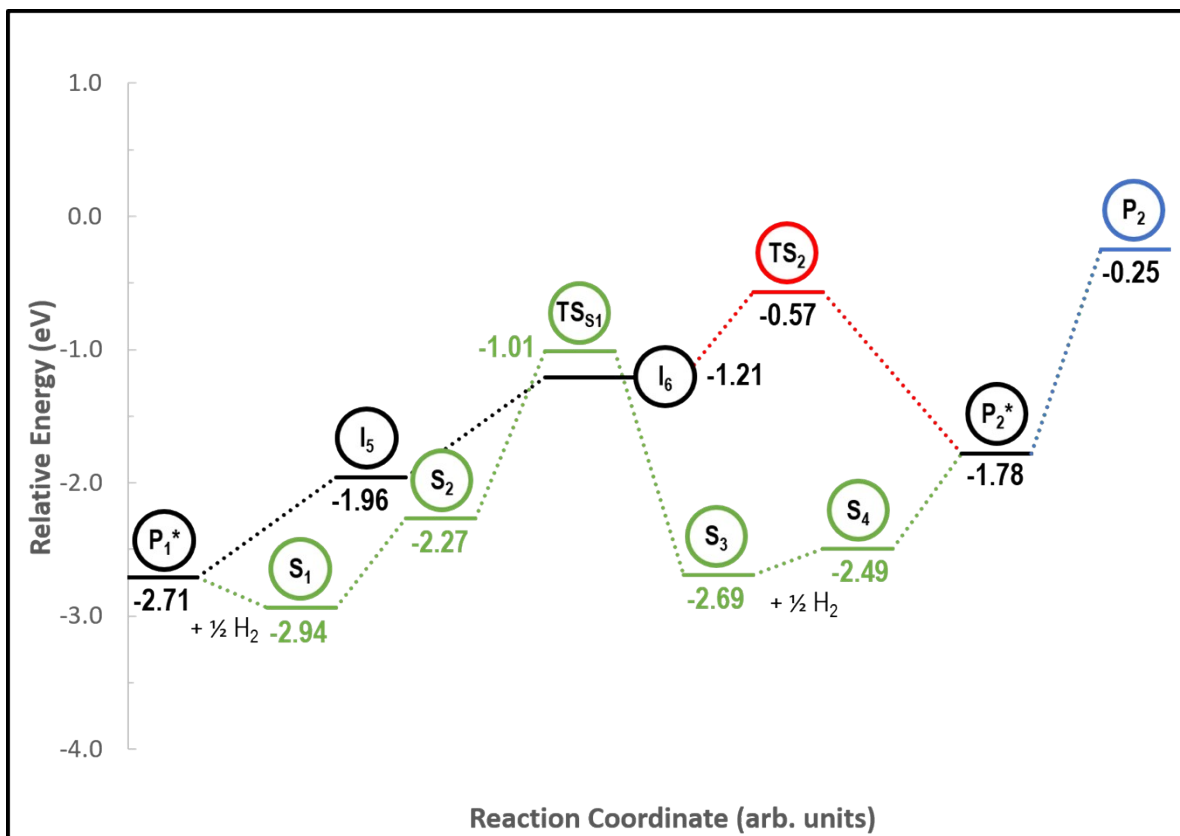


Figure S4. Alternate mechanism of benzyl alcohol formation from benzaldehyde is shown in green, where the first H atom is added to C via H migration from O_{3C} (i.e., not the hydride). Ti is depicted in gray, O in red, C in black, and H in white.

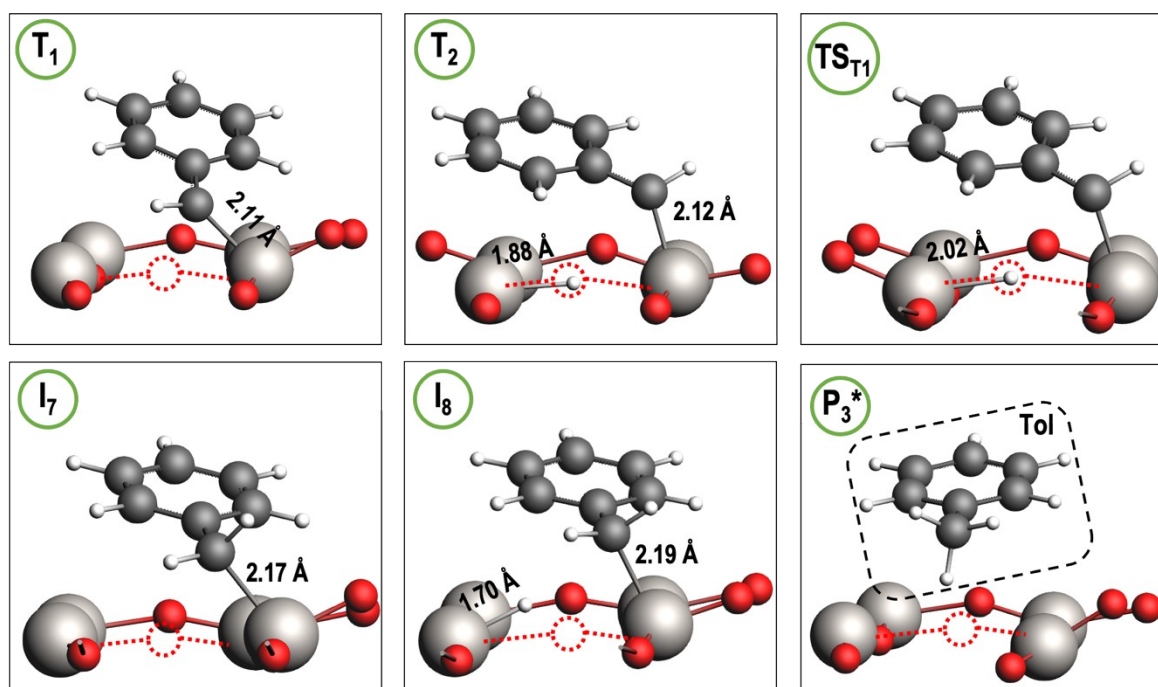
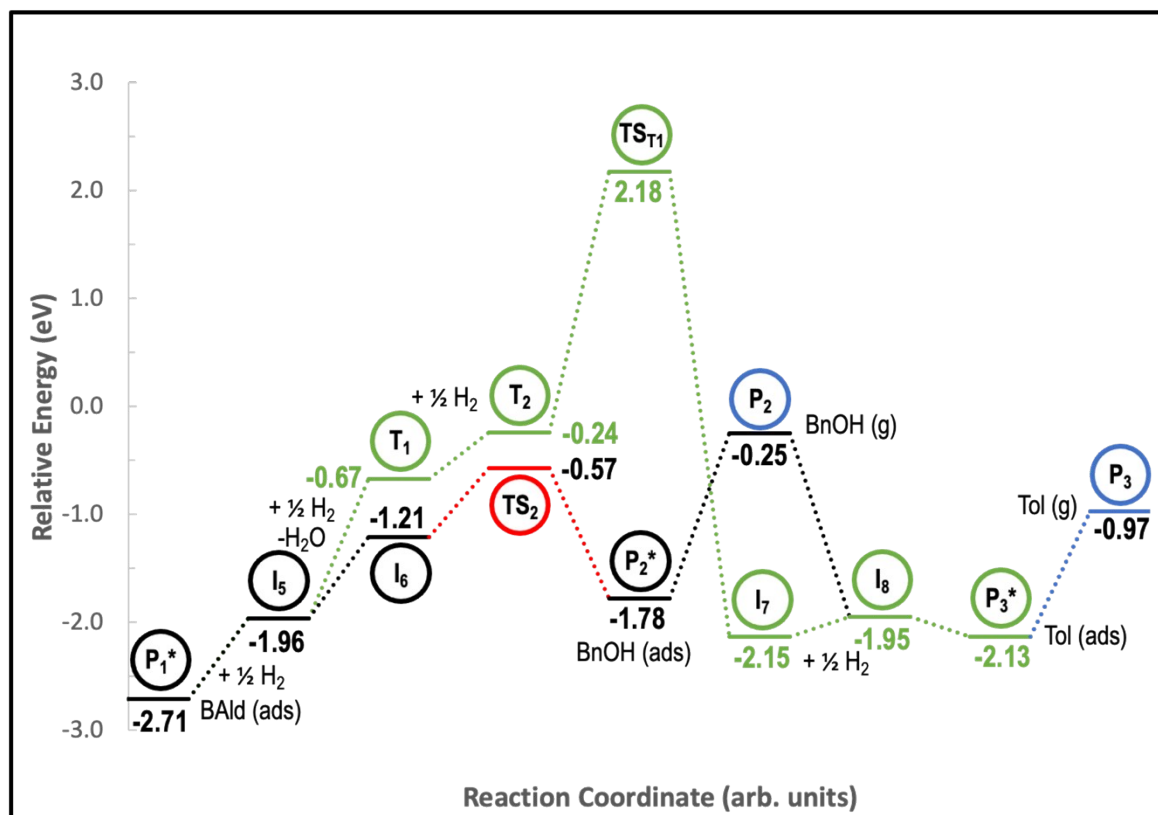


Figure S5. Alternative mechanism of toluene formation directly from benzaldehyde and bypassing benzyl alcohol is shown in green. Ti is depicted in gray, O in red, C in black, and H in white.

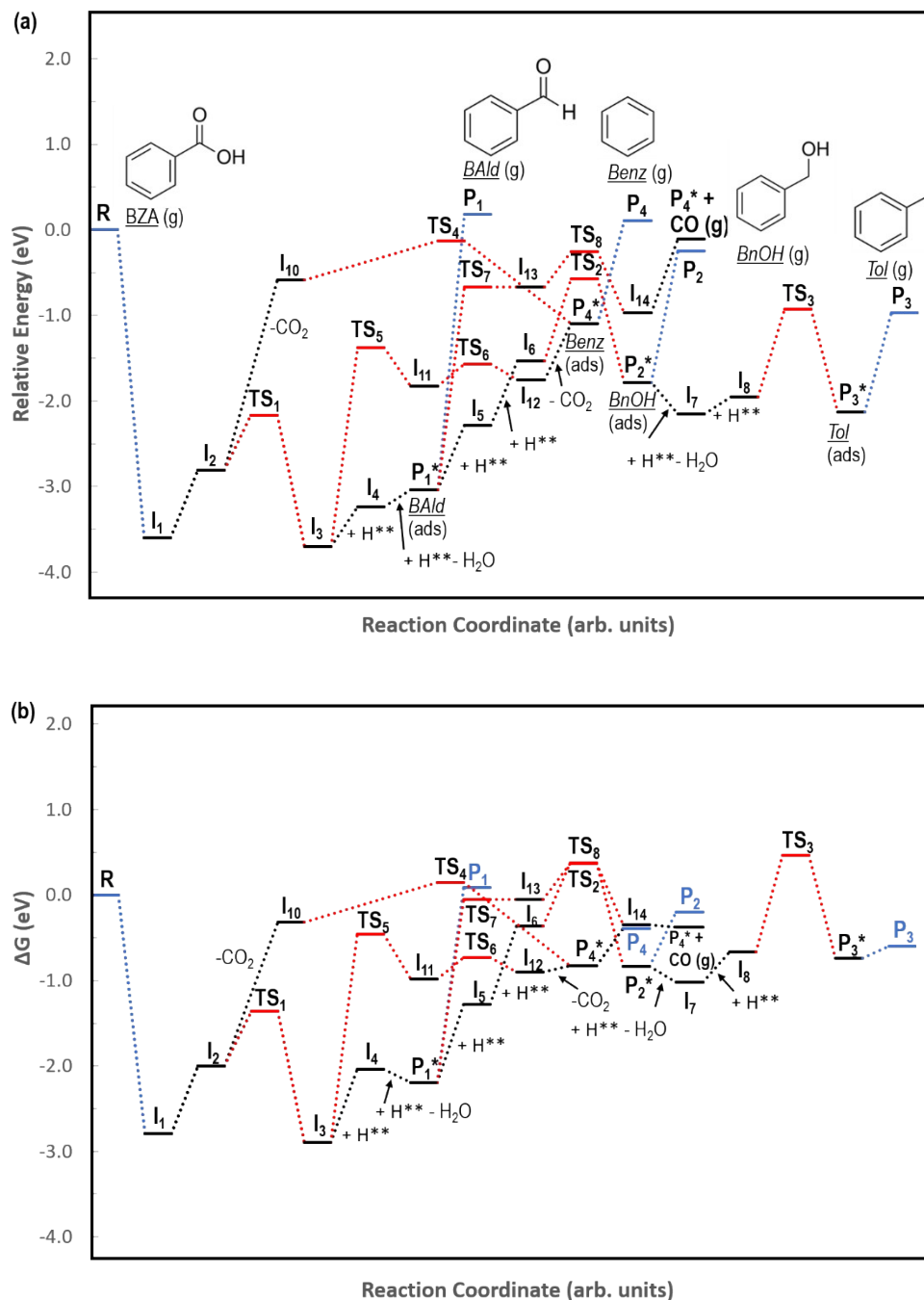


Figure S6. (a) Overall reaction energy diagram using DFT-calculated ΔE for benzoic acid hydrogenation to benzaldehyde (P_1), benzyl alcohol (P_2), toluene (P_3), and benzene (P_4) with hydrogen provided from adsorbed hydrogen on lattice O sites (H^{**}); (b) Gibbs free energy diagram along the reaction 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.

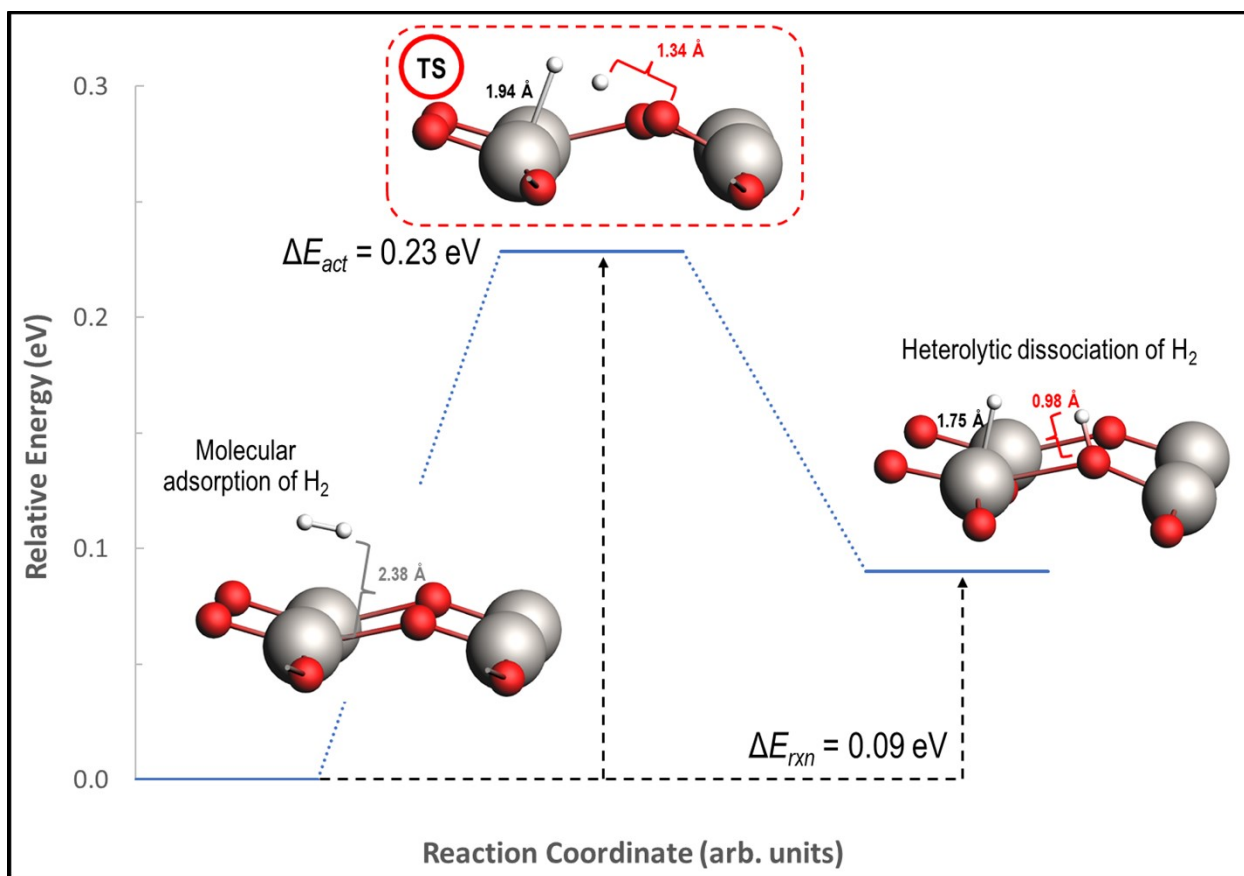


Figure S7. Reaction energy diagram of the heterolytic dissociation of H₂ on anatase TiO₂ (001) following H₂ molecular adsorption. Ti is depicted in gray, O in red, C in black, and H in white. The coordination of adsorbed H species (H^{**}) considered in the MKM is provided in the Appendix. Hydrogen spillover on anatase titania can involve activation barriers of 1.10 eV on the (001) surface.⁷ 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 TiO₂ 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 TiO₂ is kinetically favorable.⁸ It is also worth noting that once H spills over 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 TiO₂.⁹ 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.

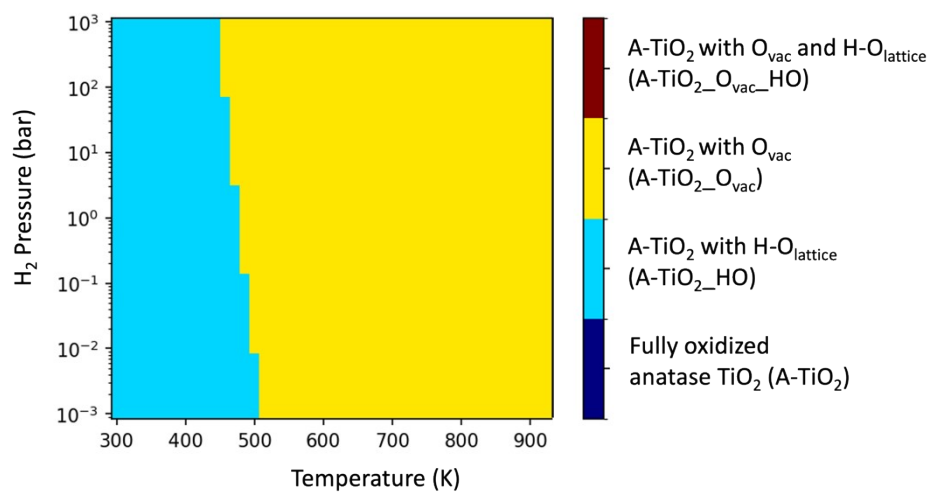


Figure S8. Phase diagram of anatase TiO₂ surface under dry conditions (water pressure was fixed at 10⁻²⁰ bar).

Kinetic Model Differential Equations:

(Eqns. S3)

$$r_0 = k_0 \theta_{**}^2 P_{H2} - k_{-0} \theta_{H**}^2$$

$$r_1 = k_1 \theta_{*} P_{BZA} - k_{-1} \theta_1$$

$$r_2 = k_2 \theta_1 - k_{-2} \theta_2$$

$$r_3 = k_3 \theta_2 - k_{-3} \theta_3$$

$$r_4 = k_4 \theta_3 \theta_{H**} - k_{-4} \theta_4 \theta_{**}$$

$$r_5 = k_5 \theta_4 \theta_{H**} - k_{-5} \theta_{P1} \theta_{**} P_{H2O}$$

$$r_6 = k_6 \theta_{P1} - k_{-6} \theta_{*} P_{BAld}$$

$$r_7 = k_7 \theta_{P1} \theta_{H**} - k_{-7} \theta_5 \theta_{**}$$

$$r_8 = k_8 \theta_5 \theta_{H**} - k_{-8} \theta_6 \theta_{**}$$

$$r_9 = k_9 \theta_6 - k_{-9} \theta_{P2}$$

$$r_{10} = k_{10} \theta_{P2} - k_{-10} \theta_{*} P_{BnOH}$$

$$r_{11} = k_{11} \theta_{P2} \theta_{H**} - k_{-11} \theta_7 \theta_{**} P_{H2O}$$

$$r_{12} = k_{12} \theta_7 \theta_{H**} - k_{-12} \theta_8 \theta_{**}$$

$$r_{13} = k_{13} \theta_8 - k_{-13} \theta_{P3}$$

$$r_{14} = k_{14} \theta_{P3} - k_{-14} \theta_{*} P_{Tot}$$

$$r_{15} = k_{15} \theta_2 - k_{-15} \theta_{10} P_{CO_2}$$

$$r_{16} = k_{16} \theta_{10} - k_{-16} \theta_{P4}$$

$$r_{17} = k_{17} \theta_3 - k_{-17} \theta_{11}$$

$$r_{18} = k_{18} \theta_{11} - k_{-18} \theta_{12}$$

$$r_{19} = k_{19} \theta_{12} - k_{-19} \theta_{P4} P_{CO_2}$$

$$r_{20} = k_{20} \theta_{P1} - k_{-20} \theta_{13}$$

$$r_{21} = k_{21} \theta_{13} - k_{-21} \theta_{14}$$

$$r_{22} = k_{22} \theta_{14} - k_{-22} \theta_{P4} P_{CO}$$

$$r_{23} = k_{23} \theta_{P4} - k_{-23} \theta_{*} P_{Benz}$$

$$\frac{d\theta^{**}}{dt} = -2r_0 + r_4 + r_5 + r_7 + r_8 + r_{11} + r_{12}$$

$$\frac{d\theta^*}{dt} = -r_1 + r_6 + r_{10} + r_{14} + r_{23}$$

$$\frac{d\theta_{H^{**}}}{dt} = 2r_0 - r_4 - r_5 - r_7 - r_8 - r_{11} - r_{12}$$

$$\frac{d\theta_1}{dt} = r_1 - r_2$$

$$\frac{d\theta_2}{dt} = r_2 - r_3 - r_{15}$$

$$\frac{d\theta_3}{dt} = r_3 - r_4 - r_{17}$$

$$\frac{d\theta_4}{dt} = r_4 - r_5$$

$$\frac{d\theta_{P1}}{dt} = r_5 - r_6 - r_7 - r_{20}$$

$$\frac{d\theta_5}{dt} = r_7 - r_8$$

$$\frac{d\theta_6}{dt} = r_8 - r_9$$

$$\frac{d\theta_{P2}}{dt} = r_9 - r_{10} - r_{11}$$

$$\frac{d\theta_7}{dt} = r_{11} - r_{12}$$

$$\frac{d\theta_8}{dt} = r_{12} - r_{13}$$

$$\frac{d\theta_{P3}}{dt} = r_{13} - r_{14}$$

$$\frac{d\theta_{10}}{dt} = r_{15} - r_{16}$$

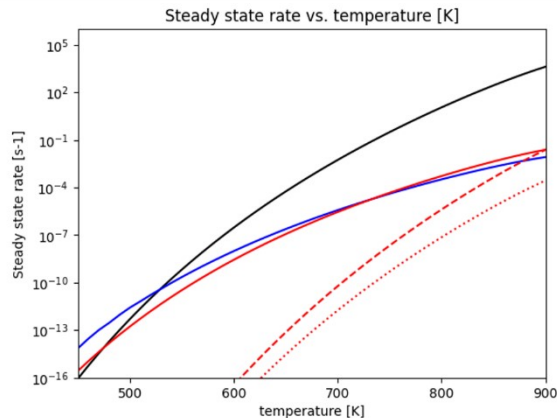
$$\frac{d\theta_{11}}{dt} = r_{17} - r_{18}$$

$$\frac{d\theta_{12}}{dt} = r_{18} - r_{19} \quad (a)$$

$$\frac{d\theta_{13}}{dt} = r_{20} - r_{21}$$

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

$$\frac{d\theta_{P4}}{dt} = r_{16} + r_{19} + r_{21}$$



Initial value
balance):

At $t = 0$,
, with all
such that:

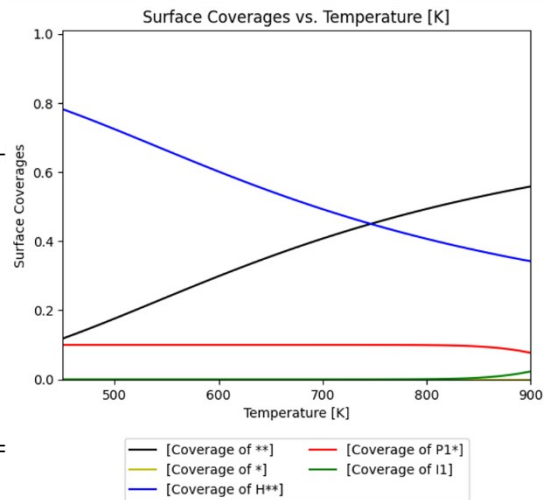
$$\theta_{**} + \theta_* + \theta_{H**} + \theta_R + \theta_{P1} = 1$$

Kinetic

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

$$P_{H2O} = P_{BAld} = P_{BnOH} = P_{Tol} =$$

(b)



constraint (site

$$\theta_{**} = 0.9, \theta_* = 0.1$$

others = 0

**Model
Parameters:**

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 $T = 450\text{-}900$ K.

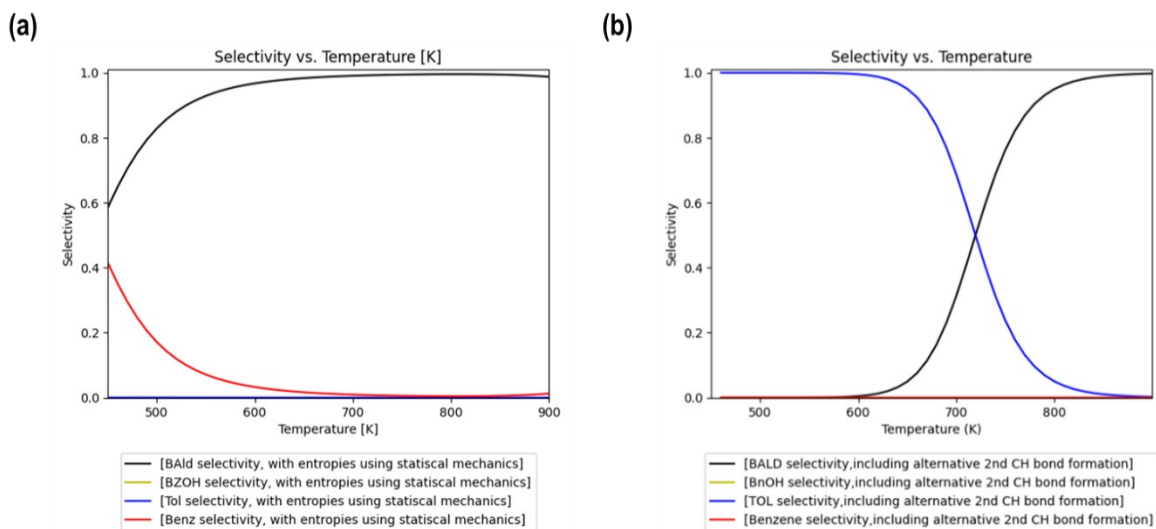


Figure S10. (a) Selectivity of products from the MKM results with entropies of surface species and transition states calculated with statistical mechanics (as described in Eqns. S4, including a desorption transition state where 1-dimensional translational degree of freedom is lost relative to gas phase). 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 O_{vac} , this alternative mechanism without hydride (i.e., S_2 to 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 ω 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 cm^{-1} .³

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

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 σ 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_i)

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

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

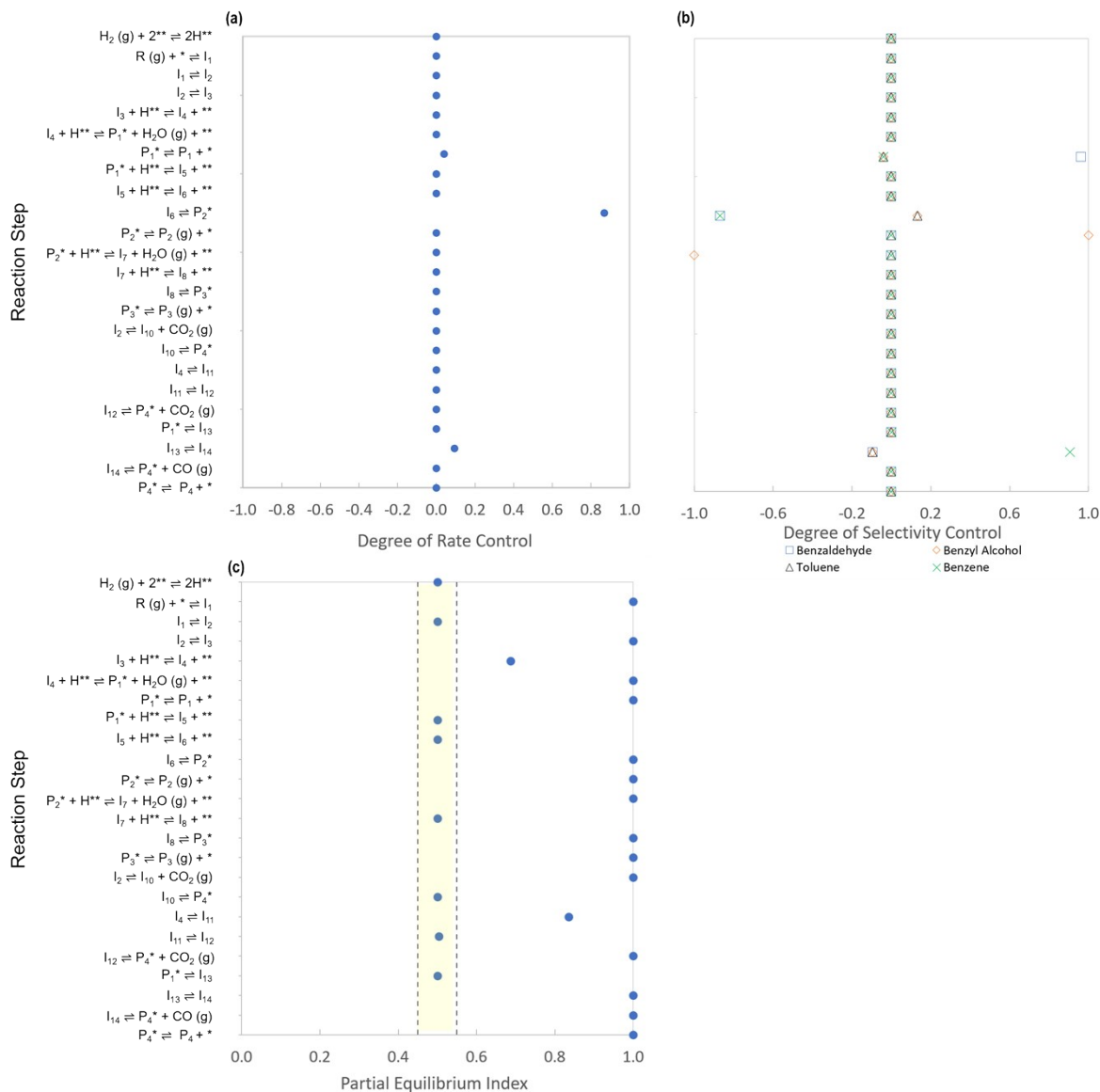


Figure S11. (a) Partial equilibrium index; (b) Degree of Rate control (DRC); and (c) Degree of selectivity control (DSC) respect to benzaldehyde, benzyl alcohol, toluene, and benzene formation, calculated for each reaction step in the kinetic model corresponding to Table 1 at 540 K. A reaction step with 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

l1

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
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.7045629647073106 5.8050497114584809 9.8954982590173053 T T T
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
5.6839945756824664 5.9011484503928431 10.2809760572694238 T T T
1.9637989958592177 5.0423151927664884 13.9669895681810274 T T T
1.8913621144673265 2.8042327426885256 13.9064130120709049 T T T
4.3194835476536273 2.5871586153301305 15.3064218046929046 T T T
5.6274381167640577 2.5353535598166115 15.7825625404381285 T T T
6.3295802294656118 3.7154314082290019 16.0580775536660845 T T T

5.6981608528596013 4.9544551366412346 15.8868473960268410 T T T
 4.3924171815845492 5.0218266822930371 15.4071971649109365 T T T
 2.4478302087394206 3.9016477774251963 14.3377384127151579 T T T
 3.6937783282848540 3.8360194507237408 15.0816498237980046 T T T
 3.7796417311729078 1.6706916510761123 15.0607761436985115 T T T
 6.1094511228315822 1.5667511642230081 15.9247018472304749 T T T
 7.3625102771271314 3.6701789503207860 16.3992609750448324 T T T
 6.2382304876549259 5.8762767445639410 16.1103965503192548 T T T
 3.9099536684329248 5.9853193195259804 15.2368740371305318 T T T
 4.5662147133482796 3.8854779475392656 12.6625163119783899 T T T

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

1.9351236307235535 1.9351235494069645 2.7933008378649218 F F F

1.8502781076096335 1.7447157488895140 12.2698271779084855 T T T

7.6980416306358164 7.6616715343923758 7.5606659825130000 T T T

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
3.8349313230988140 7.6595222183339100 7.5624579050578973 T T T
5.7674373045115850 7.7363812039499944 5.1749288277675962 T T T
3.8702473227661907 1.9351238062798457 0.3938262668217468 F F F
3.7731466388208865 1.8481876453816788 9.9290518975224735 T T T
1.9351236307235535 5.8053727258701802 2.7933008378649218 F F F
1.8147584788034021 5.8267865456537997 12.3279251623724448 T T T
7.7037742805058702 3.8015059158527458 7.5587190981892407 T T T
1.8976206374851023 3.8660715218132156 5.1742219405760368 T T T
7.7404950271152559 5.8053732077085396 0.3938262668217468 F F F
7.6514707032567442 5.7181307592621025 9.9568067318965632 T T T
5.8053713350726186 5.8053729508356593 2.7933008378649218 F F F
5.6957513286680133 5.7974328204963728 12.2847005693557954 T T T
3.8297182352697434 3.8008699314380885 7.5569279187619740 T T T
5.7685539806477761 3.8663572727530857 5.1762159215852712 T T T
3.8702473227661907 5.8053729827430605 0.3938262668217468 F F F
3.7485959965989712 5.7142246300169885 9.9606706852177460 T T T
1.9004471740384679 1.9288963437524189 4.7857138324111057 T T T
0.0000001925857419 7.7404969978200588 0.0000000000000000 F F F
7.6008258462080027 7.6654713901086007 9.5457612580549647 T T T
1.8938345631856741 7.6732599145670264 7.1773431845959728 T T T
7.7404951940399229 1.9351242343854522 2.3994608670731532 F F F
7.6697062164814787 1.7649344391983848 11.9407986265852095 T T T
7.6979018694888390 1.8650495193507284 7.9478125850912713 T T T
1.9351236030856309 7.7404975900603716 3.1871236795975757 F F F
1.8323500363116214 7.5673990294922859 12.8060165455001300 T T T
7.7031738729400212 7.7276018873521615 5.5643354720845242 T T T
1.9351241436230258 1.9351235318700586 0.7876614242995419 F F F
1.8495249739344157 1.7467743985086464 10.3003684534164570 T T T

5.7695486837982948 1.9294151730273692 4.7859446175019205 T T T
3.8702478969348064 7.7404972227855380 0.0000000000000000 F F F
3.8284353039512635 7.6634301656831711 9.5474407044760863 T T T
5.7642359688720957 7.6698281445260275 7.1669787820238282 T T T
3.8702474896908576 1.9351240094199731 2.3994608670731532 F F F
3.7751205769966591 1.7775191667938632 11.9143094972813355 T T T
3.8309750837544976 1.8637912145958555 7.9414114060360044 T T T
5.8053713074346955 7.7404978150258508 3.1871236795975757 F F F
5.6933344751162211 7.5314243447960001 12.7964182896365273 T T T
3.8322001124984761 7.7245145776951487 5.5633779460515189 T T T
5.8053718479720899 1.9351237568355377 0.7876614242995419 F F F
5.7252584187059536 1.9306441545191013 10.3193123251055017 T T T
1.8986796423669532 5.7988651128627104 4.7854023160674330 T T T
0.0000001925857419 3.8702478213568439 0.0000000000000000 F F F
7.6881698303589472 3.7968263262418782 9.5556046375711290 T T T
1.8935000347838653 3.8044907737290585 7.1684479631652751 T T T
7.7404951940399229 5.8053734108486674 2.3994608670731532 F F F
7.6461477874137298 5.6261433674541461 11.9444857184626194 T T T
7.6957986626116517 5.7316696379264851 7.9543674112181861 T T T
1.9351236030856309 3.8702484135971562 3.1871236795975757 F F F
1.8874353182589270 4.8094246475290481 14.0829024333022854 T T T
7.7023388566066053 3.8584081390651983 5.5642212178558168 T T T
1.9351241436230258 5.8053727083332740 0.7876614242995419 F F F
1.8332758245826413 5.8424776786664241 10.3328663505543492 T T T
5.7711623479499181 5.7984504482132628 4.7847937227467519 T T T
3.8702478969348064 3.8702480463223226 0.0000000000000000 F F F
3.7413627405457972 3.7944218646567447 9.5525004304469103 T T T
5.7646792985935003 3.8086509975212923 7.1765965998459196 T T T
3.8702474896908576 5.8053731858831883 2.3994608670731532 F F F

3.7488639566527331 5.5988237239979135 11.9458857832341803 T T T
 3.8199741354583554 5.7294685810371986 7.9556198658225359 T T T
 5.8053713074346955 3.8702486385626353 3.1871236795975757 F F F
 5.7255514738389648 3.6594819894645716 12.7385789746637581 T T T
 3.8331633853003306 3.8601516008720678 5.5636484586596886 T T T
 5.8053718479720899 5.8053729332987523 0.7876614242995419 F F F
 5.7034623854056798 5.7680103446489772 10.3501463642729128 T T T
 2.1605745745424052 2.5639613819008087 14.1465889730427481 T T T
 3.8058809968587006 3.9605970291902222 15.1715510763154136 T T T
 4.5836693895321501 2.8779506215063115 15.6108581409219056 T T T
 5.8526098588690099 3.1060398064223236 16.1458499704413363 T T T
 6.3595951709505885 4.4064361285309532 16.2279982417448743 T T T
 5.5841369435936663 5.4892298958466750 15.7988165867630350 T T T
 4.3069637926227982 5.2691109430659218 15.2863231865702449 T T T
 2.5323454162331500 3.7554490881526390 14.4335169432319095 T T T
 4.1945159508815912 1.8638095620137418 15.5052864582956289 T T T
 6.4642882450116117 2.2661375468638294 16.4788399333175768 T T T
 7.3638640101083652 4.5798628495327431 16.6165175268318599 T T T
 5.9748142903213148 6.5062390895649163 15.8520763534866251 T T T
 3.6949975519208356 6.1036700219128264 14.9438973183189248 T T T
 1.7987905552145431 3.5709489245563848 11.9880306216205597 T T T

TS1

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

1.9351236307235535 1.9351235494069645 2.7933008378649218 F F F
1.9496377423196323 1.8061525330927990 12.3857677805689192 T T T
7.7214041567944367 7.7016005254119140 7.5749248878196962 T T T
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
3.8520551776683707 7.6912192022927703 7.5786172429981216 T T T
5.7858749425050942 7.7378553236600540 5.1821523560360285 T T T
3.8702473227661907 1.9351238062798457 0.3938262668217468 F F F
3.8658226690849236 1.8672155245072786 9.9775240931380402 T T T
1.9351236307235535 5.8053727258701802 2.7933008378649218 F F F
1.8880061403098665 5.9458785815466966 12.3638555008388824 T T T
7.7225132890906849 3.8332486698662955 7.5685818043798596 T T T
1.9199350778105917 3.8674000729574596 5.1821952049985525 T T T
7.7404950271152559 5.8053732077085396 0.3938262668217468 F F F
7.7330087362221205 5.7567095298922064 9.9644802129501269 T T T
5.8053713350726186 5.8053729508356593 2.7933008378649218 F F F
5.7874568171823828 5.8694821411050029 12.3063622836577018 T T T
3.8525272254187990 3.8232396903261314 7.5833807222509497 T T T
5.7848893951631846 3.8671028309127093 5.1820857302088470 T T T
3.8702473227661907 5.8053729827430605 0.3938262668217468 F F F
3.8343480253433624 5.7443947758492442 9.9825190987063070 T T T
1.9186353845896813 1.9315769217044405 4.7882157716550715 T T T
0.0000001925857419 7.7404969978200588 0.0000000000000000 F F F

7.7425878610841998 7.7095761631300990 9.5725201222882728 T T T
1.9181794744178986 7.6981621230294461 7.1813579589928951 T T T
7.7404951940399229 1.9351242343854522 2.3994608670731532 F F F
7.7906390774667189 1.9023965089971095 11.9678724608556770 T T T
7.7374079539992424 1.9003486792535595 7.9693087383786736 T T T
1.9351236030856309 7.7404975900603716 3.1871236795975757 F F F
1.9152906352777626 7.6768457656256102 12.8571244721397928 T T T
7.7234121511397769 7.7360015636595998 5.5768834962448581 T T T
1.9351241436230258 1.9351235318700586 0.7876614242995419 F F F
1.9512840991249034 1.8980704895724030 10.3755947406028159 T T T
5.7868692776964572 1.9316318647393238 4.7876836729414691 T T T
3.8702478969348064 7.7404972227855380 0.0000000000000000 F F F
3.8601383853340625 7.6952210621970796 9.5645207294428349 T T T
5.7883720761672839 7.7052637891677040 7.1827516835098111 T T T
3.8702474896908576 1.9351240094199731 2.3994608670731532 F F F
3.8914192949546931 1.7233422038076895 11.9639842791439452 T T T
3.8534024909582874 1.8915306582394389 7.9758722284592878 T T T
5.8053713074346955 7.7404978150258508 3.1871236795975757 F F F
5.8434684123260441 7.5973692877500278 12.8264443750800385 T T T
3.8536811381578135 7.7310363867468430 5.5754910291449420 T T T
5.8053718479720899 1.9351237568355377 0.7876614242995419 F F F
5.8257010498525901 1.9308334796480489 10.3452575095283095 T T T
1.9176296178064871 5.8012497541155179 4.7877095386685387 T T T
0.0000001925857419 3.8702478213568439 0.0000000000000000 F F F
7.7502396644312057 3.8374263271747777 9.5675468723104355 T T T
1.9188580025892084 3.8343752407686411 7.1817270435112759 T T T
7.7404951940399229 5.8053734108486674 2.3994608670731532 F F F
7.7399416164637049 5.6905630750631486 11.9454174711563539 T T T
7.7130697022786530 5.7693265129217730 7.9658687945740621 T T T

1.9351236030856309 3.8702484135971562 3.1871236795975757 F F F
1.6896350847307862 4.8928402857458089 14.0382914852385383 T T T
7.7237289385931245 3.8640861875368890 5.5748370823070408 T T T
1.9351241436230258 5.8053727083332740 0.7876614242995419 F F F
1.9150167551383004 5.8217067606310540 10.3653602106746341 T T T
5.7876262651712453 5.8012493874361706 4.7883768250127821 T T T
3.8702478969348064 3.8702480463223226 0.0000000000000000 F F F
3.8572993074648072 3.8258167258198283 9.5859999621118082 T T T
5.7886944907389930 3.8278537468598612 7.1841666463197891 T T T
3.8702474896908576 5.8053731858831883 2.3994608670731532 F F F
3.8256122703654816 5.7404605500890975 11.9715815530069136 T T T
3.8485200129020125 5.7576725894184095 7.9762570546721330 T T T
5.8053713074346955 3.8702486385626353 3.1871236795975757 F F F
5.8046887493413486 3.7404167206944376 12.6697941670678915 T T T
3.8541530793016969 3.8616174586083543 5.5804763754203730 T T T
5.8053718479720899 5.8053729332987523 0.7876614242995419 F F F
5.7856858328873670 5.8345056249912037 10.3655085294667177 T T T
1.8252597351777058 2.5892697038859231 14.2206550045491174 T T T
3.7348550801108358 3.9450118536410272 14.7945963121294302 T T T
4.4521423613145714 2.8408252783955930 15.2787901176420835 T T T
5.6807564855149408 3.0242519473568028 15.9224227458603043 T T T
6.2146277863753454 4.3056809440008328 16.0761737328781109 T T T
5.4991367956531594 5.4135115368345215 15.6092076578826138 T T T
4.2607243342872367 5.2353207368561145 14.9889097166482763 T T T
2.3871344502288387 3.7806836864179609 14.1461077339739258 T T T
4.0333086206210416 1.8394891755414324 15.1666110049445386 T T T
6.2293603820117349 2.1628837544583552 16.3064609870328354 T T T
7.1805192208914779 4.4460530572504346 16.5629188326066981 T T T
5.8940809049661613 6.4221859272997612 15.7421759875863287 T T T

3.6883158522457800 6.1080378703997562 14.6763957302565959 T T T
2.5614669099686571 3.6057285035519167 12.3843573648770757 T T T

I3

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

1.7433372997667471 1.7605819239477858 12.3263847661551917 T T T

-0.0921859036306795 0.0370005916048161 7.5588215441773619 T T T

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

3.6789536552211808 1.9706247215615231 9.9436595350747687 T T T

1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F

1.7572296046748828 6.0418291194977343 12.3539439515784686 T T T

-0.0914714751162602 3.9116532486667670 7.5576923711652135 T T T

1.8484600199372667 3.8727853613681207 5.1753171298214022 T T T
7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
-0.1558151549641285 5.8363235736256183 9.9491618141745786 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.6278917530761579 5.9667643124304011 12.2684282595327190 T T T
3.7788384464795617 3.9100598027559266 7.5591702494832447 T T T
5.7171731472404934 3.8729996629829899 5.1744305300351359 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.6798526731675691 5.8329736557357030 9.9522105862128960 T T T
1.8554697072681394 1.9387979761030165 4.7847606424325608 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
-0.1561032923546466 0.0412470922520744 9.5490781178411357 T T T
1.8421398051522542 0.0362252364124177 7.1721228038572713 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
-0.1703627843686357 1.9079832373629153 11.9160386785984045 T T T
-0.1059103735388871 1.9738349215830344 7.9451542274050020 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
1.7892391456177221 0.0322089774471734 12.9047510571970854 T T T
-0.0864219955541648 0.0071312895385270 5.5627024228120892 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.7583315559119788 1.9702397753068202 10.3388232646623770 T T T
5.7206683335812354 1.9388708496124214 4.7848494063969307 T T T
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
3.7842791685254493 0.0064014219743126 5.5671433622771129 T T T
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
1.8423395747635727 3.9043142517760470 7.1725450941876172 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
-0.1503590180191878 5.8166421321474058 11.9284921847476202 T T T
-0.0964185070226706 5.8415663364289667 7.9477633161208203 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
-0.0859153576830717 3.8778268496200536 5.5637839405728045 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.7662428552507776 5.8789013293970882 10.3459193659632778 T T T
5.7205878071588803 5.8087180994785976 4.7841606313813854 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.6915342982101182 3.9119331249882068 9.5546976025976242 T T T
5.7126545503321076 3.9089746267875189 7.1719324574788956 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.6724192803427993 5.7752360511183758 11.9329144719356979 T T T
3.7703121050411972 5.8417842041513834 7.9528331878907199 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
5.6664078962927267 3.8607278435124863 12.6406379045568915 T T T
3.7840993859860408 3.8764788428612480 5.5653672169353117 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
5.6351593683357999 5.9249467152640847 10.3318976062983765 T T T
1.7550136539619881 5.0868710922680043 13.9235246309623282 T T T
1.6892530967912442 2.7912234673660552 13.8366606891831818 T T T

4.1252171104901381 2.5965229179963121 15.2026813553694176 T T T
 5.4619801246448070 2.5342290627318151 15.6096405851600650 T T T
 6.1784148123226021 3.7107833297934603 15.8413368415389844 T T T
 5.5587630844195308 4.9491401955337517 15.6674078964876298 T T T
 4.2226067264710876 5.0140405754634250 15.2590568368854829 T T T
 2.0408824851915575 3.9033847219960296 14.5954830891554845 T T T
 3.5059460079143583 3.8380877527226667 15.0185036472478668 T T T
 3.5615792546610270 1.6796603853003942 15.0233073760593214 T T T
 5.9376198628625296 1.5629400059535372 15.7560556800249270 T T T
 7.2223122693086159 3.6607372673139937 16.1477337481106566 T T T
 6.1120221276447761 5.8710298568011154 15.8515614429731979 T T T
 3.7310706136487535 5.9773540182816447 15.1180862306528425 T T T
 1.4045596910445666 3.8877591376953813 15.5057412102132179 T T T

I4

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 7

Selective dynamics

Cartesian

1.9351236277001749 1.9351235473800663 2.7933008483844719 F F F

2.0148901182266918 1.6986178549577780 12.3563812997892501 T T T

0.0230283985265525 -0.0279287878468846 7.5623228153668673 T T T

1.9585409936598872 -0.0011327641027810 5.1775576889503734 T T T

7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F
0.0826532791374178 1.9076140106001169 9.9397044472295857 T T T
5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F
5.8731481300670811 2.0273696053562169 12.2552463042022612 T T T
3.8963437110100285 -0.0270030834327570 7.5605860424926519 T T T
5.8298670731673852 -0.0003865000548377 5.1763339095983634 T T T
3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F
3.9149511503451309 1.9095969923179701 9.9329566338186446 T T T
1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F
1.9612886415974147 6.0343309678549755 12.2730515027731126 T T T
0.0253715627959100 3.8503771069701780 7.5567278563487870 T T T
1.9581811435365093 3.8689041460411611 5.1729111753859733 T T T
7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
0.0505743877852165 5.7721421461092826 9.9500461882161382 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.8171621772877193 5.9132796539962795 12.2442882177132972 T T T
3.8958988089856090 3.8491176610553177 7.5477152689833291 T T T
5.8313002912800700 3.8678300488394552 5.1736100305695780 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.8940597637657435 5.7627367320829750 9.9382664584496752 T T T
1.9569792717365764 1.9326191134785409 4.7854107391162684 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
0.0439724270447388 -0.0156715510243256 9.5586596624153124 T T T
1.9600464866000462 -0.0275370904459783 7.1754229914077783 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
0.0975093874565542 1.8883529633631919 11.9417593000809426 T T T
0.0398443966064290 1.9151609618236796 7.9503967977928118 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
2.0751755516178787 0.0146339756724193 12.9779324171202948 T T T

0.0236719846283311 -0.0041323395330757 5.5654358220438320 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.9979676004009361 1.8824973948890287 10.3578783870782942 T T T
5.8283303743679538 1.9327137768162712 4.7828443919963863 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.9165314397819908 -0.0141892482862842 9.5569926386723143 T T T
5.8312652567255219 -0.0090788731863591 7.1723419430121735 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
3.9150905566513106 1.9407096042310410 11.9283996477788783 T T T
3.8958640667247608 1.9142345500020532 7.9415689505187332 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.8382005213810277 7.6676637487605257 12.7578617604166951 T T T
3.8936038921199887 -0.0030424419973663 5.5644010433378392 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.8693405878280460 1.9759686092650408 10.3276723718884700 T T T
1.9568893948605692 5.8037102235707803 4.7854810621912724 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
0.0709535637550304 3.8485214753253527 9.5537297020306138 T T T
1.9606451914809668 3.8558574009364897 7.1674803828130011 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
0.0079424471539649 5.6847798418179973 11.9266374457123767 T T T
0.0053154646663677 5.7826342048156718 7.9439756202375511 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
0.0239084467851023 3.8662129491435353 5.5611699688429157 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.9727960801297482 5.8247645407593343 10.2705929517428753 T T T
5.8288818628074104 5.8036398557000295 4.7861377942294832 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.8956525259852244 3.8454588467511419 9.5408079687204275 T T T

5.8319517973153259 3.8387163841189045 7.1696893702810520 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.9157456879331587 5.6532184470252593 11.9177841983823463 T T T
3.9105698824925876 5.7824558475374603 7.9352922455173474 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
5.9225147650830747 3.7506155154428931 12.7838045975158927 T T T
3.8943997007713236 3.8644291344922395 5.5559939543774322 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
5.8370984260155945 5.8521376960729325 10.3054330067214135 T T T
1.4122013855499551 4.9025474967602705 14.0199517195391330 T T T
2.0226386271447634 2.6739326085364112 13.9537204866060680 T T T
4.3024412269481145 3.1593475814801639 15.6102588035023064 T T T
5.5974669387559413 3.4400423963558930 16.0456882361120670 T T T
6.0839088030777031 4.7486440438715345 15.9977081144581241 T T T
5.2608388450826089 5.7730033963264633 15.5218869126279309 T T T
3.9469990153797228 5.4964968653755566 15.1173251788146565 T T T
2.0576458985056481 3.7929931795722327 14.7263456008816416 T T T
3.4665612845131082 4.1841197241214694 15.1442066580253396 T T T
3.9311891458792023 2.1322860825083718 15.6205041472630430 T T T
6.2327692098378638 2.6324672483292124 16.4120878638364616 T T T
7.0975871763306841 4.9764947271257167 16.3339060582824906 T T T
5.6304223806011784 6.7984877543488489 15.4676142696130334 T T T
3.3145914080901315 6.3200554396740865 14.7832463237874467 T T T
1.4333919126082704 3.6315355821372708 15.6300888345546891 T T T
0.4880301303459864 4.6211159021945303 13.8200253059468139 T T T

P1*

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 6

Selective dynamics

Cartesian

1.9351236277001749 1.9351235473800663 2.7933008483844719 F F F
1.8972824097266723 1.7414329428896302 12.2722646548102485 T T T
7.7259369989646904 7.6529194215390897 7.5525269877030645 T T T
1.9210892179764596 7.7375837613963130 5.1733955524887474 T T T
7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F
7.7218285881981510 1.8392639717309112 9.9128574938402316 T T T
5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F
5.7854153718610215 1.9743872943610334 12.2162269880735632 T T T
3.8576624672220365 7.6684599071449879 7.5509702941192014 T T T
5.7925735668932745 -0.0023438216408976 5.1730950486223302 T T T
3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F
3.8421164215466015 1.8652961091002027 9.9157350745261734 T T T
1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F
1.9493073147708255 6.0233788615052068 12.3143173753896065 T T T
7.7261422680261367 3.7965897582231229 7.5552884612991731 T T T
1.9200694833801328 3.8682787082915091 5.1727793632352572 T T T
7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
0.0161295883501004 5.7106428507788856 9.9578237414490651 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.8021705854863912 5.8569823995659238 12.2984409566794657 T T T
3.8565347474447185 3.8072729898551314 7.5479235086869858 T T T

5.7924549969220420 3.8679753827260490 5.1736191077799667 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.8643846980813672 5.7302698971316781 9.9402745577869620 T T T
1.9188062164833963 1.9296905154979167 4.7857064804147154 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
7.7342165177985649 7.6625918191933673 9.5362159809373317 T T T
1.9217992750601318 7.6661140869559299 7.1686722577031015 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
-0.0257638580160387 1.7083710157541163 11.8762343266530692 T T T
7.7280159480315538 1.8629398248347633 7.9268187816764035 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
1.9743373033369891 -0.0082367038569475 12.9881254675175484 T T T
7.7283245135956342 7.7191157809144046 5.5561610953171785 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.9124673821707454 1.8675277233101988 10.3091497318159444 T T T
5.7949907815307133 1.9298655340603392 4.7839563037260699 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.8597860083034528 7.6780012537739548 9.5413478072389086 T T T
5.7931590245577125 7.6763823579171913 7.1664918974814844 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
3.8362335816984601 1.8281544200500615 11.8960675429956417 T T T
3.8449948447863234 1.8732955576621366 7.9272455377576501 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.7880031511524788 7.5979376303310557 12.7798082169855007 T T T
3.8572892577599283 -0.0097753374866245 5.5572869245637833 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.7806214637770035 1.9098298462319425 10.2753530716573334 T T T
1.9227718239132419 5.7992051263393796 4.7836697565808493 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F

0.0037695007034011 3.7979391356896297 9.5566851296686988 T T T
1.9216782459129009 3.8145439293731287 7.1690646755360055 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
0.0437360774797463 5.7210476529534091 11.9755666717860496 T T T
7.7196635146302590 5.7282735178408029 7.9547143161028133 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
7.7276823098222289 3.8613197986954377 5.5625344110091568 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.9344281144969850 5.7825729692309125 10.3129343148523311 T T T
5.7912866707482946 5.7992669225334605 4.7832064627630411 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.8481435983791172 3.8113218234736230 9.5449409380108801 T T T
5.7923565538963731 3.8044858887728377 7.1695203027460286 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.8456401936498925 5.7269974634623324 11.9120776726426314 T T T
3.8751645219694040 5.7415080731762336 7.9370101252059095 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
5.8542871019816110 3.7191837207039451 12.6002606266437631 T T T
3.8570374001269547 3.8594385910726974 5.5567465901354982 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
5.8158572016903598 5.7950801713493698 10.3541896215785343 T T T
1.7643945848085445 3.2752069194687277 13.2704255426283115 T T T
3.9309677810977197 3.0612604976587772 14.9767220809700898 T T T
5.1824747931747099 2.8859538939435363 15.5692620819586036 T T T
6.0124685459225287 3.9850463531917990 15.8044497670880713 T T T
5.5523805267665951 5.2633462058128435 15.4734779612254183 T T T
4.2891868874009864 5.4404301028795015 14.8883108730671836 T T T
2.1534281496755554 4.4717536930163018 13.8875358609135375 T T T
3.4637116695773318 4.3334019215335857 14.6060255803368335 T T T

3.3031532688093566 2.1880041897073328 14.7922560013989148 T T T
 5.5078677612892566 1.8803325003403937 15.8436790863365342 T T T
 7.0052183891378839 3.8452393947330741 16.2347267285438335 T T T
 6.1726303010704635 6.1383233121581897 15.6735058294436218 T T T
 3.9544781096310477 6.4520864515793388 14.6461131822459993 T T T
 1.3454427118257588 4.7945968458250814 14.5784542984819065 T T T

l10

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

1.9351236277001749 1.9351235473800663 2.7933008483844719 F F F

1.9899664430798680 1.7231842551298513 12.1414811118731141 T T T

0.0259012161915985 7.7172608899240984 7.5538109715198987 T T T

1.9617449886962346 7.7400363686599469 5.1744233136643398 T T T

7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F

0.0426741422549600 1.9291087564744973 9.8858728629951802 T T T

5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F

5.8579785102688797 2.0355214755262070 12.2345669284535656 T T T

3.8989709177974645 7.7148011909339163 7.5516126646098103 T T T

5.8320580951607219 7.7394794284887247 5.1734736420568721 T T T

3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F

3.9344550198365260 1.9268992499028952 9.8833106350979509 T T T
1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F
1.9864744116344988 6.0579188252600344 12.4328885347908606 T T T
0.0265012763124530 3.8771085833445920 7.5430070160221643 T T T
1.9620120305230169 3.8697355731885419 5.1703925908283308 T T T
7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
0.0941929616030290 5.7828134103742439 9.9649878664871210 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.8579988449357927 5.9184320958941399 12.2678537449810658 T T T
3.8984998099658261 3.8754478329630300 7.5435176817997140 T T T
5.8323786069191534 3.8705458480511390 5.1701885731076738 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.8801558480783709 5.7832875444714160 9.9636394780182993 T T T
1.9606404618563200 1.9344367062626309 4.7845477389977713 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
0.0443366117104093 7.7327437536740842 9.5444423750247065 T T T
1.9630192089093219 7.7329690901715100 7.1692804882840901 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
0.0678334076340557 1.8959171281877620 11.8773550545059958 T T T
0.0130760221388719 1.9298646594082314 7.9130575652162713 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
1.9838761765018085 0.0491981971062866 12.9411549049844492 T T T
0.0263939384668181 7.7325469153376920 5.5572423399518325 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.9871954693913771 1.9297428363220264 10.2177066469937312 T T T
5.8307356845025495 1.9346539747570073 4.7854201149414486 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.9239242033051136 7.7304700902805621 9.5402189614660227 T T T
5.8337212565587162 7.7182503910675422 7.1663395173066791 T T T

3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
3.9113888472989138 1.8812617786634660 11.8716623975176070 T T T
3.9192606920686477 1.9281957661156004 7.9115241664384772 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.8605502994168601 7.6600756704760942 12.7515435210556483 T T T
3.8961714390925342 7.7330013081884941 5.5560414283504258 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.8579262931327065 1.9914005161272752 10.2879793593831419 T T T
1.9613850895021860 5.8046910830702130 4.7832169631446675 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
0.0515960813311243 3.8707323386387569 9.5385125012596284 T T T
1.9627893357737973 3.8626858955427696 7.1648160208412994 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
0.0913221188083193 5.7332839197308489 11.9753105192129112 T T T
0.0355150985689293 5.7969919188444585 7.9507839884762399 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
0.0263602880218232 3.8760882389179350 5.5523590504231599 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.9845285232167293 5.8181462958223911 10.3185527721535220 T T T
5.8304625286416982 5.8046525443915922 4.7810923173211082 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.9175624753909624 3.8694369815492871 9.5372643505016583 T T T
5.8341249947306881 3.8784718813195309 7.1638428892080821 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.8882102666673850 5.7558116056053370 11.9501189723185863 T T T
3.8958961468054456 5.7955294443390244 7.9411946533698288 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
5.8600175013536733 3.7541584592916086 12.7545452127628280 T T T
3.8965046246953134 3.8742817177026070 5.5520680658426373 T T T

5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
 5.8612387374328154 5.8526342701134109 10.3591866227716949 T T T
 2.1059350441009586 5.2682017547339344 14.3829835609843091 T T T
 1.0785114908165088 4.5768824987133305 15.0500557354147055 T T T
 1.2226548185347734 4.1999696643635449 16.3886197504493545 T T T
 2.4021406198563704 4.4978801526881265 17.0797165221332072 T T T
 3.4281263689915273 5.1943549610595969 16.4351409742140930 T T T
 3.2715685497606350 5.5854687968633323 15.1030274567397882 T T T
 0.1660509463469713 4.3045945810536219 14.5121746158241010 T T T
 0.4181553945709651 3.6599420601359105 16.8906639091543163 T T T
 2.5194310358620640 4.1888442057660891 18.1197035541888170 T T T
 4.3498371412910286 5.4377893333999392 16.9696079054702871 T T T
 4.0668578551116825 6.1739232785048666 14.6348890870688368 T T T
 2.0190489433894294 3.1920744740744471 13.0218004759798731 T T T

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

1.9351236277001749 1.9351235473800663 2.7933008483844719 F F F

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
5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F
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
3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F
3.9186700548101259 1.9262520651938666 9.8538476485953002 T T T
1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F
1.9819891996601597 5.9667047555895314 12.3710308906441782 T T T
0.0254268873972254 3.8676122859064117 7.4899738410598724 T T T
1.9622007826871399 3.8701279773174342 5.1480006963677871 T T T
7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
0.0778836112426954 5.7841039517514856 9.8942687069595721 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.8535944751376947 5.9140628578566385 12.2239796606631241 T T T
3.8986156490657473 3.8676517800167338 7.4895418760837096 T T T
5.8326604514599278 3.8705224512033274 5.1461963811793634 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.8861696809216824 5.7840347210072327 9.8945600649834624 T T T
1.9595262708992516 1.9344188853978157 4.7775684912100687 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
0.0464242912327764 -0.0100909966140954 9.4956590089143802 T T T
1.9626910875645738 -0.0100444720410178 7.1355398701101755 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
0.0708396764062588 1.8968682424805756 11.8826455589845921 T T T
0.0170538552292836 1.9258694783724208 7.8798974628762579 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F

1.9821681528661159 7.7014889885766822 12.9304718077817640 T T T
0.0256234395720688 -0.0046318060977817 5.5155584776544710 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.9826208699294909 1.9223733338443869 10.2429820971283831 T T T
5.8302354703534665 1.9343150190673628 4.7774096000418185 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.9149767054752860 -0.0103557342035422 9.4950047035814364 T T T
5.8330221364147850 -0.0187823902209309 7.1341374337706602 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
3.8968851770530493 1.8943206627296147 11.8814288525242766 T T T
3.9128174723116427 1.9257768503893860 7.8790671317688830 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.8547930205132941 7.6418928078974773 12.7452739968158220 T T T
3.8961244262658554 -0.0045469395014907 5.5151708874589449 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.8529343658547841 1.9796933605019711 10.2823099149653796 T T T
1.9597155745194970 5.8047393049661951 4.7772466708319543 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
0.0400399043932133 3.8655567384149760 9.4900092427330360 T T T
1.9626769255435619 3.8587251318638840 7.1330237885287548 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
0.0780977756069236 5.7046887476933064 11.9278135102917133 T T T
0.0320692473501921 5.7939034886672207 7.8980837589286033 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
0.0257538348088453 3.8722110045368501 5.5108142001991220 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.9814543906981255 5.8113438139767020 10.3100995998807843 T T T
5.8300334027406837 5.8048083595561417 4.7756134121579965 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F

3.9217006132330368 3.8654358937110485 9.4897197690897386 T T T
 5.8330362833181448 3.8681524622968926 7.1295865894912192 T T T
 3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
 3.8867436886457876 5.7066972359041426 11.9268031726036359 T T T
 3.8964541728749751 5.7937427135014081 7.8974275047435256 T T T
 5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
 5.8543600643171363 3.7492760995652392 12.7659057297823963 T T T
 3.8960279070726012 3.8719384527776768 5.5105460990154027 T T T
 5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
 5.8520569415547863 5.8664324477173562 10.3107378375031065 T T T
 1.9869288992871845 4.8260320299006549 14.3008457826056983 T T T
 0.7811021680105469 4.8077272570827079 15.0603892379447100 T T T
 0.7837085552112431 4.8125543875866708 16.4574138456125034 T T T
 1.9903912945854796 4.8350503538584411 17.1676769193082670 T T T
 3.1930836597169030 4.9062351371592534 16.4549991607780868 T T T
 3.1919016335786408 4.8987116432984941 15.0577115321019104 T T T
 7.5604247493941221 4.7632331034175408 14.5422974749065137 T T T
 7.5751238331636204 4.7944411464413470 16.9989918473022925 T T T
 1.9936112863397997 4.7924998356733770 18.2585696030826519 T T T
 4.1420442962595647 4.9674337935148776 16.9931707013576414 T T T
 4.1530637964095716 4.9380451677037689 14.5403651815089798 T T T
 1.9965007320244423 3.4027390895489038 13.3473218805860778 T T T

P4*

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

1.9351236277001749 1.9351235473800663 2.7933008483844719 F F F
1.9806568211706481 1.3790347054565006 12.1759229138316769 T T T
0.0259288745361269 0.0455473437059947 7.5712304249232147 T T T
1.9617804266026719 0.0035356869051410 5.1803724112067133 T T T
7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F
0.0619507364711170 1.9942484045925817 9.9334067654872165 T T T
5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F
5.8563815983461200 1.9908485894270198 12.2920260059221302 T T T
3.9007338357696812 0.0444732031789468 7.5716254314150353 T T T
5.8320271862932573 0.0021421701607864 5.1787767956190844 T T T
3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F
3.9078459897290121 1.9924771826349124 9.9360680387649918 T T T
1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F
2.0131030530216112 5.9980825682864447 12.3897772491464480 T T T
0.0283460199280709 3.9268999857215703 7.5592469147104309 T T T
1.9620534393620435 3.8712773654693731 5.1756780895839976 T T T
7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
0.0888934276249281 5.8481875817315334 9.9654498280519128 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.8751952852198217 5.9451788176232601 12.2692646664630871 T T T
3.8975448298844277 3.9247302003219859 7.5601924206444098 T T T
5.8316437591495571 3.8732108050394385 5.1763473049166615 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.8992057679066483 5.8479881718819584 9.9663413423683238 T T T

1.9602900846508704 1.9395784496964390 4.7860017570435369 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
0.0280270285552552 0.0453193205227632 9.5722243937853122 T T T
1.9638047866265271 0.0575437985906264 7.1850670956447367 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
0.1019777669638174 1.8813199146534063 11.9592471554010871 T T T
0.0048846485589940 1.9860099615680675 7.9579000978387793 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
1.9662724773656808 7.6054841523166381 13.2820187745066534 T T T
0.0264182790370689 0.0072370963490105 5.5763862316765609 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.9842570436866684 1.9075366645865732 10.2396950700421279 T T T
5.8294559828619663 1.9399299684518492 4.7897160577031652 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.9467388050490322 0.0441366031209328 9.5746096638236580 T T T
5.8341107306919575 0.0271375177212888 7.1811021330010139 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
3.8676534322203220 1.8795116450919707 11.9616382362828304 T T T
3.9251200467834617 1.9843737528897598 7.9593124537615854 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.8608234381619289 7.666239926902406 12.8190449129929647 T T T
3.8964482248479473 0.0072112725712221 5.5779474427244260 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.8544416418664813 2.0574834437812655 10.3679670928323180 T T T
1.9612134473511786 5.8088807924547945 4.7886678700924028 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
0.0838927893479185 3.9267278379492252 9.5764357584378637 T T T
1.9639020619396788 3.9034797558611398 7.1788332318151964 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F

0.0645857489605816 5.6723385953397685 11.9930684088723165 T T T
0.0505528139420553 5.8492790067074667 7.9769247067392435 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
0.0257018571621129 3.8797206616309139 5.5746493903848933 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.9931214119517013 5.9603888664481106 10.3871222544976671 T T T
5.8285500518399100 5.8088381881769067 4.7866253832544530 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.8890736065520057 3.9258056066591651 9.5774621714218675 T T T
5.8338432228049246 3.9352956836977313 7.1845510149319463 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.9343393944848906 5.6575778202272531 11.9891829323384815 T T T
3.8870000241446445 5.8483121270305070 7.9780271167166736 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
5.8715178191006547 3.6590576952431477 12.9482182962308148 T T T
3.8970946335906120 3.8781291575083765 5.5751356176839302 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
5.8656911719497886 5.9304550792927841 10.3585396873095608 T T T
2.1381974150493068 4.0863098259761284 14.2962227244928606 T T T
0.9113140314570460 4.2084555792559319 14.9795279028752244 T T T
0.8978685589893187 4.7915354904974494 16.2437425561635180 T T T
2.0926954946610747 5.2337437231116173 16.8314405735480292 T T T
3.3107450761384047 5.0723322916998734 16.1655972811478392 T T T
3.3433471643870516 4.4882634150557941 14.8983887552928422 T T T
7.7353658545351331 3.8454295175405573 14.5062140484388244 T T T
7.6951848251695498 4.9061756208716831 16.7820373524081141 T T T
2.0726963259095492 5.6999903341466691 17.8164003565075006 T T T
4.2389951769060046 5.3981399378949355 16.6390788087494137 T T T
4.2837760323955933 4.3072691271494090 14.3687604226012642 T T T

2.1787097133895932 3.5523081186416459 13.3391000163856575 T T T

TS5

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

1.8233394804748975 1.6610788037593676 12.2951118612559682 T T T

7.7095501023414004 7.7336647013381405 7.5557399880148193 T T T

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

5.6987875363302747 2.0426966351298037 12.3017890534222154 T T T

3.8417798294357914 7.7348463898775544 7.5586549168150352 T T T

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

7.7121133993000885 3.8633379723567591 7.5516450097485066 T T T

1.9069278839905199 3.8696882362280443 5.1718123907120805 T T T

7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
7.6489586337074007 5.7904157116121722 9.9356385757825940 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.7010121080025087 5.8821266317543550 12.2974400933160624 T T T
3.8404873936941626 3.8648340728354640 7.5500294188153694 T T T
5.7774134592908819 3.8697280917278367 5.1727994640776380 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.7782351660578559 5.7890930820639550 9.9357299319440049 T T T
1.9099777384355394 1.9343686484746632 4.7880469173571836 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
7.6425897353409562 7.7361810486822673 9.5613981688834642 T T T
1.9025854866986724 7.7344984517030229 7.1809781813315503 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
7.6586302409590905 1.8677430513946760 11.9426020718795343 T T T
7.6990372309844339 1.9291386675875570 7.9548773411321925 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
1.8657352833141361 7.6880986140733407 12.8959563145861047 T T T
7.7122052552763378 7.7389838078955373 5.5684322577331287 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.8416329146680956 1.8996187749960434 10.3432594749471001 T T T
5.7802349306503924 1.9345581981709528 4.7878917993577828 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.7967584941611285 7.7378182590216582 9.5668435421176952 T T T
5.7730126123157683 7.7354330292229303 7.1769324041876796 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
3.7444902518544052 1.9231370765685041 11.9443081862626101 T T T
3.8378869361999195 1.9299906776779188 7.9544027598780414 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.6937134487328613 7.6147018470312400 12.7956118869658049 T T T

3.8413013800882974 7.7396637590989954 5.5697239655311481 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.7098484170837924 1.9888995145928494 10.3582364364376911 T T T
1.9100628980600742 5.8047666211999260 4.7881000386486949 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
7.6759468021412136 3.8642983707514582 9.5637230849806070 T T T
1.9027485745600350 3.8640984179640063 7.1751638198800753 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
7.6697751789833575 5.7284221519737466 11.9387905282124382 T T T
7.6993687800876014 5.7969631107231869 7.9533900227809786 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
7.7120444809921862 3.8684192815419758 5.5664641426090133 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.8443124800121307 5.8522816962858206 10.3337764911640413 T T T
5.7801682590449062 5.8046469936739671 4.7880498374974119 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.7644044735112367 3.8661769950733036 9.5567602264568254 T T T
5.7734736161753899 3.8638341563992893 7.1781873041916855 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.7443414357973892 5.6898587303019914 11.9339262515279234 T T T
3.8395723031648616 5.7987445651804252 7.9521589737018097 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
5.7293452239945060 3.7791795401670503 12.7505273160083821 T T T
3.8419845066869969 3.8688602610405063 5.5651223274217694 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
5.7135278423834324 5.8455499218195861 10.3538566614139729 T T T
1.8423877202270704 4.9566529326253441 13.9119727268581332 T T T
1.8103792312321587 2.6964977763907503 13.8955155529497691 T T T
4.1602461430803919 2.5351877574466175 15.5073178831383380 T T T

5.3944799225769646 2.5453985148509974 16.1297141158012245 T T T
 6.0535544249720061 3.7444176822712238 16.4522550753398455 T T T
 5.4410731710024951 4.9671548656937263 16.1254615865734685 T T T
 4.2067863924058289 5.0229373788165264 15.5076893097684803 T T T
 2.3233794743837186 3.8170258963710166 14.3284202849650963 T T T
 3.4850814705444262 3.7924534985374878 15.2242985316850863 T T T
 3.6518418849899086 1.6018714787213519 15.2689779141694313 T T T
 5.8686299582221153 1.5883184440008544 16.3582693713906906 T T T
 7.0281749589309079 3.7264964938942273 16.9350149970996142 T T T
 5.9548336668756745 5.9057161490135437 16.3448333976902980 T T T
 3.7356757448757181 5.9735849641147043 15.2612832086359091 T T T
 2.3676641582110149 3.8090889929608354 15.8615384312157452 T T T

I11

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

1.9198479163352733 1.5632609510395583 12.2921901042368180 T T T

-0.0052250544397771 0.0010784962924720 7.5676739733668512 T T T

1.9325909208758383 7.7393086980163899 5.1800225350933049 T T T

7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F

0.0103954905315089 1.9223843251257984 9.9678265858074599 T T T
5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F
5.7907589516029683 2.0510622234480138 12.2645615727099031 T T T
3.8712207076847234 7.7386137075010906 7.5611014858692842 T T T
5.8047179781237475 7.7390096193320375 5.1776856201855477 T T T
3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F
3.8540765763681102 1.9241550591166070 9.9556457086784054 T T T
1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F
1.9288419926029863 5.9105759457129237 12.2876583373419805 T T T
-0.0006619604804277 3.8495505176989151 7.5573101393946143 T T T
1.9327662155163206 3.8695760512546125 5.1734532720017388 T T T
7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
-0.0002947744505806 5.7817084588511474 9.9290968196418650 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.7975706172677715 5.8246691167261284 12.2834210543151734 T T T
3.8665104476710770 3.8510937700145327 7.5531736226589974 T T T
5.8044221493354620 3.8700665802953669 5.1756505091283307 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.8659016793086418 5.7864623780756972 9.9248972881084079 T T T
1.9327112844534058 1.9334323030855336 4.7858138582785097 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
7.7051180685148219 7.7337846468205456 9.5682140342843098 T T T
1.9326508024804965 7.7327858903888247 7.1806011699734764 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
7.7063255198874927 1.8895917893227501 11.9421462844523525 T T T
7.7240849226573882 1.9258385882081517 7.9505524842327091 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
1.9243576494712296 7.5549288223504636 12.9547801323844602 T T T
-0.0013334875802735 7.7394526471229677 5.5702211649513051 T T T

1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.9263981315205909 1.9047443758699594 10.3052638805503012 T T T
5.8045227591877016 1.9338563563331033 4.7866219845396563 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.8952175799145525 7.7323708386510965 9.5584727486113685 T T T
5.8036390396566535 7.7249531944200118 7.1725508836027130 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
3.8881095176501526 1.8468413479056331 11.9171897939446421 T T T
3.8794552342245807 1.9257482736932880 7.9428074566707068 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.8045865792288796 7.5380662312961304 12.8066287077209111 T T T
3.8679252164332540 7.7388569599554105 5.5663158542724931 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.7987609020883966 2.0550502632427530 10.3245724915565891 T T T
1.9324542679037444 5.8048482624544775 4.7862959692176990 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
0.0428287687557727 3.8678107508408210 9.5514737713377365 T T T
1.9324671585046449 3.8582063151342680 7.1673560895363551 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
0.0348089922714801 5.6212054757292478 11.9400829123476502 T T T
-0.0033271370951258 5.7958199934275658 7.9534618710383906 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
-0.0022466029716190 3.8674971743884510 5.5623130640100502 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.9307018451014653 5.9019370153045765 10.3269861316547207 T T T
5.8048378080372327 5.8045468678837695 4.7855552410729878 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.8161070985320613 3.8682463813750445 9.5479321753294499 T T T
5.8036703525332474 3.8667639296620271 7.1751571370409639 T T T

3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.8313713546846846 5.6398415716303028 11.9198194741211818 T T T
3.8723056665463678 5.7949810090555030 7.9448793413505214 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
5.7762643995778777 3.7756695128935180 12.8146829631316557 T T T
3.8687156508904859 3.8675134113180047 5.5600467105756115 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
5.8045783895403202 5.8267080051815041 10.3429068075373056 T T T
2.0506259974861045 4.8584246565039519 13.9512709227242375 T T T
2.1061532811069488 2.6279008956100709 13.9883413189297077 T T T
3.9989243826520675 2.5443265742625027 15.9924077024420779 T T T
5.3576079270641506 2.5786481233507121 16.1558311790540365 T T T
6.0719925287845289 3.8008308970149409 16.1881529014950942 T T T
5.3677198828229962 5.0231453562886585 16.0700149142540845 T T T
4.0107554599493502 5.0571932749956261 15.8979339233951382 T T T
2.3985718884674143 3.7474847953743966 14.4810801407421508 T T T
3.1939972266015579 3.7987809889294279 15.8054790636940865 T T T
3.4654566349304003 1.5955427295598212 15.9486814891886208 T T T
5.9018655636531623 1.6375476035071195 16.2550291417499260 T T T
7.1573375889045883 3.7992892670508054 16.2778349805456735 T T T
5.9195051963642431 5.9647890039834488 16.1081491276722204 T T T
3.4853746379886950 6.0051128456295215 15.7871664418968702 T T T
2.3819283694636884 3.8349289886638758 16.5724677616133320 T T T

TS6

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
1.9019829207822463 1.6273256078562308 12.2631037662097153 T T T
7.7183246576215607 7.7224482385963427 7.5469818440870959 T T T
1.9144343786171938 7.7393459561342173 5.1713250511466740 T T T
7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F
7.7109337683904338 1.9160317303961396 9.9208449919197328 T T T
5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F
5.7661063706098359 2.0281993496975743 12.2580640607288043 T T T
3.8506918713842944 7.7212613366672356 7.5434998745923449 T T T
5.7854849800321073 7.7396571187177194 5.1703729078682832 T T T
3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F
3.8312044699912389 1.9127179563186840 9.9160596800601546 T T T
1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F
1.8964302911257354 5.9424125594207737 12.2479688647351725 T T T
7.7200366852940778 3.8508730187085116 7.5383735721635903 T T T
1.9146868558847072 3.8691952539419692 5.1675359473729490 T T T
7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
7.7035708602967397 5.7758572308711278 9.9150856308496866 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.7628766688162907 5.8705578150056059 12.2602151414684855 T T T
3.8492210490435386 3.8498405714957751 7.5373209989265293 T T T
5.7851956764841441 3.8690399447990460 5.1682541477701456 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F

3.8336081158301458 5.7760884732687749 9.9111893415318608 T T T
1.9160172225736964 1.9332782818330179 4.7851868908050053 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
7.6951584505449802 7.7249797955086832 9.5470188675363001 T T T
1.9136257750251071 7.7219422900729038 7.1712004045747797 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
7.7317276808733544 1.8968944512796486 11.9262186421896548 T T T
7.7154029918679203 1.9176581979305432 7.9350708704304038 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
1.8975675195736752 7.6520627803628294 12.8558456788550650 T T T
7.7211299818151131 7.7379585058655627 5.5575492007102207 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.9008128552124119 1.8848820122945691 10.3030431795455790 T T T
5.7868236540948343 1.9334518591582455 4.7846403507736879 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.8459247960240783 7.7233829883542136 9.5403021279553091 T T T
5.7846029868164566 7.7267750620600220 7.1673522748586747 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
3.8152479204202017 1.8626856655009818 11.9105185616831086 T T T
3.8510240191595364 1.9168157187934916 7.9297985519434757 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.7746583841918602 7.6019500493200756 12.7509882875507401 T T T
3.8502551674447036 7.7372551824945575 5.5550677169148139 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.7726756713368994 1.9688113374510059 10.3209738533289297 T T T
1.9158281400351056 5.8037499901838787 4.7851118643450281 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
7.7231972915287086 3.8518532011931708 9.5389559619705651 T T T
1.9136843988999490 3.8540441173514774 7.1653298745776892 T T T

7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
7.7279717510832056 5.6792509224421881 11.9069486763989012 T T T
7.7083063376881187 5.7860074678264866 7.9298576816835871 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
7.7207707267771069 3.8660600145854551 5.5525830163997059 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.8983612295820662 5.8320905814597994 10.2825554543240525 T T T
5.7869995787269222 5.8036494040842674 4.7853514505083758 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.8181524972262686 3.8507433228535159 9.5379430431380410 T T T
5.7845778291315186 3.8499449170061260 7.1674474639804666 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.8105746217919028 5.7018153230965085 11.8975132978373654 T T T
3.8561718708146318 5.7847667491504238 7.9254969573737251 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
5.7550016450821637 3.7647691812725732 12.6794737011771002 T T T
3.8506104874719127 3.8658935751687644 5.5517797988673872 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
5.7698471813180001 5.8389854958095295 10.3163933972055144 T T T
1.9245799120813389 4.8475573530035696 13.8038790172331911 T T T
1.9444577472901290 2.6452418007837255 13.8790285016216082 T T T
4.2806236581967463 2.6604177839825520 16.1820968236578899 T T T
5.6462372978200266 2.6589365073030704 15.8903271539900430 T T T
6.3314668397608518 3.8690175134091191 15.7321263261250603 T T T
5.6293116222929696 5.0788264707846036 15.7831613860734095 T T T
4.2632564510660185 5.0838327351980466 16.0745158593287982 T T T
1.8052647661657060 3.7672692610778826 14.4890350157937355 T T T
3.5997695347156098 3.8762699834735419 16.3290181920964308 T T T
3.7431814860516610 1.7183881384649964 16.3090974545282705 T T T

6.1880419187599562 1.7113918962871386 15.8402516651911771 T T T
7.4124077254805938 3.8675845044153370 15.5664387397892447 T T T
6.1578439152093329 6.0265759914233330 15.6531795270533411 T T T
3.7129378046727939 6.0259158890644571 16.1187585017298680 T T T
2.5766300087709464 3.8846567969958548 16.6925842074785784 T T T

I12

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

1.8501283731802514 1.6027148283722938 12.2501693740107527 T T T

7.6988122330489173 7.7189941179097383 7.5312274981743492 T T T

1.8952837117289276 7.7390914424025015 5.1656985826660300 T T T

7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F

7.6669016832899146 1.9099562436685522 9.8979728658495052 T T T

5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F

5.7174512480690920 2.0289260185002806 12.2218412330879662 T T T

3.8308236450301756 7.7178747203713733 7.5288942408658830 T T T

5.7658711365487374 7.7392368884022025 5.1658751554460576 T T T

3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F

3.7781418973318064 1.9084054777892978 9.8973427980156554 T T T

1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F
1.8513013642176925 5.9246762723856987 12.2170704117525712 T T T
7.6999259435271563 3.8451310814721609 7.5181995542183042 T T T
1.8964067198152068 3.8685557173359841 5.1607487587889569 T T T
7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
7.6596326850539791 5.7689907081164433 9.8861916053606311 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.7198671972893402 5.8828343632618409 12.2278790340884971 T T T
3.8300331815016238 3.8443766009682880 7.5218397681634022 T T T
5.7648555609142500 3.8687829263223019 5.1608689766464497 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.7900624187860976 5.7718727341157035 9.8852174771535388 T T T
1.9000350598324958 1.9326385465482663 4.7807792953138959 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
7.6577864028805145 7.7202419345997999 9.5179588230992440 T T T
1.8932092300287788 7.7184430657320329 7.1567233789111810 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
7.6809885411144698 1.8778144094563720 11.8848396486038617 T T T
7.6929103266891286 1.9134284895500016 7.9028748997678973 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
1.8472381507427302 7.6309565559400774 12.8494643312617871 T T T
7.7018699220561215 7.7373857936502333 5.5402980872143441 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.8543506156642093 1.8834811027682337 10.2750260289309985 T T T
5.7677069376482368 1.9327467353168155 4.7811102531375154 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.7968031271410161 7.7199724878570271 9.5140760384784837 T T T
5.7635188124885133 7.7236148124232935 7.1563179407281332 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F

3.7624401023646801 1.8532223483093686 11.8854684585854713 T T T
3.8248610557382583 1.9134105951516225 7.9040535668707506 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.7341151435644111 7.6117601435174347 12.7155466111929538 T T T
3.8316354331307574 7.7374951530361544 5.5389307936529635 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.7237342340022446 1.9580359001166314 10.2819162315468606 T T T
1.9004937558241857 5.8034128029684293 4.7810011809528641 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
7.6780862723108889 3.8458784331966207 9.5088720511784715 T T T
1.8931277274184379 3.8498371907015594 7.1503454106424851 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
7.6786200700824105 5.6949177273336549 11.8618404800579622 T T T
7.6856627327085558 5.7813276984683055 7.8952641064899156 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
7.7019424672706025 3.8654905442337415 5.5310049481887500 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.8550585808082594 5.8226195638172920 10.2417543191525322 T T T
5.7672671265753142 5.8034437046025662 4.7817695472242550 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.7764481370033427 3.8464546735097347 9.5121007643050337 T T T
5.7636367235365569 3.8457023380988220 7.1517167918143896 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.7687301639926689 5.7213516753786857 11.8592360639471419 T T T
3.8361006125205304 5.7807713383805455 7.8948149107703873 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
5.7005674109323561 3.7714653956540087 12.5939811055988127 T T T
3.8316207321052649 3.8642913186296033 5.5341983377794373 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F

5.7261010903978704 5.8385398904836183 10.2755423602312952 T T T
 1.8484889471752233 4.7788152934123227 13.7083961389423354 T T T
 1.8217913912141537 2.5947791355087610 13.8739937766076906 T T T
 4.5077609217524692 2.7208891680790503 16.1259832162637622 T T T
 5.8506104453286998 2.7199890534984550 15.7380372023377149 T T T
 6.5098792843856623 3.9327551902900262 15.5229040107579408 T T T
 5.8227397137742791 5.1443805871377890 15.6343833966856742 T T T
 4.4795009476996652 5.1454061666000017 16.0248131233071369 T T T
 1.6906234751774865 3.7365863494448335 14.4669240275148159 T T T
 3.8348821598733411 3.9352141635153735 16.2998781098911500 T T T
 3.9813553070951491 1.7800386759597389 16.2969889843803379 T T T
 6.3969092473853806 1.7780180149869234 15.6346615105793330 T T T
 7.5765497942405240 3.9277251112233325 15.2753781588220523 T T T
 6.3477389404761322 6.0884770076576054 15.4632405748365791 T T T
 3.9353868536220258 6.0861014035251442 16.1272238744465533 T T T
 2.7971072552092338 3.9355902258485380 16.6239493763380217 T T T

I5

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 7

Selective dynamics

Cartesian

1.9351236277001749 1.9351235473800663 2.7933008483844719 F F F

1.9613770458368620 1.6045022560473505 12.2907655426198215 T T T
0.0153145611495328 -0.0621280663243172 7.5420685773564706 T T T
1.9520540534562172 -0.0033745986162898 5.1713915446697554 T T T
7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F
0.0519247972257048 1.8492723670952331 9.9232967774310588 T T T
5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F
5.8418745774404828 1.9621759516764461 12.2056172820219953 T T T
3.8903414917821126 -0.0418164665998885 7.5504071756683011 T T T
5.8210060924021452 -0.0029400148169844 5.1700063398233951 T T T
3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F
3.8883612439690585 1.8955180117189399 9.9302575937969344 T T T
1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F
2.0162959023761049 5.9931655241119435 12.2798087050011038 T T T
0.0178663542630869 3.8012904312755031 7.5509654467800233 T T T
1.9495707837735450 3.8675255548213632 5.1706193404332783 T T T
7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
0.0780120230631504 5.7299539658967387 9.9222669571700912 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.8586876436846937 5.8228303067101530 12.2663344100706748 T T T
3.8867275036495306 3.8168457406615057 7.5392964645919234 T T T
5.8228755282319806 3.8675085376355467 5.1721874725078649 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.9218175893105620 5.7468118607060195 9.9093271112296382 T T T
1.9489978820672236 1.9308262433415484 4.7843351274301087 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
0.0291897108581801 -0.0669227752319960 9.5240633521705291 T T T
1.9536934594911968 -0.0536584609848280 7.1660675598284218 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
7.7314466288183370 1.6701259311971997 11.8666028157055319 T T T

0.0119515504763793 1.8750893068518488 7.9189765407309398 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
2.0891493145835160 7.6132268512209329 13.0738595622823404 T T T
0.0170106280587451 -0.0151512823808877 5.5484164576198003 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.9747177195437420 1.8567087715015014 10.2941743158466092 T T T
5.8215086763825283 1.9312837551036577 4.7833732422344069 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.9357945974119768 -0.0460758013176850 9.5458592641252871 T T T
5.8244023737172759 -0.0495531396873410 7.1610123807618891 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
3.9310755804312310 1.9106061937271128 11.9085392348618786 T T T
3.8872744746718890 1.8893567427063009 7.9246588395766775 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.8178611643972156 7.5529853709576136 12.7708163508270509 T T T
3.8866232218183763 -0.0023798521799028 5.5544940382810886 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.8366808420065741 1.9621349002400403 10.2705489028849044 T T T
1.9522001521512997 5.8001828013592167 4.7841694940947672 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
0.0801852784693225 3.8111422329651763 9.5516487879691230 T T T
1.9532974119535642 3.8215088337358440 7.1638356241727887 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
0.1071952635327298 5.7078412735277633 11.9450720572250599 T T T
0.0162003834634167 5.7410934694537019 7.9381813785303539 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
0.0162135972571362 3.8600471106739231 5.5579090987497963 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.9949057600043563 5.8280025752215252 10.2854416126222628 T T T

5.8187362737623340 5.8001230963853105 4.7836158420185804 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.8831472031829501 3.8310218373099105 9.5292459105625440 T T T
5.8239686063643434 3.8186556127886506 7.1684793971510414 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.9034132209952110 5.6252577088499178 11.9036871878557839 T T T
3.9073786033491302 5.7595748290301767 7.9261183382113947 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
6.0602687765160370 3.7133431092308302 12.6987065287688399 T T T
3.8867275361416449 3.8621643567425630 5.5513045087453037 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
5.8700291620760767 5.7862240069958064 10.3347340609463600 T T T
1.2999933526646339 3.2994101173855741 13.4142896502401321 T T T
3.6705094827752500 2.9154657191863986 14.9140157975269929 T T T
4.9137444099636918 2.6873897802979227 15.5147185793633398 T T T
5.7575869458126201 3.7535055942402726 15.8289625347989293 T T T
5.3367053955866099 5.0565794888714759 15.5420500699560389 T T T
4.1022105597372507 5.2847866783224520 14.9298738030161786 T T T
1.9538684265595478 4.5142239318099584 13.9123757186555324 T T T
3.2431479025013701 4.2147919390268385 14.5936029695195604 T T T
3.0244274328748295 2.0567844705729010 14.7250976566533325 T T T
5.2154497520849805 1.6631037721954716 15.7430317045227355 T T T
6.7318944825518274 3.5738349337015456 16.2843505722967130 T T T
5.9735837228282591 5.9079450456191651 15.7880131309599960 T T T
3.7970331892578022 6.3100832953150849 14.7051910231490517 T T T
1.2473236940977801 4.9928468779609609 14.6154544230080745 T T T
0.3552250959510613 3.5108346726811912 13.1704017727222240 T T T

I6

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

1.9351236277001749 1.9351235473800663 2.7933008483844719 F F F

1.9171182209933941 1.7335092603072140 12.3081618624504738 T T T

7.7156624143900006 0.0509845225296954 7.5590111632095169 T T T

1.9118395221573712 0.0018652511384276 5.1765147257558652 T T T

7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F

7.6782770543726580 1.9654671868707929 10.0033346365886313 T T T

5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F

5.7653216566233310 2.2314791303165866 12.5013662034423234 T T T

3.8465773233589164 0.0536856757070211 7.5582845377032237 T T T

5.7817916785638239 0.0019932780572889 5.1761996996039628 T T T

3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F

3.8892678492063641 1.9763011962727495 9.9902315228775826 T T T

1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F

1.9148469315374701 6.0418926958084258 12.0924103819716429 T T T

7.7181196104878298 3.8793120222024555 7.5508713452057288 T T T

1.9111158794572982 3.8711660424866214 5.1709448149547477 T T T

7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F

7.6947757179023437 5.8283528350001639 9.8740572409161640 T T T

5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F

5.7853258705750124 5.9662984561566086 12.2127979717554478 T T T
3.8455791507036952 3.8832935789444307 7.5441031899070490 T T T
5.7830431362913686 3.8711802085652947 5.1723187581231311 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.8710025553901750 5.8309221293929205 9.8715666115251217 T T T
1.9150122684622588 1.9376285104113096 4.7831393884753437 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
7.6908107154155712 0.0433777588926814 9.5479485687082946 T T T
1.9113181711305574 0.0405953177886546 7.1746892517428025 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
0.0209616406354088 2.0451344608155728 12.0401183234479259 T T T
7.7026111274629487 1.9668569689767148 7.9773075714561195 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
1.9334567494195369 0.0068571628700212 12.8625277256783264 T T T
7.7191088320965040 0.0173489517496801 5.5613721929938249 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.9026861149004839 1.8711923657533505 10.3721692699637309 T T T
5.7824865711467357 1.9377866870723668 4.7827488178123509 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.8681399784909112 0.0458886642769746 9.5488403381065883 T T T
5.7825528227470517 0.0416408665687212 7.1679920703874744 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
3.7916235785789696 2.1079661700223573 11.9866492812700400 T T T
3.8556439621084957 1.9697063590720847 7.9625300079514085 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.7921103215530039 7.6384921282161873 12.7800704514327119 T T T
3.8473212558589256 0.0139431439159423 5.5608850481997658 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.7778558461227121 1.9907816915213161 10.4313586062184314 T T T

1.9118251772935255 5.8079183801575986 4.7868997178323873 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
7.7229131492900187 3.8901206198155118 9.5512440711062787 T T T
1.9116509219620212 3.8842640218278208 7.1677128148462996 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
0.0105836965513808 5.8543166592755727 11.8433214009463725 T T T
7.7076938548852780 5.8315704366581063 7.9062183876843024 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
7.7191399559556126 3.8621056693160276 5.5578435283777594 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.9139910065636749 5.8754256072794639 10.1857112366838880 T T T
5.7856930479377064 5.8078432133776756 4.7869025444594460 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.8403369452513170 3.8951662134530527 9.5402346224970120 T T T
5.7831467816553159 3.8846046858410324 7.1670609043289106 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.8195632285294496 5.8195446004576965 11.8504681321546705 T T T
3.8562028796682251 5.8350778598943345 7.9042615093659938 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
5.8340486235792390 4.0129202720584018 12.7453778559663462 T T T
3.8480229167579005 3.8684134092777707 5.5538283090694645 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
5.7818905710464339 5.8864401141328937 10.2479784459646392 T T T
1.9427282863474897 2.4950796434695803 14.3004437509981699 T T T
4.8771087666221886 1.9581627188198727 14.6961818588098154 T T T
6.2113444434952534 1.7685622088461779 15.1679676610931100 T T T
6.9149987606583441 2.7844082242638128 15.7946929567990040 T T T
6.2555427772371770 4.0314101894849079 16.0499738365779514 T T T
4.9398827669395926 4.2082646225101596 15.7287466729604173 T T T

2.8143512778023010 3.4017787762841434 14.9428864788802649 T T T
 4.1515071155205270 3.1631894924014783 15.1007247840214287 T T T
 4.3103686340418221 1.0629820987801739 14.4339706689015728 T T T
 6.6749825425313682 0.7923217684175494 15.0030793492475532 T T T
 0.1582611156144965 2.5956896055618124 16.2344899646352019 T T T
 6.8056965632564586 4.8420871615084389 16.5329341708799511 T T T
 4.4451124973986316 5.1514636665269302 15.9723676338200420 T T T
 2.3435070928460480 4.3432205246228435 15.2166851057764525 T T T
 1.0131325364046528 2.6739061858754369 14.6024889885408093 T T T
 1.8660018855396383 4.5357955633979810 12.9410573380255016 T T T

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

1.9351236277001749 1.9351235473800663 2.7933008483844719 F F F

1.9142326904327227 1.7689768781259654 12.2716891004754078 T T T

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

5.7571018526356044 2.1951299732560079 12.3850142712040050 T T T
3.8855301125293455 0.0322245341911074 7.5491547995760646 T T T
5.8201399754132614 0.0017313371947947 5.1709730855466773 T T T
3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F
3.8773231685056206 1.9684353923030535 9.9404441704032429 T T T
1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F
1.9736798875793922 6.1304650111055885 12.1607350348467911 T T T
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
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.8312630384349005 6.0004830654165513 12.2350065287384364 T T T
3.8840111861870992 3.8910555485628335 7.5372057265291073 T T T
5.8207633034724520 3.8709796447549185 5.1679171161098978 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.9086762154496939 5.8239138981376479 9.8934951185063920 T T T
1.9473211876368892 1.9369072626295325 4.7875812389742851 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
7.7223282964861006 0.0272741417900672 9.5622108342639418 T T T
1.9472353608249993 0.0258972215317747 7.1812533223749595 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
0.0138926135620087 2.0383534526125722 12.0042609816006376 T T T
7.7341770134270016 1.9546151993201286 7.9713523315651038 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
1.9852817408839121 0.0837537260826782 12.9291524671359639 T T T
0.0135917363202634 0.0073349760572495 5.5678778326647898 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.9148093495860465 1.8567076194890602 10.3467181478675716 T T T

5.8199183078836789 1.9371580596431843 4.7871097550200430 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.9051490637778161 0.0387032227333803 9.5572500976607646 T T T
5.8190071492068212 0.0279311183632326 7.1735767510483406 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
3.7882559839168830 2.1326363590899517 11.9759227232599450 T T T
3.8816393580878414 1.9632467441868937 7.9595494701888141 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.8116342096188660 7.7219420595965795 12.7722642074953896 T T T
3.8824355414600156 0.0109007476453664 5.5647129370460036 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.7843083484445152 2.0022525963495403 10.4135684830337780 T T T
1.9475581764088368 5.8073496437563579 4.7896931680020991 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
0.0213235732818002 3.8813351598338657 9.5616447033006473 T T T
1.9475945708839224 3.8811950981463066 7.1735578069717834 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
0.0660995346694969 5.8443201100933049 11.9162447179918818 T T T
0.0114594593818039 5.8206198488409226 7.9347033872335127 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
0.0134079545321345 3.8677394097360058 5.5636249695830688 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.9632476681861109 5.8536146682817041 10.2337679666227412 T T T
5.8199888906718176 5.8072310835636678 4.7894720344724488 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.8704955434137442 3.8941793245369798 9.5464990188724599 T T T
5.8193287992201581 3.8806849784865807 7.1739455040557756 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.8778709032684553 5.8587732891926354 11.8866827578607097 T T T

3.9015240612478514 5.8306258688757397 7.9220580136184333 T T T
 5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
 5.8511030437372611 3.9681444197279920 12.7192615893119729 T T T
 3.8832190304972998 3.8711988834231637 5.5580536250820920 T T T
 5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
 5.8368270721332252 5.8812430419329385 10.2997945239476927 T T T
 1.5203611573573330 2.7223501460930626 14.1676006219256543 T T T
 4.2749639748533097 2.1965962902368132 14.8960718216795218 T T T
 5.6142635666634018 2.0171601071363492 15.2618445724800491 T T T
 6.3723937290102430 3.0764602909025260 15.7852381285064052 T T T
 5.7537558110490181 4.3336039456542128 15.9604513467397080 T T T
 4.4209934127594401 4.5205194308446099 15.6488895730016022 T T T
 2.2733946997732972 3.7013440249101612 14.8411335247666258 T T T
 3.6208085949342745 3.4543639340014294 15.1253569514467490 T T T
 3.6955059440922815 1.3297158379127318 14.5760943537859120 T T T
 6.0470337929970928 1.0187545179951840 15.1668724967482316 T T T
 7.3937251648072486 2.9092145958701745 16.1286468099679894 T T T
 6.3297200528271329 5.1743852964284160 16.3522810870743953 T T T
 3.9617078687479710 5.5032501150136595 15.7817961555943640 T T T
 1.6826606703998457 4.4645882817255718 15.3389470901967382 T T T
 0.5729740956078671 2.9970174201846187 14.1433759047258736 T T T
 2.1172172030030461 4.8289401549568103 13.3081654910080456 T T T

P2*

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

1.9351236277001749 1.9351235473800663 2.7933008483844719 F F F
2.0347667326350090 1.7217433887751845 12.3519119237728798 T T T
0.0674932419525859 0.0218108310628592 7.5502747402024104 T T T
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
5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F
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
3.9492423785913511 1.9626498570295430 9.9448102498489597 T T T
1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F
2.0768997387039372 6.3084086180551173 12.1850734273563344 T T T
0.0725820117636622 3.8775619059580269 7.5483465521401625 T T T
2.0043996875393186 3.8721834082254323 5.1693115671506051 T T T
7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
0.1440550750214423 5.8016965040547976 9.9117860533811903 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.9282120136899552 5.9415686695349850 12.2425069629206398 T T T
3.9413169330012900 3.8889907145522393 7.5407983092366297 T T T
5.8761227190145879 3.8713982093430888 5.1705815919401337 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.9784881898195730 5.8100040686445418 9.9068241554154639 T T T
1.9997333660100027 1.9371380045169997 4.7841579193115900 T T T

0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
0.0647460022023833 0.0207472614178509 9.5319528518735677 T T T
2.0079778348177784 0.0096795763718960 7.1728251015467253 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
0.0653792009566562 1.8309249884739998 11.8904375373548330 T T T
0.0826693299401573 1.9534489313176708 7.9283012222161897 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
2.1154214093106143 0.0941119702757319 13.2742637175564102 T T T
0.0688414671616767 -0.0009213009320610 5.5543118238031228 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
2.0476091927720539 1.9092547308640959 10.3184683070281267 T T T
5.8732315526379608 1.9376529249211234 4.7814109735034833 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
4.0264517862569189 0.0340992800916887 9.5497901397986382 T T T
5.8778288279925910 0.0310661978005303 7.1599582680139662 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
4.0045630452809826 2.0152474464562244 11.9349088973685529 T T T
3.9369489712942554 1.9631017906157571 7.9360320081088744 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.8957498207257402 7.6680095651595472 12.7840166665690624 T T T
3.9377610221664217 0.0071337762912605 5.5589076283609469 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.9064394977062271 2.0649510003482021 10.2954021183445565 T T T
2.0027504299092986 5.8066770578791198 4.7832092081115114 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
0.1540806242007157 3.8881820770304611 9.5519269768977146 T T T
2.0076281756077088 3.9017152865570215 7.1626421553703929 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
0.1739024477652416 5.8363689239741436 11.9358548944852014 T T T

0.0576571702885940 5.8167782428660155 7.9345220517298278 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
0.0676738883473941 3.8724504867927751 5.5572228682114240 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
2.0570392377506637 5.9410139226061940 10.2075201591221951 T T T
5.8707066321767929 5.8063246831037585 4.7839632097061200 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.9384015370036867 3.9031283718747600 9.5379332333117564 T T T
5.8776630121634081 3.8805817190873251 7.1686763038994501 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.9527909413516196 5.7579759760443086 11.9321937877353879 T T T
3.9765130604131822 5.8294788485619993 7.9303603302325190 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
6.1041615741106066 3.8442456400370335 12.7760111562131229 T T T
3.9385243323085559 3.8727329231684604 5.5534617293431978 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
5.9271463146890548 5.8636942681725293 10.3298918169805329 T T T
1.3560715262513607 3.4848114403091537 13.4497114736562757 T T T
3.5961791168566646 2.5070358692745063 15.2552241315236241 T T T
4.9116374404544390 2.2649325027576683 15.6589210472869773 T T T
5.7607678875225510 3.3350400244658940 15.9517493719200534 T T T
5.3084777329163462 4.6468032404008541 15.8058691342467466 T T T
4.0035373684772448 4.8896409411450312 15.3694219703419748 T T T
1.7064463556555554 4.1000868583792069 14.7213368407683749 T T T
3.1334781283973898 3.8231437052592026 15.1033443948661237 T T T
2.9353310748389276 1.6582136456952474 15.0575919691670794 T T T
5.2678334983947002 1.2373017326482159 15.7524165885619247 T T T
6.7809068570266531 3.1392555136351139 16.2866900946313109 T T T
5.9733808899983734 5.4867750856122299 16.0167230367526550 T T T

3.6558424673156980 5.9175587570663737 15.2318704191324557 T T T
1.0188891424252955 3.7078231002732585 15.4873595965785125 T T T
0.3949016116258153 3.6625939349799874 13.2278199715471096 T T T
1.5408605864875484 5.1885105710857280 14.6476067946150650 T T T

TS7

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 6

Selective dynamics

Cartesian

1.9351236277001655 1.9351235473800794 2.7933008483844914 F F F

1.8937918901382300 1.7994698251668744 12.2536630895272864 T T T

7.7087104266295032 7.7216576694499635 7.5580631461269991 T T T

1.9038714548925011 7.7397001395544374 5.1736494840000091 T T T

7.7404950294138555 1.9351240318977576 0.3938262801202625 F F F

7.6990111524146609 1.9173399713436361 9.9061508035512897 T T T

5.8053713320492308 1.9351237723455583 2.7933008483844914 F F F

5.7681437831843816 2.0548975402608947 12.2210644404257298 T T T

3.8410798224805958 7.7310377675656028 7.5452292064558915 T T T

5.7781669739105910 0.0002893807823457 5.1725168846979637 T T T

3.8702473250647897 1.9351238069322787 0.3938262801202625 F F F

3.8363208575363927 1.9329767223056085 9.8997278043742121 T T T

1.9351236277001655 5.8053727238432939 2.7933008483844914 F F F

1.8691598379528176 6.1255854641980747 12.2588200936942240 T T T
7.7126066204744612 3.8749150011618552 7.5533478120654358 T T T
1.9048198745734424 3.8707284627350167 5.1708653174651085 T T T
7.7404950294138555 5.8053732083609724 0.3938262801202625 F F F
7.6701535018616775 5.7794370080741109 9.9730929987484540 T T T
5.8053713320492308 5.8053729488087731 2.7933008483844914 F F F
5.7201004400849573 5.9699758720664597 12.4156025895175670 T T T
3.8381994293291113 3.8804947386667576 7.5444834019158566 T T T
5.7776355269768205 3.8697151315144334 5.1732672181903894 T T T
3.8702473250647897 5.8053729833954932 0.3938262801202625 F F F
3.8596290373110644 5.8012440925898572 9.9437976786074955 T T T
1.9031184285371612 1.9350154804222113 4.7859208408943985 T T T
0.0000001927383357 7.7404969983392293 0.0000000000000000 F F F
7.6754240051854596 7.7344746710863426 9.5469934316890583 T T T
1.9038173333486033 7.7231412320068031 7.1709830323325052 T T T
7.7404951919642579 1.9351242331507241 2.3994608702671258 F F F
7.7266396897016980 1.8972014409798048 11.8875843670152843 T T T
7.7195237206840597 1.9305757293275776 7.9264820311298765 T T T
1.9351236044786793 7.7404975907328408 3.1871236831667402 F F F
1.9182341221547348 0.0881610748075289 12.9668859015172959 T T T
7.7128869966991562 7.7304923107093426 5.5594006142256749 T T T
1.9351241463133577 1.9351235318991127 0.7876614236504151 F F F
1.8998543699902488 1.8878319024540102 10.3052136362476290 T T T
5.7823794521384446 1.9353133745162667 4.7841128164167426 T T T
3.8702478978614496 7.7404972233047085 0.0000000000000000 F F F
3.8532963367643274 0.0027844580162012 9.5328563762692120 T T T
5.7766606193205901 0.0038137464763986 7.1645145213516654 T T T
3.8702474876151935 1.9351240081852452 2.3994608702671258 F F F
3.8099805786407210 1.9257289825467510 11.8845647227411391 T T T

3.8305372909554349 1.9379928667815598 7.9193453190692615 T T T
5.8053713088277439 7.7404978156983200 3.1871236831667402 F F F
5.7871579308715733 0.0251236331911186 12.7530843118910227 T T T
3.8414253504551445 7.7408371920575023 5.5526905683790826 T T T
5.8053718506624232 1.9351237568645918 0.7876614236504151 F F F
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
7.6851413921595579 5.7972959641501660 7.9602960787857437 T T T
1.9351236044786793 3.8702484142696258 3.1871236831667402 F F F
7.7124430560659798 3.8764204661580046 5.5594758003923301 T T T
1.9351241463133577 5.8053727083623281 0.7876614236504151 F F F
1.8778581035609112 5.8724365762758444 10.3155625425213806 T T T
5.7769716014641297 5.8046869300104600 4.7844704647305552 T T T
3.8702478978614496 3.8702480468414935 0.0000000000000000 F F F
3.7991130237133492 3.8775179729432012 9.5415267916606314 T T T
5.7766854121273834 3.8617972286245288 7.1702633734623964 T T T
3.8702474876151935 5.8053731846484604 2.3994608702671258 F F F
3.7972176937480704 5.8493672393926230 11.8926187004779393 T T T
3.8563616658321167 5.8052241560265312 7.9288706506328133 T T T
5.8053713088277439 3.8702486392351050 3.1871236831667402 F F F
5.7912970292029522 3.7816756174211545 12.6541193391703075 T T T
3.8421742898289089 3.8713914871073527 5.5537652637745110 T T T
5.8053718506624232 5.8053729333278072 0.7876614236504151 F F F
5.7656634420571038 5.825372737779914 10.3750447751542865 T T T

1.9108669430991025 3.3123948686928659 13.4402343061822691 T T T
 3.5442984769629868 4.6267510203574398 14.5748385171017443 T T T
 4.1095693089571199 3.4214910122749465 15.1960488817728372 T T T
 5.3340675754341991 3.4452080245880827 15.8119932139998500 T T T
 6.1324515232194736 4.6185510261726188 15.8623539142414103 T T T
 5.6496399643398343 5.7811832476828329 15.2758254334158678 T T T
 4.4367214635131775 5.8096443394214958 14.5571314246600583 T T T
 2.4140216153226524 4.5101188206452010 13.6143459075252125 T T T
 3.5205564114586760 2.5048517506379113 15.1650351992975292 T T T
 5.7113376419666420 2.5234760820747408 16.2614089393572492 T T T
 7.1020918110264519 4.6052699973848332 16.3580900141796555 T T T
 6.2286984221922896 6.7066119607284707 15.3326984059880385 T T T
 4.0084794606649163 6.7797908127225384 14.3010043298798557 T T T
 2.5345088587107236 4.9395398558042514 15.1675026448000256 T T T

l13

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 6

Selective dynamics

Cartesian

1.9351236277001749 1.9351235473800663 2.7933008483844719 F F F

1.8845592913036522 1.7307829814549287 12.2892188244035854 T T T

-0.0249079672442100 -0.0337870453210731 7.5602597002745933 T T T

1.9118957264516669 -0.0010741721254280 5.1757365187897744 T T T
7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F
-0.0439355601725971 1.8969498691991153 9.9333270124275188 T T T
5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F
5.7529042759033420 2.0275282062477604 12.2416525145671979 T T T
3.8482733797660593 -0.0295819756153043 7.5538917997330017 T T T
5.7839071607178276 -0.0005419906454554 5.1748459825515898 T T T
3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F
3.8179989770956060 1.9031200433854747 9.9275600754261575 T T T
1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F
1.8792504191305721 6.0572307161978722 12.3047506594859222 T T T
-0.0225037299948334 3.8428367288249112 7.5570095751224269 T T T
1.9125792256874701 3.8693237108569409 5.1744822273442432 T T T
7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
-0.0403383865617525 5.7604253351247081 9.9533075286271746 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.7432170834611798 5.9095625409501249 12.2929914154212394 T T T
3.8470502772824671 3.8459951950016813 7.5528367230360756 T T T
5.7842922285417977 3.8691305568919492 5.1755643265988205 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.8130777206742543 5.7694643594179880 9.9411448495343304 T T T
1.9130351720471535 1.9334427981420874 4.7857671901690830 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
-0.0556141445951063 -0.0279901057218213 9.5518595312714343 T T T
1.9103732397019058 -0.0293760840504799 7.1720951817177276 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
-0.0520561967896475 1.8522683159699425 11.9142633869608243 T T T
-0.0248409318183789 1.9076534024565528 7.9397844674731219 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F

1.8999519203443165 0.0072567109304122 13.0248419546816816 T T T
-0.0220629254920406 -0.0074710902742486 5.5622489603182137 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.8869371756364284 1.8760169898899202 10.3250202978656009 T T T
5.7867719727781983 1.9335670061781041 4.7856135532028770 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.8325800269914878 -0.0236536343919930 9.5429994007258667 T T T
5.7813918153336568 -0.0217505813341127 7.1692142914498547 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
3.8231169239959129 1.8482706282668733 11.9057113853164758 T T T
3.8418952930479953 1.9116736620281247 7.9346288139863841 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.7603389895784485 7.6498486079916779 12.7937965910276290 T T T
3.8480101999173946 -0.0045989470752137 5.5581872908293084 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.7573642537771770 1.9783666739826968 10.3003909697890510 T T T
1.9143557710916312 5.8025180583806018 4.7846761218603548 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
-0.0230182230227349 3.8440637394607933 9.5561794557606579 T T T
1.9105320642242545 3.8499214391497780 7.1702844172288307 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
-0.0290077716108401 5.7442485512206085 11.9586632484439992 T T T
-0.0368592703905637 5.7757954805154430 7.9518350869253158 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
-0.0221011460877563 3.8660519164768608 5.5629599102837854 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.8828558562243578 5.8250959068634938 10.3148032411103170 T T T
5.7853803024575585 5.8024921257344602 4.7856254134828387 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F

3.8009560553945061 3.8484793802380732 9.5528858534554768 T T T
5.7819607080931865 3.8432815751896374 7.1740794593852959 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.8017127374258375 5.7843000503284614 11.9178564049436453 T T T
3.8525190138434100 5.7789850936706273 7.9391713805218940 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
5.7525330555445686 3.7634776125735665 12.7246554849598468 T T T
3.8487266877250099 3.8660295898595018 5.5612111050734159 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
5.7601554559821118 5.8276572595855685 10.3468640554105971 T T T
1.9186398832426652 3.2972609979019083 13.3926581517564216 T T T
3.1651291050320580 3.4169963268464483 15.8034587217200819 T T T
4.4784051894683401 3.1409750126562859 16.0850658999840910 T T T
5.4929101212367044 4.1082338166732475 15.8983172254781362 T T T
5.1415099948573726 5.4059330429013466 15.4462674206200337 T T T
3.8489274199433354 5.7261171795095551 15.1212809906064312 T T T
2.1130184721066230 4.5145002527746350 13.7625997108132854 T T T
2.7415655679425952 4.7105938381196060 15.1897786916188018 T T T
2.3985522799861934 2.6582124958098969 15.9659358708383738 T T T
4.7423217052328059 2.1574918675378272 16.4797603312416214 T T T
6.5333818069643588 3.8631852842370122 16.1086419930109912 T T T
5.9101171484698840 6.1811842698542252 15.3784959315117451 T T T
3.5965358011542197 6.7352883829653969 14.7896450006836790 T T T
1.8937098220441493 5.1496428250632693 15.7639338770998929 T T T

TS8

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 6

Selective dynamics

Cartesian

1.9351236277001749 1.9351235473800663 2.7933008483844719 F F F
1.9301641994953518 1.7101363573558466 12.2834520204103921 T T T
7.7236156874795192 7.7212172450425216 7.5574371617018823 T T T
1.9189708638240059 7.7398806940485914 5.1741384868790599 T T T
7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F
7.7439454795243634 1.9186641934484663 9.9171310709773177 T T T
5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F
5.7977100021443677 2.0672138602861860 12.2136566812621794 T T T
3.8570186988389765 7.7291669129930645 7.5466272498660638 T T T
5.7923823895481608 7.7406454159918026 5.1725605565366175 T T T
3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F
3.8561431509855404 1.9243093216467981 9.9116901264419539 T T T
1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F
1.9387691357451384 6.0350717167451808 12.2945646884113966 T T T
7.7271101465477514 3.8667859919034040 7.5506612413806042 T T T
1.9197006897093232 3.8701256696600574 5.1708946402642963 T T T
7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
7.7482011943223403 5.7795359764017809 9.9560048330854016 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.7961532831710638 5.9658698531969172 12.2965408022844649 T T T
3.8530635853932593 3.8699393304115990 7.5462624025912080 T T T
5.7914529056979713 3.8696143211658973 5.1731673672419687 T T T

3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.8791089604211368 5.7945378829979033 9.9348085632645660 T T T
1.9192595687663956 1.9346559055684118 4.7851066262045672 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
7.7186040500148554 7.7307362801192800 9.5488517247942948 T T T
1.9209792317098098 7.7257449188432608 7.1704470395239843 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
7.7621091345600854 1.9368444656519588 11.9153201219381071 T T T
7.7318933265810834 1.9261006102918414 7.9339354236761164 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
1.9413237046591552 0.0332555129250412 13.0178018777681199 T T T
7.7276559063799999 7.7346234026418541 5.5593932297502668 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.9306411466090476 1.8405880212108052 10.3186323844239354 T T T
5.7940142729649811 1.9350187706691822 4.7840973567333531 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.8878744903143634 7.7377275226080640 9.5320639362383677 T T T
5.7928163963744526 7.7390200314827444 7.1654050006513437 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
3.8434394223450572 1.9058512578546225 11.8996723215662588 T T T
3.8481166481329399 1.9323698951658987 7.9259090512964931 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.8290607218507127 7.7415545227534572 12.7152180047881131 T T T
3.8568121094812722 7.7400972338113307 5.5531842634582755 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.8014587045159303 1.9964900935383938 10.2803570965653943 T T T
1.9215297932029018 5.8044945543342576 4.7835528652053680 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
7.7807612544641209 3.8593699907138501 9.5482312790045167 T T T

1.9210166994320812 3.8706196556985231 7.1639243966987838 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
7.7546148483801964 5.7632754616050175 11.9528172821543954 T T T
7.7158257604630043 5.7934733654716055 7.9459194443263206 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
7.7268198172244453 3.8711257925464144 5.5579326079361913 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.9319607463633519 5.8414837772295778 10.3157784782035620 T T T
5.7918010459033500 5.8042465083560995 4.7847432147746254 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.8252717874042133 3.8666087324554832 9.5471817333465410 T T T
5.7924693101347655 3.8585515165308242 7.1717951098077375 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.8697161802515412 5.8640936649812625 11.8996804201143007 T T T
3.8685745960991116 5.7984330951280887 7.9288852634032541 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
5.7779899535570420 3.8022752342249011 12.6576177365580147 T T T
3.8573790440148796 3.8700127069726751 5.5555876268869424 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
5.8113962313962535 5.8282805368310342 10.3301172388967650 T T T
2.0159922989026997 3.2116138424143195 13.5795317157626236 T T T
3.9177116613732053 3.6228014092988694 15.6991315435923244 T T T
5.2841720263587320 3.4677639702137082 15.8451645096048122 T T T
6.1681698618249081 4.5300995294412996 15.5858264832077715 T T T
5.6436312089166814 5.7601204905235104 15.1395105857387673 T T T
4.2760747334368752 5.9337569071313121 14.9568081815637868 T T T
2.2507127023020463 4.4463417204518212 13.6527918386341511 T T T
3.3343946557093602 4.8555710339314571 15.2088229744364156 T T T
3.2536938689665496 2.7917369033539341 15.9410204593604128 T T T

5.6791912227192807 2.5140994742371969 16.2029624889664774 T T T
7.2422902775927449 4.4079021714680726 15.7252098724671470 T T T
6.3085716675187982 6.6154857862334984 14.9874528919817127 T T T
3.8975771151454301 6.9136621431923695 14.6592627564438942 T T T
2.4034068870698877 5.1688585332167136 15.7038630598639113 T T T

l14

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 6

Selective dynamics

Cartesian

1.9351236277001749 1.9351235473800663 2.7933008483844719 F F F

1.8232261361781064 1.6669817405213085 12.2903252299282659 T T T

7.6763742254380620 -0.0124043879481140 7.5564512758386035 T T T

1.8764488920756277 -0.0032277466703627 5.1765815151430052 T T T

7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F

7.6399740398263196 1.9182008790076108 9.9307635352910673 T T T

5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F

5.6907482656052224 2.0020094912543178 12.2079884378485950 T T T

3.8145306575462214 -0.0119491160448743 7.5558784080015240 T T T

5.7467063179663969 -0.0032459396305897 5.1717907100623064 T T T

3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F

3.7420016870565038 1.9192184447142659 9.9292008928931264 T T T

1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F
1.8226711108811673 6.0063577595443860 12.2963708806512759 T T T
7.6827427923100302 3.8557129225469029 7.5551913551624450 T T T
1.8759936274424931 3.8676559539773874 5.1729840936423086 T T T
7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
7.6270470669315902 5.7859698848972974 9.9448482912890910 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.6886375065606556 5.8562943342168667 12.3207412461660049 T T T
3.8081959350489649 3.8551758156520486 7.5538416389682608 T T T
5.7473020460624831 3.8672757106435105 5.1747215538351403 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.7629088186204891 5.7861221548228814 9.9424999316990395 T T T
1.8781565738970434 1.9332973766695081 4.7848618835612688 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
7.5902763974037040 -0.0141947452136069 9.5443286906008673 T T T
1.8736919028903500 -0.0234370298817806 7.1749362495764997 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
7.6094871419497911 1.7903672810224274 11.8859208032205768 T T T
7.6710227941798896 1.9235604194609646 7.9280256958179702 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
1.8184009309852540 -0.1139566435798756 13.0436880284996910 T T T
7.6836897082060736 -0.0053263470794654 5.5595937615361342 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.8243893355398013 1.8918079820270053 10.2956188452861905 T T T
5.7506645756017329 1.9338010478599115 4.7848087368480421 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.8056260518635736 -0.0138586715333598 9.5434759857334601 T T T
5.7438876864176205 -0.0200401238956119 7.1626807039818328 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F

3.7762441635925206 1.7839744747762392 11.8825913212438259 T T T
3.8045049224095950 1.9241926607567670 7.9273313539936074 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.6889108516630680 -0.1338956918726961 12.7398468673370164 T T T
3.8123227159817605 -0.0054537202407993 5.5584724027106542 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.6950526154413543 2.0358218507590582 10.2692378531521360 T T T
1.8779833478627657 5.8029847842113895 4.7830190866789346 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
7.6931190648269947 3.8705506647456605 9.5543639157435081 T T T
1.8733312821821888 3.8638924948201909 7.1662436764689641 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
7.6635080614502620 5.6936547468569048 11.9573445586814451 T T T
7.6663065030292703 5.7916244678872122 7.9549894787250626 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
7.6826458848627102 3.8707410756211682 5.5613339356794507 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.8256135695998992 5.9454108431692401 10.3417029247917700 T T T
5.7503636437694512 5.8023546303452056 4.7835845319145687 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.7032506236171918 3.8707516694455166 9.5518441184825651 T T T
5.7440562683770047 3.8603204264427755 7.1746211490735954 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.7210203046575399 5.6898423923579378 11.9560836421372603 T T T
3.8154433184407002 5.7913634251539392 7.9544981576114440 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
5.6835382321919985 3.7276392823197817 12.7173040618914364 T T T
3.8131853555733715 3.8695263942236418 5.5610683444270972 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F

5.6953057139418339 5.8062829881234199 10.3672198557895943 T T T
 1.8001145334034447 4.5119556543875010 13.7491820768295199 T T T
 3.9327352467257413 4.9706761739953231 15.9544736943664951 T T T
 4.5042078972912165 3.7220142001698879 16.2115059856468520 T T T
 5.8774248615682030 3.5305437391936421 16.0340680848626924 T T T
 6.6806171803692580 4.5880988880317526 15.6060906478122483 T T T
 6.1098863776356458 5.8355778933514344 15.3308976131806940 T T T
 4.7285306283274338 6.0246319935052703 15.4984161934262517 T T T
 1.8206772122508528 3.3278646103692457 13.4393337803762947 T T T
 3.8769732233004301 2.8956407366701260 16.5487074854182907 T T T
 6.3223103725800449 2.5522940617734626 16.2276160314035920 T T T
 0.0095748771219481 4.4404653894027648 15.4663066812161549 T T T
 6.7352781590105195 6.6710512314412052 15.0124165610560070 T T T
 4.2816681288764817 6.9964097622823074 15.2808032940645315 T T T
 2.8631460221784901 5.1202478993759346 16.0993138517539407 T T T

17

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 7 7

Selective dynamics

Cartesian

1.9351236277001749 1.9351235473800663 2.7933008483844719 F F F

1.9301206987725241 1.7980092196227475 12.3248451061492368 T T T

7.7317216650840432 0.0795215976812474 7.5485861769528064 T T T
1.9269879854912486 0.0032838477987489 5.1726210813133324 T T T
7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F
0.0100255747512625 2.0040649802106700 9.9343999649851682 T T T
5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F
5.7907146053017504 2.1732017052339687 12.2665465381477237 T T T
3.8644150790256697 0.0789035082552498 7.5431300924737066 T T T
5.7985702071032392 0.0049345893862275 5.1709047299769271 T T T
3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F
3.8494783949070324 2.0021422798638229 9.9234288542865841 T T T
1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F
1.9325115817320730 6.3053620921315421 12.1569262738059987 T T T
7.7330890442626306 3.9407866267795453 7.5366845817078554 T T T
1.9271086937080744 3.8752807335493089 5.1667248252688127 T T T
7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
0.0030054045189220 5.8609479149096577 9.9030489490413487 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.7943577210593711 6.0054956535575634 12.2266489281720219 T T T
3.8634377365128740 3.9393447002839723 7.5317645506921815 T T T
5.7984155788683776 3.8749689030712764 5.1661682329595706 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.8565724457199453 5.8595454742665343 9.8958602170139418 T T T
1.9277324179572333 1.9413086612326813 4.7836453486807597 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
7.7215708579254239 0.0841589013917912 9.5361843385561098 T T T
1.9272378068561808 0.0600812268104816 7.1662038579952929 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
0.0197678722692456 2.0081598406609547 11.9503104699875227 T T T
0.0022066406238171 2.0098986309850804 7.9343498242588844 T T T

1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
1.9598520319324000 0.1807021701194147 13.1408184955089542 T T T
7.7338601930549915 0.0161971094510215 5.5532966214764610 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.9260193704701583 1.9966409295566867 10.3058921245827015 T T T
5.7981879102463569 1.9415763235002701 4.7810395888478983 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.8776391313373741 0.0825616285095809 9.5291981662637646 T T T
5.7992194795537646 0.0808776013847465 7.1606714063238943 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
3.8419164651084303 2.0015004433255776 11.9001232033543047 T T T
3.8522894524426183 2.0083879976662176 7.9200688703824742 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.7961674785701192 -0.0143192474570939 12.7586641519738073 T T T
3.8633174134055719 0.0125787034638113 5.5494465090391643 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.8049112463011117 2.0579263937611332 10.3278416698884872 T T T
1.9262861927662722 5.8122375583752346 4.7828431708146315 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
0.0030035881458871 3.9455592795973438 9.5363911947379485 T T T
1.9271147752593847 3.9461914107251701 7.1583516012430666 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
0.0411825786656537 5.8598418941842025 11.9110713437388593 T T T
7.7079934555233782 5.8740352573690089 7.9187873374939430 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
7.7336381086097807 3.8798558345099310 5.5470651191744365 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.9289478419964805 5.9563117542123187 10.1850845991350649 T T T
5.7995834656148189 5.8122478927450798 4.7832529786181430 T T T

3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.8578274114434792 3.9438603442032321 9.5292167293112122 T T T
5.7993398677895556 3.9242960227974333 7.1574911809116193 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.8212261055972401 5.8456582546612026 11.8943861100249553 T T T
3.8859973736505529 5.8728274137260277 7.9106874068490383 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
5.8301830626951778 3.9318476573771752 12.6154561217070551 T T T
3.8633909467342171 3.8814306584985232 5.5438521685615463 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
5.8005928289579796 5.9569693273498032 10.2981736206537793 T T T
4.1854822086508392 2.2630943454769992 14.8870327771889457 T T T
5.4610852839037767 2.4378812889818322 15.4341538031275061 T T T
5.9238360410610600 3.7195639082919167 15.7523522655723944 T T T
5.0909717423508081 4.8171978551532089 15.5258471321175726 T T T
3.8186963762519612 4.6394756062565818 14.9721356167648008 T T T
2.0036906498169644 3.1673531765111305 14.0014737272880136 T T T
3.3329713067327971 3.3638834548447138 14.6314393414570691 T T T
3.8336698469575068 1.2543641391756490 14.6593174851692467 T T T
6.0914078796666109 1.5651367344519840 15.6216893952717992 T T T
6.9201260997682565 3.8569704682687340 16.1712821205265520 T T T
5.4286808625748870 5.8217272747858706 15.7945652247319526 T T T
3.1771300445482722 5.5140359127969356 14.8285114150693378 T T T
1.3316304092030211 2.5530993408666531 14.6301567298124446 T T T
1.4717111903761249 4.1127496299864310 13.7983526742893243 T T T

I8

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 7 8

Selective dynamics

Cartesian

1.9351236277001749 1.9351235473800663 2.7933008483844719 F F F

1.9068055796261947 1.5981048257379880 12.4255352608284859 T T T

0.0052385945426949 0.0121909914082411 7.5611083585832493 T T T

1.9394179626124028 -0.0010270006233240 5.1755473506086549 T T T

7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F

0.0064055745259885 1.9307742142286060 9.9956004190545045 T T T

5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F

5.7731925660879329 2.0546447617538628 12.3637521008296165 T T T

3.8745652852967685 0.0149873708018672 7.5569920725357012 T T T

5.8107588528799301 -0.0001985816262933 5.1756790888361452 T T T

3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F

3.8331570067374914 1.9302928529253276 9.9895093253672993 T T T

1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F

1.9362576046101920 5.9243235766803277 12.1290577374486404 T T T

0.0034748730921911 3.8454880640845590 7.5537469368502865 T T T

1.9395320931712587 3.8691266262534305 5.1740884727551464 T T T

7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F

-0.0172554051670747 5.7892658442359188 9.8862011473774363 T T T

5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F

5.8025591643973744 5.8542471094263675 12.2268807679778000 T T T

3.8760044714182262 3.8454169617382168 7.5501926639670316 T T T

5.8105578265631044 3.8680077854894885 5.1723417200027697 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.8844676270913112 5.7899815345364702 9.8813101293544516 T T T
1.9398271019801472 1.9343666873614305 4.7836895830465380 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
0.0016739720831989 0.0043694756725191 9.5572027687024281 T T T
1.9382206023769699 -0.0032946850380367 7.1717545265968115 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F
0.0117482763307707 1.8753543339038610 12.0291525578665137 T T T
0.0068224839956206 1.9298845665139273 7.9746986521526209 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
1.9446491802830261 -0.1473643135895994 12.9371811226079636 T T T
0.0040755100452580 0.0092976813098396 5.5645163129546518 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.9133238834922683 1.9423417764361421 10.3703892800632680 T T T
5.8102563297110299 1.9341796808653775 4.7820460453236953 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.8550324520019941 0.0055956580255950 9.5507824791848428 T T T
5.8099613388527462 0.0157403361087473 7.1724087325954304 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
3.8169208906913608 1.8761162830270193 11.9714441839324337 T T T
3.8654731191812464 1.9306096522761984 7.9583829463129918 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.8088856356851135 7.5388268604573785 12.7926981689617172 T T T
3.8745882241682272 0.0069163254564349 5.5613386783413494 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.7955925887619886 1.9626336372132778 10.4120393711195227 T T T
1.9377018081846615 5.8044361169987688 4.7855593744005800 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F

-0.0220227735499259 3.8586525245416570 9.5490766685066646 T T T
1.9382183672219924 3.8622783626067623 7.1714243760031451 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
0.0241063254336823 5.7157674332169170 11.8672384832641029 T T T
-0.0138679945671272 5.7986283684519480 7.9167004762250892 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
0.0042351535883199 3.8567854196109130 5.5601305500221514 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F
1.9334564677205150 5.8114434320396793 10.2055698625921298 T T T
5.8126433500568266 5.8045113010171656 4.7874738621732584 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.8777614210896041 3.8584789033233120 9.5439021548678653 T T T
5.8098023981222164 3.8428269072038859 7.1669011871712867 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.8454246940844508 5.7207523752675105 11.8626427830725483 T T T
3.8958258616859065 5.7992749209552645 7.9132417030927922 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
5.7994610511567553 3.8142247356518286 12.7090908108769334 T T T
3.8743005710104850 3.8613806975877325 5.5571046239316484 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
5.8033501423201077 5.8662250502683362 10.2753690476673363 T T T
4.3652287823421743 1.6387297351770165 14.8956932327261082 T T T
5.6770236962872866 1.8955417874368614 15.3169944710366384 T T T
6.0281293982673478 3.1621336567579070 15.8034386992225411 T T T
5.0569145675461673 4.1647279888777682 15.8391577209792391 T T T
3.7536817558797066 3.9149369132327410 15.3974634732731825 T T T
1.9946343740611172 2.3623989757189734 14.4619009027731220 T T T
3.3665698516395266 2.6449789606540022 14.9277984234655339 T T T
4.1023634567137703 0.6372119069385648 14.5507242318523637 T T T

6.4072812053424650 1.0836057395535288 15.2980599746300499 T T T
7.0460976416953445 3.3565954228037134 16.1429583976550042 T T T
5.3110329984924318 5.1533036021488927 16.2261281929041488 T T T
3.0088515145493937 4.7125709317427615 15.4366890402552297 T T T
1.5861011664624267 1.4489357829774865 14.9246510773935785 T T T
1.9431554232844310 4.4466356213160259 13.0133986333548375 T T T
1.2991855184023657 3.1966856435254929 14.6020364364644148 T T T

TS3

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 7 8

Selective dynamics

Cartesian

1.9351236277001731 1.9351235473800639 2.7933008483844639 F F F

1.9361278607704813 1.5628777648303662 12.3313505679105404 T T T

7.7333180604617082 0.0130430714862928 7.5542166803248492 T T T

1.9344735223956175 7.7401402633155492 5.1759628137538165 T T T

7.7404950294138475 1.9351240318977809 0.3938262801202403 F F F

0.0336529456391989 1.9286490039341451 9.9372140139935308 T T T

5.8053713320492388 1.9351237723455428 2.7933008483844639 F F F

5.8056833878067051 2.0080086768410039 12.2331123763704817 T T T

3.8758511960981967 0.0141118250136984 7.5529102686377314 T T T

5.8046549500733979 7.7395943001457255 5.1720871998679057 T T T

3.8702473250647822 1.9351238069323018 0.3938262801202403 F F F

3.8332785182990166 1.9328722715771234 9.9305247209542760 T T T
1.9351236277001731 5.8053727238432788 2.7933008483844639 F F F
1.9225140637108780 6.1810133496781141 12.2218989455112066 T T T
7.7393957031535328 3.8613279541229941 7.5434776302496029 T T T
1.9345998458819955 3.8709112085817701 5.1678548571610765 T T T
7.7404950294138475 5.8053732083609955 0.3938262801202403 F F F
0.0353737581927190 5.7916629231512475 9.9001975458970222 T T T
5.8053713320492388 5.8053729488087580 2.7933008483844639 F F F
5.7998632397563039 5.8594705396362015 12.2184133192491995 T T T
3.8699320666015988 3.8648551379233775 7.5416252172563505 T T T
5.8046596620672508 3.8715794672688491 5.1703690363926897 T T T
3.8702473250647822 5.8053729833955172 0.3938262801202403 F F F
3.8286407574736874 5.7947205327549396 9.9032776214734461 T T T
1.9339589194356082 1.9356770544193331 4.7842461553261080 T T T
0.0000001927383101 7.7404969983392524 0.0000000000000000 F F F
7.6834782884765804 0.0063964723829664 9.5346670495258152 T T T
1.9334501835101865 0.0055315323324700 7.1751557752355426 T T T
7.7404951919642428 1.9351242331507164 2.3994608702670819 F F F
0.0387778066701886 1.8555054855575632 11.9395975021492582 T T T
7.7226905327436883 1.9397634074122974 7.9279564645875693 T T T
1.9351236044786559 7.7404975907328488 3.1871236831667957 F F F
1.9592539961184878 0.0041985684932831 13.2324693384421987 T T T
0.0002470451687141 7.7374373982752180 5.5579011185441933 T T T
1.9351241463133810 1.9351235318990974 0.7876614236504124 F F F
1.9318524127662557 1.8615627533826553 10.2598229336115541 T T T
5.8056032583728294 1.9362136575034852 4.7846418678399623 T T T
3.8702478978614421 7.7404972233047316 0.0000000000000000 F F F
3.9211183427452316 0.0085271514099103 9.5312049479210703 T T T
5.8053465144329950 7.7332614001703153 7.1605542957274109 T T T

3.8702474876151780 1.9351240081852374 2.3994608702670819 F F F
3.8401693049285064 1.8685306589843818 11.9038395013739837 T T T
3.8872824856331292 1.9413550429078730 7.9178644160568155 T T T
5.8053713088277208 7.7404978156983280 3.1871236831667957 F F F
5.8044343854783502 7.5871871036125356 12.7403087517812867 T T T
3.8685530692690113 7.7394168079742105 5.5561600282397929 T T T
5.8053718506624463 1.9351237568645763 0.7876614236504124 F F F
5.8106167929042334 1.9942146881109433 10.3257781002212905 T T T
1.9346103418022003 5.8053061394279126 4.7844283064131794 T T T
0.0000001927383101 3.8702478218760379 0.0000000000000000 F F F
0.0391755931923083 3.8688841719386828 9.5409740700637151 T T T
1.9336756349927484 3.8709535869485463 7.1619337878827523 T T T
7.7404951919642428 5.8053734096139307 2.3994608702670819 F F F
0.0753790936933301 5.7229827008245175 11.9601530419606359 T T T
7.7373578301887278 5.8035696538934074 7.9306629454590833 T T T
1.9351236044786559 3.8702484142696338 3.1871236831667957 F F F
7.7396792281074012 3.8726712872616469 5.5543154562836872 T T T
1.9351241463133810 5.8053727083623130 0.7876614236504124 F F F
1.9343219281935231 5.9087039845771931 10.1838543280297067 T T T
5.8049526880072806 5.8048321284402036 4.7826657203123526 T T T
3.8702478978614421 3.8702480468415166 0.0000000000000000 F F F
3.8266132354905245 3.8700693045434167 9.5358509206660784 T T T
5.8052515788839525 3.8844388003814583 7.1678840191703355 T T T
3.8702474876151780 5.8053731846484524 2.3994608702670819 F F F
3.8002263798494016 5.7255728604677119 11.9455905042346515 T T T
3.8710557589375867 5.8054739849459427 7.9255848627881926 T T T
5.8053713088277208 3.8702486392351125 3.1871236831667957 F F F
5.8551211874432507 3.7663962586619029 12.5944564799440215 T T T
3.8697178234082417 3.8729162409653810 5.5520071783267060 T T T

5.8053718506624463 5.8053729333277921 0.7876614236504124 F F F
 5.8068470319624081 5.8519222474011370 10.3255198682262304 T T T
 4.2601691629909011 2.1478432516042987 14.8415289746960504 T T T
 5.5814755378686680 2.3162290268297601 15.2801256222738679 T T T
 6.0476717941606459 3.5854400307091789 15.6436574215469566 T T T
 5.1738578529235681 4.6729264864631812 15.5897196997554968 T T T
 3.8552047537950926 4.5044991816490842 15.1573721679307329 T T T
 2.0065720246921948 3.0995696308076965 14.1978262337653973 T T T
 3.3746263926087932 3.2453028509232134 14.7533914087107494 T T T
 1.9234844318264226 4.2505571748821245 13.1121723952651426 T T T
 1.2482035737990991 3.6946127079182260 14.7210943286709259 T T T
 3.9105514046053171 1.1426146822388030 14.5887542901908720 T T T
 6.2343352921059418 1.4429759530630040 15.3533510361907304 T T T
 7.0843107768188336 3.7242677291437554 15.9549750697784898 T T T
 5.5196976038796892 5.6675728547905555 15.8823813057236247 T T T
 3.1862467452703074 5.3687799489515875 15.1256492309839281 T T T
 1.6389470989395607 2.0410498041941971 14.3697886555669427 T T T

P3*

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 7 8

Selective dynamics

Cartesian

1.9351236277001749 1.9351235473800663 2.7933008483844719 F F F
1.9206741482855592 1.4737062518995065 12.2263583499188471 T T T
-0.0011404460798955 -0.0253710734506617 7.5631409643457861 T T T
1.9384529621893485 -0.0019970941273853 5.1792841278199573 T T T
7.7404950294138510 1.9351240318977847 0.3938262801202403 F F F
-0.0013535420897043 1.9102766287405304 9.9402713475754503 T T T
5.8053713320492397 1.9351237723455452 2.7933008483844719 F F F
5.7881699643498488 2.0380446686257949 12.2901592191328692 T T T
3.8782459335374884 -0.0229485032179645 7.5617144738928772 T T T
5.8089256674005396 -0.0023827475497802 5.1750381642009646 T T T
3.8702473250647857 1.9351238069323058 0.3938262801202403 F F F
3.8528126089712069 1.9115128676411681 9.9364429582142506 T T T
1.9351236277001749 5.8053727238432815 2.7933008483844719 F F F
1.9363904197737374 6.0900892724773676 12.2474201916709671 T T T
0.0028025001768384 3.8419060239234817 7.5511431109826246 T T T
1.9385872963350195 3.8681893715852405 5.1728639407719088 T T T
7.7404950294138510 5.8053732083609990 0.3938262801202403 F F F
0.0153068348158017 5.7656725694430300 9.9303907401513243 T T T
5.8053713320492397 5.8053729488087606 2.7933008483844719 F F F
5.8009278523863452 5.8604786320783901 12.2477798506556361 T T T
3.8738460938507204 3.8431930598282555 7.5494434218420867 T T T
5.8090575223518872 3.8688314839112090 5.1734776120553043 T T T
3.8702473250647857 5.8053729833955199 0.3938262801202403 F F F
3.8525553990216919 5.7662128048023975 9.9272533239407519 T T T
1.9397935683636058 1.9327880302323497 4.7848899217409908 T T T
0.0000001927383101 7.7404969983392551 0.0000000000000000 F F F
7.6873083065244483 -0.0215036605692713 9.5535283444205508 T T T
1.9375836437388949 -0.0173741943758690 7.1797427548669841 T T T
7.7404951919642402 1.9351242331507126 2.3994608702670819 F F F

0.0195546714024155 1.8867035406328025 11.9625971395984791 T T T
-0.0175260718715760 1.9125495219272819 7.9460192170150412 T T T
1.9351236044786593 7.7404975907328515 3.1871236831668068 F F F
1.9449721590929903 7.6451273273235190 13.2697590601305002 T T T
0.0040794087446503 -0.0043070670708007 5.5644146864211779 T T T
1.9351241463133819 1.9351235318990987 0.7876614236504124 F F F
1.9260585945289297 1.8302335727014676 10.2489429002811843 T T T
5.8083853814419149 1.9332529643398075 4.7846300728976390 T T T
3.8702478978614385 7.7404972233047342 0.0000000000000000 F F F
3.9177754632520956 -0.0207675918416530 9.5517882108809502 T T T
5.8086981406429183 -0.0272583740938184 7.1651231389047254 T T T
3.8702474876151753 1.9351240081852337 2.3994608702670819 F F F
3.8316569831539686 1.8853410960477355 11.9394390127643710 T T T
3.8914607641238197 1.9134398660907768 7.9401552592667111 T T T
5.8053713088277235 7.7404978156983306 3.1871236831668068 F F F
5.7998842059605975 7.5890012291915108 12.7733253517273244 T T T
3.8722868423721231 -0.0037642644548967 5.5637131990176290 T T T
5.8053718506624472 1.9351237568645778 0.7876614236504124 F F F
5.7995033554325346 1.9840005988108489 10.3574780867993059 T T T
1.9391685162850274 5.8026285754774065 4.7862673584067759 T T T
0.0000001927383101 3.8702478218760397 0.0000000000000000 F F F
0.0219585004828173 3.8445527420461856 9.5505616069508417 T T T
1.9375735310059328 3.8393432590186669 7.1692839901404204 T T T
7.7404951919642402 5.8053734096139271 2.3994608702670819 F F F
0.0337142237966528 5.6865390520486541 11.9363968911135068 T T T
-0.0019804558895052 5.7776789552141006 7.9381885929392304 T T T
1.9351236044786593 3.8702484142696365 3.1871236831668068 F F F
0.0031584123246908 3.8628423266668586 5.5605208846684535 T T T
1.9351241463133819 5.8053727083623139 0.7876614236504124 F F F

1.9339928749855555 5.8706132075576596 10.2424940479739099 T T T
5.8090868217319755 5.8022573189429760 4.7841826378662393 T T T
3.8702478978614385 3.8702480468415188 0.0000000000000000 F F F
3.8423223651505971 3.8455135484355414 9.5472597073822030 T T T
5.8084941077832628 3.8503184453917889 7.1708100139005237 T T T
3.8702474876151753 5.8053731846484489 2.3994608702670819 F F F
3.8332922353939618 5.6777824573401938 11.9342663998247183 T T T
3.8794964503956311 5.7788454835669691 7.9366498358606110 T T T
5.8053713088277235 3.8702486392351152 3.1871236831668068 F F F
5.8070993724200539 3.7834363992796920 12.7359748503531609 T T T
3.8732519322564989 3.8656463439002842 5.5594641414505572 T T T
5.8053718506624472 5.8053729333277921 0.7876614236504124 F F F
5.8032871841258125 5.8210625445691262 10.3249538602358832 T T T
4.0841094540526903 1.9448085469919940 15.1674568166724129 T T T
5.4457680815768263 1.9133457855161233 15.4957331614256564 T T T
6.0824532520704464 3.0689960253333655 15.9556519430882240 T T T
5.3643342646646204 4.2620582581741857 16.0538143272662417 T T T
4.0110124770105253 4.2935124790401318 15.7133600201477357 T T T
1.8835460507631439 3.1816356077427330 14.9475197134986750 T T T
3.3488736475202598 3.1341314485435512 15.2838616913164280 T T T
3.5895702031037802 1.0300099654897259 14.8315067229571902 T T T
5.9927774670625302 0.9722644180422231 15.4099985269557163 T T T
7.1336298716849464 3.0363349218394635 16.2369749374762335 T T T
5.8551868062210941 5.1705453866233935 16.4075426410027703 T T T
3.4505388358320430 5.2283669399769375 15.8004532645811526 T T T
1.4183047337030052 2.1840827630469426 14.9830118256283598 T T T
1.7112548685659472 3.6036198790743335 13.9363763894737005 T T T
1.3304236946132195 3.8356768398048224 15.6361085275996050 T T T

H**

Ti O H

1.0000000000000000

7.7404954086981297 0.0000004499309580 0.0000000000000000

0.0000000000000000 7.7404983529264300 0.0000000000000000

0.0000000000000000 0.0000000000000000 27.7849839816825011

Ti O H

24 48 1

Selective dynamics

Cartesian

1.9351236307235535 1.9351235494069645 2.7933008378649218 F F F

1.9099060220484316 1.6661681955764147 12.3176289178463829 T T T

-0.0165546991154937 0.0302330524878281 7.5581514854796570 T T T

1.9207786863274894 0.0013940589500539 5.1752010939680595 T T T

7.7404950271152559 1.9351240312453248 0.3938262668217468 F F F

0.0022868310189495 1.9494084818953914 9.9678196614428867 T T T

5.8053713350726186 1.9351237743724437 2.7933008378649218 F F F

5.7870645912676917 2.0644345260883190 12.2566873380646673 T T T

3.8582125683010324 0.0260103695434179 7.5539250165157146 T T T

5.7920191233607490 0.0016165135339370 5.1736222026221137 T T T

3.8702473227661907 1.9351238062798457 0.3938262668217468 F F F

3.8348451867034030 1.9400278338079477 9.9647893123424094 T T T

1.9351236307235535 5.8053727258701802 2.7933008378649218 F F F

1.9031355666844916 5.8212239918089965 12.2178760888015248 T T T

-0.0126171945875623 3.8691644398711991 7.5490971563187470 T T T

1.9222843408577313 3.8720293602069447 5.1718721572403226 T T T

7.7404950271152559 5.8053732077085396 0.3938262668217468 F F F

-0.0221997845828095 5.8089741750475197 9.9046432235527178 T T T

5.8053713350726186 5.8053729508356593 2.7933008378649218 F F F
5.7937440735936576 5.8671379556166565 12.2636816439312604 T T T
3.8542796340531673 3.8723217176685027 7.5556489490480798 T T T
5.7905695783474780 3.8721245055128346 5.1741456175102210 T T T
3.8702473227661907 5.8053729827430605 0.3938262668217468 F F F
3.8708461693218226 5.8158046169510760 9.9144648180826795 T T T
1.9221915729555807 1.9362386083146259 4.7845986120065351 T T T
0.0000001925857419 7.7404969978200588 0.0000000000000000 F F F
-0.0397610597839941 0.0151065493644573 9.5534865708282375 T T T
1.9210453030833234 0.0149499416513665 7.1740409623188377 T T T
7.7404951940399229 1.9351242343854522 2.3994608670731532 F F F
-0.0601446344391621 1.9083791270739978 11.9362479951717315 T T T
-0.0204141252851438 1.9485250959075862 7.9424215383853847 T T T
1.9351236030856309 7.7404975900603716 3.1871236795975757 F F F
1.8867568171310281 7.5334834920771856 12.8701017053793976 T T T
-0.0128104197394181 0.0050422832894437 5.5618885689247923 T T T
1.9351241436230258 1.9351235318700586 0.7876614242995419 F F F
1.9164339026965436 1.8994171823709021 10.3149085506321505 T T T
5.7921570080625973 1.9366937015305394 4.7843170434015034 T T T
3.8702478969348064 7.7404972227855380 0.0000000000000000 F F F
3.8846462259864225 0.0141873764770852 9.5446220055523874 T T T
5.7917727929089908 0.0167432971256098 7.1677659215459908 T T T
3.8702474896908576 1.9351240094199731 2.3994608670731532 F F F
3.8964096400469126 1.8336280221133983 11.9319188699941847 T T T
3.8573217943162761 1.9486889167449577 7.9445727465463731 T T T
5.8053713074346955 7.7404978150258508 3.1871236795975757 F F F
5.8193234122067361 7.5714305083273530 12.7964570479173734 T T T
3.8567288809739106 0.0037287502514685 5.5593133716894148 T T T
5.8053718479720899 1.9351237568355377 0.7876614242995419 F F F

5.7868277863175379 2.0633004447652912 10.3140899528579144 T T T
1.9216200628997737 5.8069722797145822 4.7852715090359679 T T T
0.0000001925857419 3.8702478213568439 0.0000000000000000 F F F
0.0266950978813261 3.8872475001271316 9.5395023454386934 T T T
1.9213148923829202 3.8840535207769835 7.1660500849388402 T T T
7.7404951940399229 5.8053734108486674 2.3994608670731532 F F F
0.0053188215890228 5.6182746140211570 11.9150944605100886 T T T
-0.0200563271844936 5.8181098486701277 7.9383747913921185 T T T
1.9351236030856309 3.8702484135971562 3.1871236795975757 F F F
2.1405501107169753 3.8434824178717344 12.9015466659798363 T T T
-0.0133589746210689 3.8684942633647910 5.5568918863859382 T T T
1.9351241436230258 5.8053727083332740 0.7876614242995419 F F F
1.9192468919944361 5.9013314997106940 10.3029784353395879 T T T
5.7927569061019488 5.8066672174455052 4.7852872702953766 T T T
3.8702478969348064 3.8702480463223226 0.0000000000000000 F F F
3.8179853210407431 3.8885021763233776 9.5508247766521208 T T T
5.7915887900967356 3.8834018406662745 7.1723844493067013 T T T
3.8702474896908576 5.8053731858831883 2.3994608670731532 F F F
3.8467405088640310 5.7181436922158406 11.9037952519556089 T T T
3.8620373632518286 5.8172507226100976 7.9360043818665247 T T T
5.8053713074346955 3.8702486385626353 3.1871236795975757 F F F
5.7176632093335265 3.7952068705498498 12.8269291992993448 T T T
3.8573609748091373 3.8689939460356486 5.5592655968095990 T T T
5.8053718479720899 5.8053729332987523 0.7876614242995419 F F F
5.7980432596465450 5.8654768944066724 10.3132942965081185 T T T
3.1213295271519863 3.8215119297138216 12.9722928060752967 T T T

- (1) Vorotnikov, V.; Wang, S.; Vlachos, D. G. Group Additivity for Estimating Thermochemical Properties of Furanic Compounds on Pd(111). *Ind Eng Chem Res* **2014**, *53* (30), 11929–11938. <https://doi.org/10.1021/ie502049a>.
- (2) Eds. P.J. Linstrom; W.G. Mallard. *NIST Chemistry WebBook, NIST Standard Reference Database Number 69*, 20899th ed.; National Institute of Standards and Technology: Gaithersburg MD.
- (3) De Moor, B. A.; Reyniers, M.-F.; Marin, G. B. Physisorption and Chemisorption of Alkanes and Alkenes in H-FAU: A Combined Ab Initio–Statistical Thermodynamics Study. *Physical Chemistry Chemical Physics* **2009**, *11* (16), 2939–2958. <https://doi.org/10.1039/b905015a>.
- (4) Grimme, S. Supramolecular Binding Thermodynamics by Dispersion-Corrected Density Functional Theory. *Chemistry - A European Journal* **2012**, *18* (32), 9955–9964. <https://doi.org/10.1002/chem.201200497>.
- (5) Eyring, H. The Activated Complex in Chemical Reactions. *J Chem Phys* **1935**, *3* (2), 63–71. <https://doi.org/10.1063/1.1749604>.
- (6) Eyring, H. The Transmission Coefficient in Reaction Rate Theory. *Rev Mod Phys* **1962**, *34* (4), 616–619.
- (7) Wei, B.; Calatayud, M. Hydrogen Activation on Anatase TiO₂: Effect of Surface Termination. *Catal Today* **2022**, *397–399*, 113–120. <https://doi.org/10.1016/j.cattod.2021.11.020>.
- (8) Karim, W.; Spreafico, C.; Kleibert, A.; Gobrecht, J.; Vandevondele, J.; Ekinici, Y.; Van Bokhoven, J. A. Catalyst Support Effects on Hydrogen Spillover. *Nature* **2017**, *541* (7635), 68–71. <https://doi.org/10.1038/nature20782>.
- (9) Liu, K.; Hou, G.; Gao, P.; Nie, X.; Bai, S.; Janik, M. J.; Zhang, Z. C. Evolution of Multiple Spillover Hydrogen Species on Anatase Titanium Dioxide. *Cell Rep Phys Sci* **2022**, *3* (12). <https://doi.org/10.1016/j.xcrp.2022.101190>.