

Supplementary Materials for:
Bond Insertion at Distorted Si(001) Subsurface Atoms

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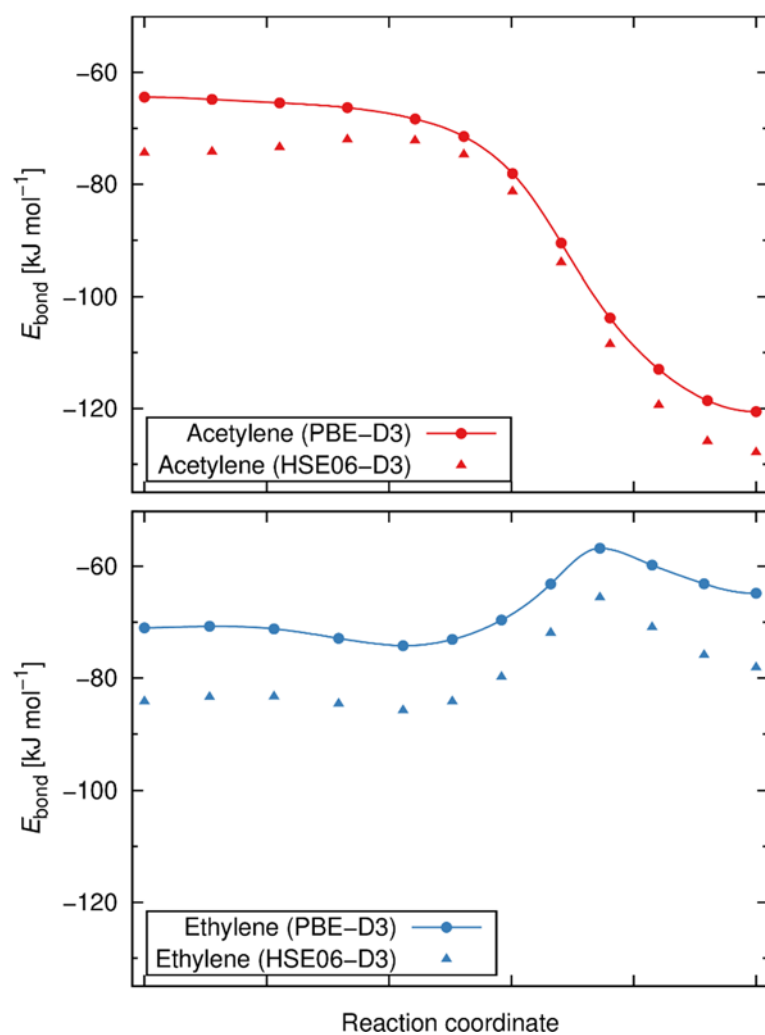


Figure S1. HSE06-D3 energies of the full π complex \rightarrow *sublayer* reaction paths, calculated on PBE-D3 structures.

Computational Setup of Ab Initio Molecular Dynamics Simulations

All simulations were performed in VASP 5.3.5 using the same setup described for the structural optimizations in the main article, except for a less accurate SCF convergence criterion of 10^{-5} eV. Trajectories were calculated using the velocity Verlet integrator [1, 2] with a time step of $\Delta t = 1$ fs. A canonical *NVT* ensemble ($T = 300$ K) was simulated using the Nosé thermostat [3–5] with a thermostat mass set to a value so that the energy oscillation frequency was equal to the frequency of the lowest energy vibrations of the system (≈ 600 fs $\triangleq 55$ cm $^{-1}$). Initially, molecule and slab were simulated separately for 20 ps starting in their respective minimum geometry to approach thermodynamic equilibrium without interference of each other. After this, coordinates and velocities were written out 10 times in intervals of 3 ps to obtain qualitatively different states of thermal excitation. At this point, molecule/surface sets were arbitrarily paired, the z coordinate of the molecular center of mass was placed 5.5 Å above the equilibrium position of an Si_{up} atom while the x and y coordinates were displaced randomly using a true random number generator [6]. Additionally, a translation velocity vector was added to the molecule to simulate the effect of gas escaping a nozzle into ultra-high vacuum. The absolute value of the vector was chosen as the mean speed $\langle v \rangle$ of a Maxwell-Boltzmann distribution of the molecule, while the direction was again chosen randomly using a true number generator. As a restriction, the z component of the vector was ensured to point into the direction of the surface.

The ten simulations performed this way are attached as xyz trajectories. It should be noted that only every tenth set of coordinates was written into this file, therefore the interval between two structures is $\Delta t = 10$ fs.

References

1. Verlet, L. Computer “Experiments” on Classical Fluids: I. Thermodynamical Properties of Lennard-Jones Molecules. *Phys. Rev.* **1967**, *159*, 98–103.
2. Swope, W. C.; Andersen, H. C.; Berens, P. H.; Wilson, K. R. A Computer Simulation Method for the Calculation of Equilibrium Constants for the Formation of Physical Clusters of Molecules: Application to Small Water Clusters. *J. Chem. Phys.* **1982**, *76*, 637–649.

3. Nosé, S. A Unified Formulation of the Constant Temperature Molecular Dynamics Methods. *J. Chem. Phys.* **1984**, *81*, 511–519.
4. Nosé, S. Constant Temperature Molecular Dynamics Methods. *Prog. Theor. Phys. Suppl.* **1991**, *103*, 1–46.
5. Bylander, D. M.; Kleinman, L. Energy Fluctuations Induced by the Nosé Thermostat *Phys. Rev. B* **1992**, *46*, 13756–13761.
6. Random Decimal Fraction Generator. <http://www.random.org/decimal-fractions>.

Cartesian Coordinates and Total Energies

Acetylene molecule: E(PBE-D3) = -22.980927 eV, E(HSE06-D3) = -26.699781 eV

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0.0000000000000000 15.3244190216000007 0.0000000000000000
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Ethylene molecule: E(PBE-D3) = -32.031858 eV, E(HSE06-D3) = -36.940415 eV

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0.2564074460701332 0.4410812097376029 0.5537097041945112
0.1957663619288062 0.5655380467621491 0.5537102818415032
0.1957658427890995 0.4785471266497333 0.5537096090751004
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Slab 4x4 cell: E(PBE-D3) = -627.241303 eV, E(HSE06-D3) = -725.272510 eV

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Si H
96 32
Selective dynamics
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Acetylene pi complex TS: E(PBE-D3) = -650.88722 eV, E(HSE06-D3) = -752.7432 eV

1.0000000000000000
15.3244190216000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 15.3244190216000007 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.6720000000000006

Si H C

96 34 2

Selective dynamics

Direct

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0.7418401878981852	0.7446102963963611	0.2963389661328085	T	T	T
0.1249944776216103	0.0412848143315799	0.3646572308578727	T	T	T
0.6249888364716513	0.0389594455940073	0.3673442815771293	T	T	T
0.3761847746411511	0.0620932023598332	0.3303227194163778	T	T	T
0.8737979136033609	0.0620947708251618	0.3303206565096906	T	T	T
0.1249986693518464	0.1880788738743027	0.3310280480346278	T	T	T
0.6250215609221003	0.1930134623913310	0.3425948858738429	T	T	T
0.3762024966172945	0.2096995797949958	0.3627293235849394	T	T	T
0.8737869673267661	0.2097031023775195	0.3627236418788335	T	T	T

0.3750647064440678	0.5406614736473180	0.3651791069488279	T	T	T
0.8749373344237427	0.5406648041097856	0.3651782179999635	T	T	T
0.1250005711602141	0.5624277406225555	0.3308332246074486	T	T	T
0.6250021957802936	0.5626273627747990	0.3308625499446856	T	T	T
0.3751360069331382	0.6878647062912273	0.3309419797246219	T	T	T
0.8748644926023625	0.6878662500181026	0.3309403591398191	T	T	T
0.1249990894899861	0.7094028571092931	0.3649604633478431	T	T	T
0.6250001052296020	0.7096297870973695	0.3650112454148698	T	T	T
0.0000000000000000	0.1711555913671532	0.0044116832779651	F	F	F
0.5000000319229088	0.1711555913671532	0.0044116832779651	F	F	F
0.0000000000000000	0.3288444405557556	0.0044116832779651	F	F	F
0.5000000319229088	0.3288444405557556	0.0044116832779651	F	F	F
0.0000000000000000	0.4211559336052488	0.0044116832779651	F	F	F
0.5000000319229088	0.4211559336052488	0.0044116832779651	F	F	F
0.0000000000000000	0.0788440983176599	0.0044116832779651	F	F	F
0.5000000319229088	0.0788440983176599	0.0044116832779651	F	F	F
0.2500003422380956	0.0788440983176599	0.0044116832779651	F	F	F
0.7500003741610044	0.0788440983176599	0.0044116832779651	F	F	F
0.2500003422380956	0.1711555913671532	0.0044116832779651	F	F	F
0.7500003741610044	0.1711555913671532	0.0044116832779651	F	F	F
0.2500003422380956	0.3288444405557556	0.0044116832779651	F	F	F
0.7500003741610044	0.3288444405557556	0.0044116832779651	F	F	F
0.2500003422380956	0.4211559336052488	0.0044116832779651	F	F	F
0.7500003741610044	0.4211559336052488	0.0044116832779651	F	F	F
0.0000000000000000	0.6711556232900620	0.0044116832779651	F	F	F
0.5000000319229088	0.6711556232900620	0.0044116832779651	F	F	F
0.0000000000000000	0.8288444724786572	0.0044116832779651	F	F	F
0.5000000319229088	0.8288444724786572	0.0044116832779651	F	F	F
0.0000000000000000	0.9211559655281576	0.0044116832779651	F	F	F
0.5000000319229088	0.9211559655281576	0.0044116832779651	F	F	F
0.0000000000000000	0.5788441302405616	0.0044116832779651	F	F	F
0.5000000319229088	0.5788441302405616	0.0044116832779651	F	F	F
0.2500003422380956	0.5788441302405616	0.0044116832779651	F	F	F
0.7500003741610044	0.5788441302405616	0.0044116832779651	F	F	F
0.2500003422380956	0.6711556232900620	0.0044116832779651	F	F	F
0.7500003741610044	0.6711556232900620	0.0044116832779651	F	F	F
0.2500003422380956	0.8288444724786572	0.0044116832779651	F	F	F
0.7500003741610044	0.8288444724786572	0.0044116832779651	F	F	F
0.2500003422380956	0.9211559655281576	0.0044116832779651	F	F	F
0.7500003741610044	0.9211559655281576	0.0044116832779651	F	F	F
0.7347491047282571	0.2659729259038536	0.4357473417513883	T	T	T
0.5151598367667323	0.2665647614155204	0.4355958559534798	T	T	T
0.6653961093038254	0.2616152726014087	0.4256566728919626	T	T	T
0.5845236592269664	0.2619078744210209	0.4256272656677248	T	T	T

Acetylene sublayer mode: E(PBE-D3) = -651.46949 eV, E(HSE06-D3) = -753.2978 eV

1.0000000000000000

15.3244190216000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 15.3244190216000007 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.6720000000000006

Si H C

96 34 2

Selective dynamics

Direct

0.0000000000000000 0.0000000000000000 0.0438344633914134 F F F

0.5000000000000000 0.0000000000000000 0.0438344633914134 F F F

0.0000000000000000	0.2500001695033731	0.0438344633914134	F	F	F
0.5000000000000000	0.2500001695033731	0.0438344633914134	F	F	F
0.2500001695034015	0.0000000000000000	0.0438344633914134	F	F	F
0.7500001695034015	0.0000000000000000	0.0438344633914134	F	F	F
0.0000000000000000	0.5000000319229088	0.0438344633914134	F	F	F
0.5000000000000000	0.5000000319229088	0.0438344633914134	F	F	F
0.2500001695034015	0.2500001695033731	0.0438344633914134	F	F	F
0.7500001695034015	0.2500001695033731	0.0438344633914134	F	F	F
0.0000000000000000	0.7500002014262819	0.0438344633914134	F	F	F
0.5000000000000000	0.7500002014262819	0.0438344633914134	F	F	F
0.2500001695034015	0.5000000319229088	0.0438344633914134	F	F	F
0.7500001695034015	0.5000000319229088	0.0438344633914134	F	F	F
0.2500001695034015	0.7500002014262819	0.0438344633914134	F	F	F
0.7500001695034015	0.7500002014262819	0.0438344633914134	F	F	F
0.1249999139362856	0.0000000000000000	0.1063344608391595	F	F	F
0.6249999139362927	0.0000000000000000	0.1063344608391595	F	F	F
0.1249999139362856	0.2500001695033731	0.1063344608391595	F	F	F
0.6249999139362927	0.2500001695033731	0.1063344608391595	F	F	F
0.3750000834396943	0.0000000000000000	0.1063344608391595	F	F	F
0.8750000834396942	0.0000000000000000	0.1063344608391595	F	F	F
0.1249999139362856	0.5000000319229088	0.1063344608391595	F	F	F
0.6249999139362927	0.5000000319229088	0.1063344608391595	F	F	F
0.3750000834396943	0.2500001695033731	0.1063344608391595	F	F	F
0.8750000834396942	0.2500001695033731	0.1063344608391595	F	F	F
0.1249999139362856	0.7500002014262819	0.1063344608391595	F	F	F
0.6249999139362927	0.7500002014262819	0.1063344608391595	F	F	F
0.3750000834396943	0.5000000319229088	0.1063344608391595	F	F	F
0.8750000834396942	0.5000000319229088	0.1063344608391595	F	F	F
0.3750000834396943	0.7500002014262819	0.1063344608391595	F	F	F
0.8750000834396942	0.7500002014262819	0.1063344608391595	F	F	F
0.1261415107111612	0.1241787674019322	0.1656371503079389	T	T	T
0.6248046258157458	0.1250746016190846	0.1666604729294092	T	T	T
0.3815779330764969	0.1264720419717380	0.1686784745484638	T	T	T
0.8783561410645134	0.1248197848760952	0.1651050688976819	T	T	T
0.3714993558802586	0.3756984349476303	0.1699934416296596	T	T	T
0.8726399606328915	0.3747468728429205	0.1718450179606317	T	T	T
0.1225766523267358	0.3750158648644865	0.1727593413306285	T	T	T
0.6227487357193862	0.3750249336679288	0.1727747604747005	T	T	T
0.3749538828648186	0.6245336527622103	0.1658684261489172	T	T	T
0.8749590921902926	0.6242509690819675	0.1659886858723530	T	T	T
0.1250450605672485	0.6255348772924492	0.1660005647700134	T	T	T
0.6252927364674002	0.6256350720813491	0.1659322018642159	T	T	T
0.1259487816336666	0.8747650240616407	0.1712930064888697	T	T	T
0.6254175858691771	0.8748704526495947	0.1714039330266842	T	T	T
0.3763318995192552	0.8753254551827133	0.1731059818843307	T	T	T
0.8765942770882926	0.8744031601938808	0.1720695518520027	T	T	T
0.0018999353294191	0.1237993697875384	0.2276596988300613	T	T	T
0.5061466758748585	0.1320929875916838	0.2350210604519200	T	T	T
0.2521687169914515	0.1237017444796345	0.2246354796886945	T	T	T
0.7528344085848691	0.1206827341930428	0.2226272570798284	T	T	T
0.4938883073100476	0.3788808500173526	0.2348857296375180	T	T	T
0.9963899317026081	0.3738507628325412	0.2379931749470892	T	T	T
0.2481690004753853	0.3757847317042090	0.2364568549402109	T	T	T
0.7479030606477202	0.3735199666894716	0.2378452440341037	T	T	T
0.5001059373213367	0.6276988802128526	0.2263908028019989	T	T	T
0.9999618159858650	0.6240626471842198	0.2267102000391062	T	T	T
0.2500806142507304	0.6248723073751534	0.2266646802386839	T	T	T

0.7501388657012467	0.6231258580381033	0.2268217640836583	T	T	T
0.0021663614394673	0.8737574040550212	0.2371194112118881	T	T	T
0.5024775718985892	0.8783096015397511	0.2386065460528874	T	T	T
0.2499922078204480	0.8745500697988013	0.2368702869943923	T	T	T
0.7510217482659894	0.8716083824054690	0.2352897672929847	T	T	T
0.2455653968888287	0.0056640106373767	0.2946984534054443	T	T	T
0.7475776088663099	0.0018508338776546	0.2922968612985273	T	T	T
0.0126058644671690	0.0029851859735496	0.2974436688398458	T	T	T
0.5155435066993848	0.0080002655720492	0.3007077187026028	T	T	T
0.4827716296267632	0.2572428228873596	0.3010042609250104	T	T	T
0.9853204486965441	0.2435167337743266	0.2984764290787107	T	T	T
0.2481757889110223	0.2430249900043041	0.2921448507331763	T	T	T
0.7570867848349476	0.2369618738232973	0.2899580275634130	T	T	T
0.4897474095831694	0.5079635524207619	0.2953692427015128	T	T	T
0.9904367379293074	0.5048696805563576	0.2969085219276767	T	T	T
0.2570603765454252	0.5056407898183715	0.2962683298471347	T	T	T
0.7563252437265937	0.5041601079946193	0.2970196201334492	T	T	T
0.0085509275571758	0.7433210722263024	0.2965343112200777	T	T	T
0.5086068284436995	0.7464043629019868	0.2968191794246031	T	T	T
0.2422172956641577	0.7442659906447439	0.2961866348132046	T	T	T
0.7422766558654786	0.7428511462208467	0.2960459301780818	T	T	T
0.1294107583306045	0.0388163485213541	0.3654559953589215	T	T	T
0.6383872220665412	0.0219960546370578	0.3697573446880640	T	T	T
0.3783273000097200	0.0625462156553129	0.3299925766132889	T	T	T
0.8791974158505181	0.0593821945717815	0.3292815864625318	T	T	T
0.1179154752391464	0.1854334708476076	0.3302755602197758	T	T	T
0.6531754358573235	0.1741029068190143	0.3541384313510717	T	T	T
0.3619626808655597	0.2081033681862765	0.3611417880051667	T	T	T
0.8685637495118025	0.2049873828075982	0.3664376783502495	T	T	T
0.3740122331050568	0.5410740062802066	0.3651087026070530	T	T	T
0.8736321368349769	0.5398839891988175	0.3654036201481987	T	T	T
0.1238400661394556	0.5618480196989659	0.3308676846531249	T	T	T
0.6232659383096834	0.5623054845528008	0.3306287982952766	T	T	T
0.3754427072450251	0.6884162424323598	0.3308831253378904	T	T	T
0.8751938014535359	0.6868557020359529	0.3309564319902261	T	T	T
0.1254562195346998	0.7088421639724375	0.3650490000545644	T	T	T
0.6252807010032283	0.7094760566914998	0.3650984223777274	T	T	T
0.0000000000000000	0.1711556604610038	0.0044115609559584	F	F	F
0.5000000000000000	0.1711556604610038	0.0044115609559584	F	F	F
0.0000000000000000	0.3288443714619048	0.0044115609559584	F	F	F
0.5000000000000000	0.3288443714619048	0.0044115609559584	F	F	F
0.0000000000000000	0.4211558299644409	0.0044115609559584	F	F	F
0.5000000000000000	0.4211558299644409	0.0044115609559584	F	F	F
0.0000000000000000	0.0788442019584679	0.0044115609559584	F	F	F
0.5000000000000000	0.0788442019584679	0.0044115609559584	F	F	F
0.2500001695034015	0.0788442019584679	0.0044115609559584	F	F	F
0.7500001695034015	0.0788442019584679	0.0044115609559584	F	F	F
0.2500001695034015	0.1711556604610038	0.0044115609559584	F	F	F
0.7500001695034015	0.1711556604610038	0.0044115609559584	F	F	F
0.2500001695034015	0.3288443714619048	0.0044115609559584	F	F	F
0.7500001695034015	0.3288443714619048	0.0044115609559584	F	F	F
0.2500001695034015	0.4211558299644409	0.0044115609559584	F	F	F
0.7500001695034015	0.4211558299644409	0.0044115609559584	F	F	F
0.0000000000000000	0.6711556923839126	0.0044115609559584	F	F	F
0.5000000000000000	0.6711556923839126	0.0044115609559584	F	F	F
0.0000000000000000	0.8288444033848066	0.0044115609559584	F	F	F
0.5000000000000000	0.8288444033848066	0.0044115609559584	F	F	F

0.0000000000000000	0.9211558618873497	0.0044115609559584	F	F	F
0.5000000000000000	0.9211558618873497	0.0044115609559584	F	F	F
0.0000000000000000	0.5788442338813695	0.0044115609559584	F	F	F
0.5000000000000000	0.5788442338813695	0.0044115609559584	F	F	F
0.2500001695034015	0.5788442338813695	0.0044115609559584	F	F	F
0.7500001695034015	0.5788442338813695	0.0044115609559584	F	F	F
0.2500001695034015	0.6711556923839126	0.0044115609559584	F	F	F
0.7500001695034015	0.6711556923839126	0.0044115609559584	F	F	F
0.2500001695034015	0.8288444033848066	0.0044115609559584	F	F	F
0.7500001695034015	0.8288444033848066	0.0044115609559584	F	F	F
0.2500001695034015	0.9211558618873497	0.0044115609559584	F	F	F
0.7500001695034015	0.9211558618873497	0.0044115609559584	F	F	F
0.6262127334521922	0.2772907677210865	0.4517579679696315	T	T	T
0.5007046449882774	0.3492133568743228	0.3954567731282916	T	T	T
0.6053361569280216	0.2575820985616151	0.4055473082064011	T	T	T
0.5387753895739246	0.2953842962511297	0.3749619467652137	T	T	T

Acetylene TS sublayer -> on-top: E(PBE-D3) = -650.7846 eV, E(HSE06-D3) = -752.53247 eV

1.0000000000000000		
15.3244190216000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.3244190216000007	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.6720000000000006

Si H C

96 34 2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0438344558453004	F	F	F
0.5000000106409601	0.0000000000000000	0.0438344558453004	F	F	F
0.0000000000000000	0.2500002270816140	0.0438344558453004	F	F	F
0.5000000106409601	0.2500002270816140	0.0438344558453004	F	F	F
0.2500002270816424	0.0000000000000000	0.0438344558453004	F	F	F
0.7500002377226025	0.0000000000000000	0.0438344558453004	F	F	F
0.0000000000000000	0.5000000319229088	0.0438344558453004	F	F	F
0.5000000106409601	0.5000000319229088	0.0438344558453004	F	F	F
0.2500002270816424	0.2500002270816140	0.0438344558453004	F	F	F
0.7500002377226025	0.2500002270816140	0.0438344558453004	F	F	F
0.0000000000000000	0.7500002590045227	0.0438344558453004	F	F	F
0.5000000106409601	0.7500002590045227	0.0438344558453004	F	F	F
0.2500002270816424	0.5000000319229088	0.0438344558453004	F	F	F
0.7500002377226025	0.5000000319229088	0.0438344558453004	F	F	F
0.2500002270816424	0.7500002590045227	0.0438344558453004	F	F	F
0.7500002377226025	0.7500002590045227	0.0438344558453004	F	F	F
0.1249998909050021	0.0000000000000000	0.1063344541437864	F	F	F
0.6249999015459693	0.0000000000000000	0.1063344541437864	F	F	F
0.1249998909050021	0.2500002270816140	0.1063344541437864	F	F	F
0.6249999015459693	0.2500002270816140	0.1063344541437864	F	F	F
0.3750001179866302	0.0000000000000000	0.1063344541437864	F	F	F
0.8750001286275904	0.0000000000000000	0.1063344541437864	F	F	F
0.1249998909050021	0.5000000319229088	0.1063344541437864	F	F	F
0.6249999015459693	0.5000000319229088	0.1063344541437864	F	F	F
0.3750001179866302	0.2500002270816140	0.1063344541437864	F	F	F
0.8750001286275904	0.2500002270816140	0.1063344541437864	F	F	F
0.1249998909050021	0.7500002590045227	0.1063344541437864	F	F	F
0.6249999015459693	0.7500002590045227	0.1063344541437864	F	F	F
0.3750001179866302	0.5000000319229088	0.1063344541437864	F	F	F
0.8750001286275904	0.5000000319229088	0.1063344541437864	F	F	F

0.3750001179866302	0.7500002590045227	0.1063344541437864	F	F	F
0.8750001286275904	0.7500002590045227	0.1063344541437864	F	F	F
0.1249565772743677	0.1244666780861497	0.1660757377659307	T	T	T
0.6251150836838409	0.1244389968180124	0.1656838808599388	T	T	T
0.3749917713406570	0.1253027111433476	0.1659018499106283	T	T	T
0.8748652021908213	0.1253266804734669	0.1660021405452370	T	T	T
0.3745635913060868	0.3751535350258343	0.1713342389290700	T	T	T
0.8754163284951695	0.3751733233689173	0.1713042555854437	T	T	T
0.1249610824649340	0.3748808034783275	0.1727869635171236	T	T	T
0.6250691859259754	0.3752269915083896	0.1724955639208778	T	T	T
0.3751327765125574	0.6244644522367060	0.1659499626948567	T	T	T
0.8751653608167638	0.6244310454250309	0.1659026172955448	T	T	T
0.1251820125143802	0.6256006558545150	0.1659790846722028	T	T	T
0.6253168757789251	0.6256582025062841	0.1659409540505629	T	T	T
0.1248744726192559	0.8750644478770929	0.1717161443933017	T	T	T
0.6249226564807608	0.8750640014676956	0.1716871326574474	T	T	T
0.3751887247215598	0.8752964098702625	0.1731780910076322	T	T	T
0.8744448058012815	0.8753553330790736	0.1732374272940867	T	T	T
-0.0000835129478577	0.1251023267739841	0.2267545867650903	T	T	T
0.5001291474363477	0.1250117950363907	0.2257762903888066	T	T	T
0.2499360183460499	0.1251372367502205	0.2267504085722870	T	T	T
0.7501135674590141	0.1255675268534379	0.2263403883767359	T	T	T
0.4987805862148207	0.3753386693606562	0.2364688296654248	T	T	T
0.9991481614893908	0.3748474071842171	0.2373158577049096	T	T	T
0.2507778853864525	0.3749126303215061	0.2372699385619310	T	T	T
0.7512619749116622	0.3757842263603024	0.2365245202708661	T	T	T
0.5003008821337515	0.6259702972306755	0.2265340181994734	T	T	T
1.0001173567334454	0.6250331493908170	0.2266819813261780	T	T	T
0.2502219973917278	0.6249883301811519	0.2267634520438344	T	T	T
0.7502480611925385	0.6257494141698906	0.2267266947324894	T	T	T
0.0006910272243053	0.8752355600545068	0.2374540750717127	T	T	T
0.5012247346561057	0.8766101984312521	0.2378988706938139	T	T	T
0.2490083545773407	0.8753545467980515	0.2375782056583236	T	T	T
0.7483037319998532	0.8770370954904716	0.2381853329260670	T	T	T
0.2418637520631149	0.0061430179096319	0.2968824184624617	T	T	T
0.7391976488426473	0.0082356832449417	0.2978468534409006	T	T	T
0.0072213773882427	0.0060394969998920	0.2966071353153629	T	T	T
0.5091992106537010	0.0081356633038003	0.2972372076627458	T	T	T
0.4913300543858921	0.2434787753243456	0.2933031324198179	T	T	T
0.9917859331699057	0.2444299034229676	0.2964836709413234	T	T	T
0.2585138739790671	0.2444908219963614	0.2965096872436800	T	T	T
0.7584083335557767	0.2446483104585987	0.2937835470394623	T	T	T
0.4913060266305163	0.5061090309902530	0.2958399823194244	T	T	T
0.9916343814460060	0.5055486877918922	0.2963634407547784	T	T	T
0.2580558389109112	0.5054840253045045	0.2963184524802738	T	T	T
0.7583829769844304	0.5059102400398269	0.2961535801799292	T	T	T
0.0078923758619012	0.7443539235555018	0.2964150041006844	T	T	T
0.5078775171754691	0.7450773440406099	0.2965210806658618	T	T	T
0.2417707773625388	0.7443981002147547	0.2965672690374979	T	T	T
0.7418560140170176	0.7452984183458379	0.2965798777966638	T	T	T
0.1244950792103951	0.0409669096486819	0.3649143190371750	T	T	T
0.6238364068762499	0.0443459705552593	0.3689415025005016	T	T	T
0.3752486245567198	0.0636480825707565	0.3304920614589369	T	T	T
0.8735962679697803	0.0631543115674323	0.3304525091759994	T	T	T
0.1251073981163393	0.1879147535697229	0.3310721091095626	T	T	T
0.6254448773638963	0.1975642352736933	0.3350449247106782	T	T	T
0.3767121569553534	0.2105345405142748	0.3641295017523362	T	T	T

0.8735887626914381	0.2101964092004935	0.3639517198429705	T	T	T
0.3748562171491224	0.5403872383219004	0.3651546358224858	T	T	T
0.8747952316915741	0.5405807208616692	0.3651575029536424	T	T	T
0.1248528730451856	0.5620153407206163	0.3308050903988103	T	T	T
0.6250481901023138	0.5627460649193019	0.3303685945226053	T	T	T
0.3748933151711764	0.6877249046228223	0.3310681355430666	T	T	T
0.8747433055992165	0.6877739693207433	0.3310272646410116	T	T	T
0.1247706575446592	0.7090005454066953	0.3649999853559557	T	T	T
0.6247888707613000	0.7092946658100943	0.3647495176745575	T	T	T
0.0000000000000000	0.1711556374297203	0.0044116017299559	F	F	F
0.5000000106409601	0.1711556374297203	0.0044116017299559	F	F	F
0.0000000000000000	0.3288443944931885	0.0044116017299559	F	F	F
0.5000000106409601	0.3288443944931885	0.0044116017299559	F	F	F
0.0000000000000000	0.4211558645113769	0.0044116017299559	F	F	F
0.5000000106409601	0.4211558645113769	0.0044116017299559	F	F	F
0.0000000000000000	0.0788441674115319	0.0044116017299559	F	F	F
0.5000000106409601	0.0788441674115319	0.0044116017299559	F	F	F
0.2500002270816424	0.0788441674115319	0.0044116017299559	F	F	F
0.7500002377226025	0.0788441674115319	0.0044116017299559	F	F	F
0.2500002270816424	0.1711556374297203	0.0044116017299559	F	F	F
0.7500002377226025	0.1711556374297203	0.0044116017299559	F	F	F
0.2500002270816424	0.3288443944931885	0.0044116017299559	F	F	F
0.7500002377226025	0.3288443944931885	0.0044116017299559	F	F	F
0.2500002270816424	0.4211558645113769	0.0044116017299559	F	F	F
0.7500002377226025	0.4211558645113769	0.0044116017299559	F	F	F
0.0000000000000000	0.6711556693526290	0.0044116017299559	F	F	F
0.5000000106409601	0.6711556693526290	0.0044116017299559	F	F	F
0.0000000000000000	0.8288444264160901	0.0044116017299559	F	F	F
0.5000000106409601	0.8288444264160901	0.0044116017299559	F	F	F
0.0000000000000000	0.9211558964342856	0.0044116017299559	F	F	F
0.5000000106409601	0.9211558964342856	0.0044116017299559	F	F	F
0.0000000000000000	0.5788441993344335	0.0044116017299559	F	F	F
0.5000000106409601	0.5788441993344335	0.0044116017299559	F	F	F
0.2500002270816424	0.5788441993344335	0.0044116017299559	F	F	F
0.7500002377226025	0.5788441993344335	0.0044116017299559	F	F	F
0.2500002270816424	0.6711556693526290	0.0044116017299559	F	F	F
0.7500002377226025	0.6711556693526290	0.0044116017299559	F	F	F
0.2500002270816424	0.8288444264160901	0.0044116017299559	F	F	F
0.7500002377226025	0.8288444264160901	0.0044116017299559	F	F	F
0.2500002270816424	0.9211558964342856	0.0044116017299559	F	F	F
0.7500002377226025	0.9211558964342856	0.0044116017299559	F	F	F
0.6763469363541685	0.2239297734069160	0.4692377441797675	T	T	T
0.5710074171503404	0.3758444545652663	0.3862230758893999	T	T	T
0.6418800711161210	0.2685531314052011	0.4400780369911038	T	T	T
0.6027688318801424	0.3239202285224577	0.4106836088300584	T	T	T

Acetylene TS sublayer -> bridge: E(PBE-D3) = -651.10272 eV, E(HSE06-D3) = -752.79363 eV

1.0000000000000000

15.3244190216000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 15.3244190216000007 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.6720008849999992

Si H C

96 34 2

Selective dynamics

Direct

0.0000000000000000 0.0000000000000000 0.0438344579628804 F F F

0.5000000070939734	0.0000000000000000	0.0438344579628804	F	F	F
0.0000000000000000	0.2500002078888670	0.0438344579628804	F	F	F
0.5000000070939734	0.2500002078888670	0.0438344579628804	F	F	F
0.2500002078888954	0.0000000000000000	0.0438344579628804	F	F	F
0.7500002149828688	0.0000000000000000	0.0438344579628804	F	F	F
0.0000000000000000	0.5000000319229088	0.0438344579628804	F	F	F
0.5000000070939734	0.5000000319229088	0.0438344579628804	F	F	F
0.2500002078888954	0.2500002078888670	0.0438344579628804	F	F	F
0.7500002149828688	0.2500002078888670	0.0438344579628804	F	F	F
0.0000000000000000	0.7500002398117758	0.0438344579628804	F	F	F
0.5000000070939734	0.7500002398117758	0.0438344579628804	F	F	F
0.2500002078888954	0.5000000319229088	0.0438344579628804	F	F	F
0.7500002149828688	0.5000000319229088	0.0438344579628804	F	F	F
0.2500002078888954	0.7500002398117758	0.0438344579628804	F	F	F
0.7500002149828688	0.7500002398117758	0.0438344579628804	F	F	F
0.1249998985820966	0.0000000000000000	0.1063344554106251	F	F	F
0.6249999056760771	0.0000000000000000	0.1063344554106251	F	F	F
0.1249998985820966	0.2500002078888670	0.1063344554106251	F	F	F
0.6249999056760771	0.2500002078888670	0.1063344554106251	F	F	F
0.3750001064709849	0.0000000000000000	0.1063344554106251	F	F	F
0.8750001135649583	0.0000000000000000	0.1063344554106251	F	F	F
0.1249998985820966	0.5000000319229088	0.1063344554106251	F	F	F
0.6249999056760771	0.5000000319229088	0.1063344554106251	F	F	F
0.3750001064709849	0.2500002078888670	0.1063344554106251	F	F	F
0.8750001135649583	0.2500002078888670	0.1063344554106251	F	F	F
0.1249998985820966	0.7500002398117758	0.1063344554106251	F	F	F
0.6249999056760771	0.7500002398117758	0.1063344554106251	F	F	F
0.3750001064709849	0.5000000319229088	0.1063344554106251	F	F	F
0.8750001135649583	0.5000000319229088	0.1063344554106251	F	F	F
0.3750001064709849	0.7500002398117758	0.1063344554106251	F	F	F
0.8750001135649583	0.7500002398117758	0.1063344554106251	F	F	F
0.1212438908492006	0.1243614880943508	0.1650941687318076	T	T	T
0.6187048257112372	0.1255240454554788	0.1692595303812920	T	T	T
0.3728550308028560	0.1259338357933562	0.1670220032985089	T	T	T
0.8707843877969171	0.1251426411928550	0.1661690863608142	T	T	T
0.3752401633530249	0.3752579484143334	0.1704960742241991	T	T	T
0.8753035910556760	0.3747758494492204	0.1717503936334936	T	T	T
0.1257082243225764	0.3750475959012828	0.1725239926222591	T	T	T
0.6280293146069683	0.3758561715426985	0.1713769046526094	T	T	T
0.3752619381103913	0.6244108117391558	0.1658326116775056	T	T	T
0.8752691551073474	0.6243242428993709	0.1659358356425935	T	T	T
0.1253482998394193	0.6255321864438510	0.1659837413939054	T	T	T
0.6258232227842588	0.6255978935463945	0.1658534256602159	T	T	T
0.1250012553644799	0.8744770002514094	0.1710068091441296	T	T	T
0.6261375703076497	0.8746203499725959	0.1712616816156299	T	T	T
0.3757827959316250	0.8746867459351874	0.1726801711862280	T	T	T
0.8758534645299298	0.8746057520094197	0.1723958453600946	T	T	T
0.9969550168868733	0.1236805781567486	0.2261397622894679	T	T	T
0.4907781029227275	0.1249560669788700	0.2350757772132005	T	T	T
0.2455575734296411	0.1222842175433152	0.2249942679209463	T	T	T
0.7468340459865331	0.1256988611198084	0.2275779475592505	T	T	T
0.5014914033910699	0.3789355972638863	0.2328837657423331	T	T	T
0.0003016636806358	0.3747585608014579	0.2368834530231742	T	T	T
0.2521242180496719	0.3752678911260888	0.2366911424752995	T	T	T
0.7518695318923343	0.3734112054772840	0.2383613586207477	T	T	T
0.5005213415453390	0.6254917513521911	0.2260525787095818	T	T	T
0.0003324789459414	0.6244910777084530	0.2266101803392419	T	T	T

0.2504812480412250	0.6240501946682511	0.2266606023106269	T	T	T
0.7505414422279568	0.6244345445519137	0.2269442323786376	T	T	T
0.0016685405340574	0.8744385086857078	0.2370312260342174	T	T	T
0.5022693463618042	0.8741266050423533	0.2368268084337838	T	T	T
0.2491567384583105	0.8723630227158427	0.2360481719174950	T	T	T
0.7506255060402263	0.8742057183968683	0.2366870744303247	T	T	T
0.2422667576414913	0.0026809444234756	0.2936015909851878	T	T	T
0.7445451590692924	0.0043257048775223	0.2952267159935669	T	T	T
0.0106415668160849	0.0047028072374959	0.2960622810499044	T	T	T
0.5140531484859162	0.0000931959598431	0.3002437573924797	T	T	T
0.5137749915605028	0.2547972620100541	0.2949422222077870	T	T	T
0.9972034742352347	0.2432984224853217	0.2946985863403052	T	T	T
0.2626615362356318	0.2430440870382694	0.2934504415406541	T	T	T
0.7600577118993739	0.2419004243699643	0.2969220726019149	T	T	T
0.4939614388849499	0.5061889992789829	0.2951049868034373	T	T	T
0.9930925312704515	0.5051125509363099	0.2962225834178123	T	T	T
0.2597310681083055	0.5049542334253406	0.2966953341879708	T	T	T
0.7595648854076973	0.5047602291080232	0.2966954746116647	T	T	T
0.0085952985902093	0.7438123749905950	0.2961795649031329	T	T	T
0.5089629356981805	0.7438829654213185	0.2961972123925406	T	T	T
0.2423061737619470	0.7431458600814488	0.2964758098763903	T	T	T
0.7424248648933676	0.7441029921647753	0.2963913521676209	T	T	T
0.1283489383572278	0.0383022633726251	0.3646003857563343	T	T	T
0.6324300869909291	0.0348209273448957	0.3670436141853783	T	T	T
0.3782023715866971	0.0508001210522630	0.3280192175834105	T	T	T
0.8775319205240985	0.0611472784587381	0.3295449653931627	T	T	T
0.1313019930638294	0.1847974322465832	0.3287549443881447	T	T	T
0.6362788044658151	0.1906264749764283	0.3495220496817721	T	T	T
0.3750350522574075	0.1987317768428554	0.3624487848495312	T	T	T
0.8802074717402274	0.2074177019600055	0.3623219279209191	T	T	T
0.3773974425332199	0.5393893896650139	0.3647118543475713	T	T	T
0.8764149907892518	0.5402325925198064	0.3651273001309133	T	T	T
0.1262902359125815	0.5616054162898083	0.3307918398959330	T	T	T
0.6268276746034507	0.5622593655392468	0.3306527909878008	T	T	T
0.3758705961683625	0.6870124235162786	0.3306747989633287	T	T	T
0.8754839417414619	0.6873519197400360	0.3308726745480226	T	T	T
0.1253371065256960	0.7085926341108030	0.3650009307253695	T	T	T
0.6255713421923926	0.7093729179934375	0.3652035778665504	T	T	T
0.0000000000000000	0.1711556451068148	0.0044115880985913	F	F	F
0.5000000070939734	0.1711556451068148	0.0044115880985913	F	F	F
0.0000000000000000	0.3288443868160940	0.0044115880985913	F	F	F
0.5000000070939734	0.3288443868160940	0.0044115880985913	F	F	F
0.0000000000000000	0.4211558529957315	0.0044115880985913	F	F	F
0.5000000070939734	0.4211558529957315	0.0044115880985913	F	F	F
0.0000000000000000	0.0788441789271772	0.0044115880985913	F	F	F
0.5000000070939734	0.0788441789271772	0.0044115880985913	F	F	F
0.2500002078888954	0.0788441789271772	0.0044115880985913	F	F	F
0.7500002149828688	0.0788441789271772	0.0044115880985913	F	F	F
0.2500002078888954	0.1711556451068148	0.0044115880985913	F	F	F
0.7500002149828688	0.1711556451068148	0.0044115880985913	F	F	F
0.2500002078888954	0.3288443868160940	0.0044115880985913	F	F	F
0.7500002149828688	0.3288443868160940	0.0044115880985913	F	F	F
0.2500002078888954	0.4211558529957315	0.0044115880985913	F	F	F
0.7500002149828688	0.4211558529957315	0.0044115880985913	F	F	F
0.0000000000000000	0.6711556770297236	0.0044115880985913	F	F	F
0.5000000070939734	0.6711556770297236	0.0044115880985913	F	F	F
0.0000000000000000	0.8288444187389956	0.0044115880985913	F	F	F

0.5000000070939734	0.8288444187389956	0.0044115880985913	F	F	F
0.0000000000000000	0.9211558849186403	0.0044115880985913	F	F	F
0.5000000070939734	0.9211558849186403	0.0044115880985913	F	F	F
0.0000000000000000	0.5788442108500789	0.0044115880985913	F	F	F
0.5000000070939734	0.5788442108500789	0.0044115880985913	F	F	F
0.2500002078888954	0.5788442108500789	0.0044115880985913	F	F	F
0.7500002149828688	0.5788442108500789	0.0044115880985913	F	F	F
0.2500002078888954	0.6711556770297236	0.0044115880985913	F	F	F
0.7500002149828688	0.6711556770297236	0.0044115880985913	F	F	F
0.2500002078888954	0.8288444187389956	0.0044115880985913	F	F	F
0.7500002149828688	0.8288444187389956	0.0044115880985913	F	F	F
0.2500002078888954	0.9211558849186403	0.0044115880985913	F	F	F
0.7500002149828688	0.9211558849186403	0.0044115880985913	F	F	F
0.5948694350231909	0.2674467380771594	0.4592604030337912	T	T	T
0.4629687375796962	0.3384315369935382	0.3993097109342664	T	T	T
0.5805034270003926	0.2565607991604557	0.4103822414680550	T	T	T
0.5088607388794395	0.2897345347648079	0.3810635174714335	T	T	T

Ethylene pi complex starting rotamer: E(PBE-D3) = -660.00949 eV, E(HSE06-D3) = -763.08529 eV

1.0000000000000000		
15.3244190216000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.3244190216000007	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.6720008849999992

Si H C

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Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0438344616013850	F	F	F
0.5000000000000000	0.0000000000000000	0.0438344616013850	F	F	F
0.0000000000000000	0.2500001695033731	0.0438344616013850	F	F	F
0.5000000000000000	0.2500001695033731	0.0438344616013850	F	F	F
0.2500001695034015	0.0000000000000000	0.0438344616013850	F	F	F
0.7500001695034015	0.0000000000000000	0.0438344616013850	F	F	F
0.0000000000000000	0.5000000319229088	0.0438344616013850	F	F	F
0.5000000000000000	0.5000000319229088	0.0438344616013850	F	F	F
0.2500001695034015	0.2500001695033731	0.0438344616013850	F	F	F
0.7500001695034015	0.2500001695033731	0.0438344616013850	F	F	F
0.0000000000000000	0.7500002014262819	0.0438344616013850	F	F	F
0.5000000000000000	0.7500002014262819	0.0438344616013850	F	F	F
0.2500001695034015	0.5000000319229088	0.0438344616013850	F	F	F
0.7500001695034015	0.5000000319229088	0.0438344616013850	F	F	F
0.2500001695034015	0.7500002014262819	0.0438344616013850	F	F	F
0.7500001695034015	0.7500002014262819	0.0438344616013850	F	F	F
0.1249999139362856	0.0000000000000000	0.1063344564968744	F	F	F
0.6249999139362927	0.0000000000000000	0.1063344564968744	F	F	F
0.1249999139362856	0.2500001695033731	0.1063344564968744	F	F	F
0.6249999139362927	0.2500001695033731	0.1063344564968744	F	F	F
0.3750000834396943	0.0000000000000000	0.1063344564968744	F	F	F
0.8750000834396942	0.0000000000000000	0.1063344564968744	F	F	F
0.1249999139362856	0.5000000319229088	0.1063344564968744	F	F	F
0.6249999139362927	0.5000000319229088	0.1063344564968744	F	F	F
0.3750000834396943	0.2500001695033731	0.1063344564968744	F	F	F
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0.3750000834396943	0.5000000319229088	0.1063344564968744	F	F	F

0.8750000834396942	0.5000000319229088	0.1063344564968744	F	F	F
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0.8750000834396942	0.7500002014262819	0.1063344564968744	F	F	F
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0.8749922160864051	0.3749671130206654	0.1715180168309974	T	T	T
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0.3749942283885082	0.6243977317884259	0.1659202240257387	T	T	T
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0.6250062459031624	0.6256095615477677	0.1659633684295142	T	T	T
0.1249911686904755	0.8749972577278282	0.1715559930159128	T	T	T
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0.8748215326260306	0.8750874917354124	0.1729165894078042	T	T	T
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0.2582048931663212	0.5057343601099472	0.2964342424761808	T	T	T
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0.0080465102029712	0.7445183314644790	0.296417627271853	T	T	T
0.5080653101741902	0.7447556452861798	0.2963590207244703	T	T	T
0.2419315512943148	0.7445135368002732	0.2964244994620328	T	T	T
0.7419165006349832	0.7447868715435340	0.2963689132155966	T	T	T
0.1249635287832681	0.0408335950264673	0.3650451688362436	T	T	T
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0.3755748346061833	0.0621935534206719	0.3299560792403808	T	T	T
0.8743364961348469	0.0622745573959532	0.3299856595404869	T	T	T
0.1249833729832965	0.1877051797910552	0.3309395488022328	T	T	T
0.6251338557881398	0.1940956518121121	0.3420957495312466	T	T	T

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0.8749957045742343	0.5406429362544938	0.3652234696421168	T	T	T
0.1249926470932593	0.5623103043191356	0.3308382368990430	T	T	T
0.6250001213360209	0.5626547467557861	0.3307313809311170	T	T	T
0.3750668227935339	0.6878728011837300	0.3309749975709896	T	T	T
0.8749090289106599	0.6878817929017697	0.3309759076756013	T	T	T
0.1249869290216475	0.7092826069964968	0.3649429444232537	T	T	T
0.6249905906202289	0.7095407604177626	0.3648872783050080	T	T	T
0.0000000000000000	0.1711556604610038	0.0044115607758073	F	F	F
0.5000000000000000	0.1711556604610038	0.0044115607758073	F	F	F
0.0000000000000000	0.3288443714619048	0.0044115607758073	F	F	F
0.5000000000000000	0.3288443714619048	0.0044115607758073	F	F	F
0.0000000000000000	0.4211558299644409	0.0044115607758073	F	F	F
0.5000000000000000	0.4211558299644409	0.0044115607758073	F	F	F
0.0000000000000000	0.0788442019584679	0.0044115607758073	F	F	F
0.5000000000000000	0.0788442019584679	0.0044115607758073	F	F	F
0.2500001695034015	0.0788442019584679	0.0044115607758073	F	F	F
0.7500001695034015	0.0788442019584679	0.0044115607758073	F	F	F
0.2500001695034015	0.1711556604610038	0.0044115607758073	F	F	F
0.7500001695034015	0.1711556604610038	0.0044115607758073	F	F	F
0.2500001695034015	0.3288443714619048	0.0044115607758073	F	F	F
0.7500001695034015	0.3288443714619048	0.0044115607758073	F	F	F
0.2500001695034015	0.4211558299644409	0.0044115607758073	F	F	F
0.7500001695034015	0.4211558299644409	0.0044115607758073	F	F	F
0.0000000000000000	0.6711556923839126	0.0044115607758073	F	F	F
0.5000000000000000	0.6711556923839126	0.0044115607758073	F	F	F
0.0000000000000000	0.8288444033848066	0.0044115607758073	F	F	F
0.5000000000000000	0.8288444033848066	0.0044115607758073	F	F	F
0.0000000000000000	0.9211558618873497	0.0044115607758073	F	F	F
0.5000000000000000	0.9211558618873497	0.0044115607758073	F	F	F
0.0000000000000000	0.5788442338813695	0.0044115607758073	F	F	F
0.5000000000000000	0.5788442338813695	0.0044115607758073	F	F	F
0.2500001695034015	0.5788442338813695	0.0044115607758073	F	F	F
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0.2500001695034015	0.6711556923839126	0.0044115607758073	F	F	F
0.7500001695034015	0.6711556923839126	0.0044115607758073	F	F	F
0.2500001695034015	0.8288444033848066	0.0044115607758073	F	F	F
0.7500001695034015	0.8288444033848066	0.0044115607758073	F	F	F
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0.7500001695034015	0.9211558618873497	0.0044115607758073	F	F	F
0.7057735197705570	0.2034413965512052	0.4487031039681164	T	T	T
0.5408297639578326	0.2067215698026896	0.4471788361909456	T	T	T
0.7081614275696660	0.3162530659814012	0.4176824972500174	T	T	T
0.5441466715978752	0.3194427993793918	0.4160991552901577	T	T	T
0.6698332544854314	0.2584123658001449	0.4289972823172469	T	T	T
0.5797185904949412	0.2601341152164178	0.4281217952915836	T	T	T

Ethylene pi complex minimum rotamer: E(PBE-D3) = -660.04322 eV, E(HSE06-D3) = -763.1027 eV

1.0000000000000000

15.3244190216000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 15.3244190216000007 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.6720008849999992

Si H C

96 36 2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0438344616013850	F F F
0.5000000000000000	0.0000000000000000	0.0438344616013850	F F F
0.0000000000000000	0.2500001695033731	0.0438344616013850	F F F
0.5000000000000000	0.2500001695033731	0.0438344616013850	F F F
0.2500001695034015	0.0000000000000000	0.0438344616013850	F F F
0.7500001695034015	0.0000000000000000	0.0438344616013850	F F F
0.0000000000000000	0.5000000319229088	0.0438344616013850	F F F
0.5000000000000000	0.5000000319229088	0.0438344616013850	F F F
0.2500001695034015	0.2500001695033731	0.0438344616013850	F F F
0.7500001695034015	0.2500001695033731	0.0438344616013850	F F F
0.0000000000000000	0.7500002014262819	0.0438344616013850	F F F
0.5000000000000000	0.7500002014262819	0.0438344616013850	F F F
0.2500001695034015	0.5000000319229088	0.0438344616013850	F F F
0.7500001695034015	0.5000000319229088	0.0438344616013850	F F F
0.2500001695034015	0.7500002014262819	0.0438344616013850	F F F
0.7500001695034015	0.7500002014262819	0.0438344616013850	F F F
0.1249999139362856	0.0000000000000000	0.1063344564968744	F F F
0.6249999139362927	0.0000000000000000	0.1063344564968744	F F F
0.1249999139362856	0.2500001695033731	0.1063344564968744	F F F
0.6249999139362927	0.2500001695033731	0.1063344564968744	F F F
0.3750000834396943	0.0000000000000000	0.1063344564968744	F F F
0.8750000834396942	0.0000000000000000	0.1063344564968744	F F F
0.1249999139362856	0.5000000319229088	0.1063344564968744	F F F
0.6249999139362927	0.5000000319229088	0.1063344564968744	F F F
0.3750000834396943	0.2500001695033731	0.1063344564968744	F F F
0.8750000834396942	0.2500001695033731	0.1063344564968744	F F F
0.1249999139362856	0.7500002014262819	0.1063344564968744	F F F
0.6249999139362927	0.7500002014262819	0.1063344564968744	F F F
0.3750000834396943	0.5000000319229088	0.1063344564968744	F F F
0.8750000834396942	0.5000000319229088	0.1063344564968744	F F F
0.3750000834396943	0.7500002014262819	0.1063344564968744	F F F
0.8750000834396942	0.7500002014262819	0.1063344564968744	F F F
0.1253062458061499	0.1244762194783450	0.1660862554691410	T T T
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0.3755315554000208	0.1253784305624478	0.1660562522998101	T T T
0.8749530517449021	0.1252693426773984	0.1661033412854108	T T T
0.3752636578446279	0.3748259847705429	0.1717637315805712	T T T
0.8750743772225159	0.3750926284217602	0.1714583367030071	T T T
0.1251065453395438	0.3750144035382327	0.1728005892111847	T T T
0.6249330727610405	0.3751426361428207	0.1727870488417692	T T T
0.3749101023630881	0.6243919335519159	0.1659293246892611	T T T
0.8748916672230769	0.6244202004461644	0.1659315954759821	T T T
0.1249312062026288	0.6256076353579285	0.1659763039870562	T T T
0.6249218649597333	0.6256090704833884	0.1659584270417376	T T T
0.1246844254801634	0.8750434557184624	0.1716003200199364	T T T
0.6248804998912241	0.8750989931009353	0.1715748948221948	T T T
0.3747588531652825	0.8750479557086650	0.1727826096265784	T T T
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0.2510213249346308	0.3749796102174752	0.2374110573335545	T T T

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0.2500001695034015 0.1711556604610038 0.0044115607758073 F F F
0.7500001695034015 0.1711556604610038 0.0044115607758073 F F F
0.2500001695034015 0.3288443714619048 0.0044115607758073 F F F
0.7500001695034015 0.3288443714619048 0.0044115607758073 F F F
0.2500001695034015 0.4211558299644409 0.0044115607758073 F F F
0.7500001695034015 0.4211558299644409 0.0044115607758073 F F F

0.0000000000000000	0.6711556923839126	0.0044115607758073	F F F
0.5000000000000000	0.6711556923839126	0.0044115607758073	F F F
0.0000000000000000	0.8288444033848066	0.0044115607758073	F F F
0.5000000000000000	0.8288444033848066	0.0044115607758073	F F F
0.0000000000000000	0.9211558618873495	0.0044115607758073	F F F
0.5000000000000000	0.9211558618873495	0.0044115607758073	F F F
0.0000000000000000	0.5788442338813695	0.0044115607758073	F F F
0.5000000000000000	0.5788442338813695	0.0044115607758073	F F F
0.2500001695034015	0.5788442338813695	0.0044115607758073	F F F
0.7500001695034015	0.5788442338813695	0.0044115607758073	F F F
0.2500001695034015	0.6711556923839126	0.0044115607758073	F F F
0.7500001695034015	0.6711556923839126	0.0044115607758073	F F F
0.2500001695034015	0.8288444033848066	0.0044115607758073	F F F
0.7500001695034015	0.8288444033848066	0.0044115607758073	F F F
0.2500001695034015	0.9211558618873495	0.0044115607758073	F F F
0.7500001695034015	0.9211558618873495	0.0044115607758073	F F F
0.6169556051454086	0.1837268893381068	0.4671402759557181	T T T
0.5255701173145310	0.3017786981354900	0.4204036019045159	T T T
0.7182132899092851	0.2390712997379205	0.4397585143496763	T T T
0.6259744443504718	0.3570814967298076	0.3913475847061352	T T T
0.6468321879340192	0.2343963910870428	0.4387819476062640	T T T
0.5961301222829493	0.2998797782720393	0.4129142684956868	T T T

Ethylene TS pi complex -> sublayer: E(PBE-D3) = -659.86181 eV, E(HSE06-D3) = -762.89265 eV

1.0000000000000000		
15.3244190216000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.3244190216000007	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.6720008849999992

Si H C

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Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0438344616013850	F F F
0.5000000000000000	0.0000000000000000	0.0438344616013850	F F F
0.0000000000000000	0.2500001695033731	0.0438344616013850	F F F
0.5000000000000000	0.2500001695033731	0.0438344616013850	F F F
0.2500001695034015	0.0000000000000000	0.0438344616013850	F F F
0.7500001695034015	0.0000000000000000	0.0438344616013850	F F F
0.0000000000000000	0.5000000319229088	0.0438344616013850	F F F
0.5000000000000000	0.5000000319229088	0.0438344616013850	F F F
0.2500001695034015	0.2500001695033731	0.0438344616013850	F F F
0.7500001695034015	0.2500001695033731	0.0438344616013850	F F F
0.0000000000000000	0.7500002014262819	0.0438344616013850	F F F
0.5000000000000000	0.7500002014262819	0.0438344616013850	F F F
0.2500001695034015	0.5000000319229088	0.0438344616013850	F F F
0.7500001695034015	0.5000000319229088	0.0438344616013850	F F F
0.2500001695034015	0.7500002014262819	0.0438344616013850	F F F
0.7500001695034015	0.7500002014262819	0.0438344616013850	F F F
0.1249999139362856	0.0000000000000000	0.1063344564968744	F F F
0.6249999139362927	0.0000000000000000	0.1063344564968744	F F F
0.1249999139362856	0.2500001695033731	0.1063344564968744	F F F
0.6249999139362927	0.2500001695033731	0.1063344564968744	F F F
0.3750000834396943	0.0000000000000000	0.1063344564968744	F F F
0.8750000834396942	0.0000000000000000	0.1063344564968744	F F F
0.1249999139362856	0.5000000319229088	0.1063344564968744	F F F
0.6249999139362927	0.5000000319229088	0.1063344564968744	F F F

0.3750000834396943	0.2500001695033731	0.1063344564968744	F	F	F
0.8750000834396942	0.2500001695033731	0.1063344564968744	F	F	F
0.1249999139362856	0.7500002014262819	0.1063344564968744	F	F	F
0.6249999139362927	0.7500002014262819	0.1063344564968744	F	F	F
0.3750000834396943	0.5000000319229088	0.1063344564968744	F	F	F
0.8750000834396942	0.5000000319229088	0.1063344564968744	F	F	F
0.3750000834396943	0.7500002014262819	0.1063344564968744	F	F	F
0.8750000834396942	0.7500002014262819	0.1063344564968744	F	F	F
0.1263273739482406	0.1243966507575915	0.1658887535952898	T	T	T
0.6261678828245267	0.1246884153093835	0.1658519346749228	T	T	T
0.3785767018058230	0.1260864727357516	0.1671603316824312	T	T	T
0.8766140183790471	0.1250699356001225	0.1659348921115544	T	T	T
0.3739859713844780	0.3748355957965017	0.1712465652933144	T	T	T
0.8745178236485243	0.3749862174065705	0.1715783997423607	T	T	T
0.1245264913806801	0.3749876511626180	0.1728536114250329	T	T	T
0.6243279350928718	0.3750905648296763	0.1727471854455787	T	T	T
0.3744983254047361	0.6244484670073318	0.1658163929833026	T	T	T
0.8747807484989655	0.6243700227310424	0.1659550797029297	T	T	T
0.1247645130801920	0.6256008393336573	0.1659925437666850	T	T	T
0.6250212698701451	0.6256130693099872	0.1658701642660849	T	T	T
0.1246949613634236	0.8749336500793601	0.1714893335249195	T	T	T
0.6250502654833247	0.8749936697207269	0.1714386981494267	T	T	T
0.3747033261233801	0.8749739392997232	0.1726481910738088	T	T	T
0.8747668469351534	0.8750799320464001	0.1728854287431579	T	T	T
0.0015542891158885	0.1247365180422829	0.2268375784685072	T	T	T
0.5041554303480902	0.1268630162824951	0.2292484917577662	T	T	T
0.2517413688421526	0.1248703043318887	0.2262077681903820	T	T	T
0.7514896482859547	0.1246411493214426	0.2254012169210281	T	T	T
0.4975859991778830	0.3747747609903402	0.2366907104311190	T	T	T
0.9985512982660905	0.3748172287820064	0.2374171480295534	T	T	T
0.2503478427405019	0.3749849227896767	0.2373799784427237	T	T	T
0.7500509518018946	0.3748035108691424	0.2371988049784974	T	T	T
0.4996763399963082	0.6257436692544476	0.2261067487144352	T	T	T
0.9997231745792213	0.6249085785096581	0.2267280359264812	T	T	T
0.2497434474864166	0.6249189562903380	0.2267639952156497	T	T	T
0.7498193295672066	0.6251128293285209	0.2268036902875388	T	T	T
0.0007110797587814	0.8751478269829229	0.2374091955075847	T	T	T
0.5006779589019926	0.8754410782590724	0.2367561517272357	T	T	T
0.2486726589294696	0.8749057693282548	0.2371371673344777	T	T	T
0.7487895218236607	0.8757901284978544	0.2374189174534941	T	T	T
0.2410571901081148	0.0055294464883075	0.2960638814404302	T	T	T
0.7398987341651263	0.0069374291063237	0.2964193477387691	T	T	T
0.0076110672885792	0.0056794974221299	0.2967206317285275	T	T	T
0.5088582078249925	0.0054452210642414	0.2965026948871578	T	T	T
0.4954315029618983	0.2462407042599012	0.2995987838850835	T	T	T
0.9911589466101186	0.2442761311360148	0.2966620689897705	T	T	T
0.2569656326094142	0.2439011804498968	0.2958752239579188	T	T	T
0.7561487290199124	0.2416612744271145	0.2928939627284671	T	T	T
0.4910095606252931	0.5063313777000789	0.2954782123690463	T	T	T
0.9913688436211421	0.5055263930086903	0.2964775807960564	T	T	T
0.2578655847728096	0.5056068881658230	0.2964895910283946	T	T	T
0.7575503703857153	0.5054986084561680	0.2965540999610540	T	T	T
0.0077365938220974	0.7443235837146785	0.2963714265095612	T	T	T
0.5076567428492776	0.7448113091855021	0.2961273972443648	T	T	T
0.2414981191738563	0.7443793924996968	0.2964373038038731	T	T	T
0.7415432718080824	0.7448323894260623	0.2963910180273792	T	T	T
0.1247544461547204	0.0403986926316616	0.3651373127102342	T	T	T

0.6227753707137319	0.0338435258710418	0.3687767194251692	T	T	T
0.3746842974166370	0.0605671628750996	0.3295860508605173	T	T	T
0.8739176398726722	0.0627237822137034	0.3301791105270878	T	T	T
0.1239876114721453	0.1873727589913742	0.3311241786346257	T	T	T
0.6347786813011439	0.1907092627878210	0.3498500620065837	T	T	T
0.3741815151297984	0.2062714832076050	0.3625131538595716	T	T	T
0.8724816453153669	0.2094858039947970	0.3629659125229665	T	T	T
0.3749734444460723	0.5405470030876086	0.3650335342892457	T	T	T
0.8745009433776619	0.5406656595937389	0.3651362224524008	T	T	T
0.1245822478683961	0.5621335578005385	0.3308888832155660	T	T	T
0.6242998904703382	0.5631451992402434	0.3304312236229028	T	T	T
0.3746686679217897	0.6878148942105728	0.3308462659682486	T	T	T
0.8745115525780019	0.6878325717269222	0.3309392274751912	T	T	T
0.1245973434691777	0.7091397639446347	0.3649660849002218	T	T	T
0.6244497834737347	0.7100553808612734	0.3649436757482379	T	T	T
0.0000000000000000	0.1711556604610038	0.0044115607758073	F	F	F
0.5000000000000000	0.1711556604610038	0.0044115607758073	F	F	F
0.0000000000000000	0.3288443714619048	0.0044115607758073	F	F	F
0.5000000000000000	0.3288443714619048	0.0044115607758073	F	F	F
0.0000000000000000	0.4211558299644409	0.0044115607758073	F	F	F
0.5000000000000000	0.4211558299644409	0.0044115607758073	F	F	F
0.0000000000000000	0.0788442019584679	0.0044115607758073	F	F	F
0.5000000000000000	0.0788442019584679	0.0044115607758073	F	F	F
0.2500001695034015	0.0788442019584679	0.0044115607758073	F	F	F
0.7500001695034015	0.0788442019584679	0.0044115607758073	F	F	F
0.2500001695034015	0.1711556604610038	0.0044115607758073	F	F	F
0.7500001695034015	0.1711556604610038	0.0044115607758073	F	F	F
0.2500001695034015	0.3288443714619048	0.0044115607758073	F	F	F
0.7500001695034015	0.3288443714619048	0.0044115607758073	F	F	F
0.2500001695034015	0.4211558299644409	0.0044115607758073	F	F	F
0.7500001695034015	0.4211558299644409	0.0044115607758073	F	F	F
0.0000000000000000	0.6711556923839126	0.0044115607758073	F	F	F
0.5000000000000000	0.6711556923839126	0.0044115607758073	F	F	F
0.0000000000000000	0.8288444033848066	0.0044115607758073	F	F	F
0.5000000000000000	0.8288444033848066	0.0044115607758073	F	F	F
0.0000000000000000	0.9211558618873497	0.0044115607758073	F	F	F
0.5000000000000000	0.9211558618873497	0.0044115607758073	F	F	F
0.0000000000000000	0.5788442338813695	0.0044115607758073	F	F	F
0.5000000000000000	0.5788442338813695	0.0044115607758073	F	F	F
0.2500001695034015	0.5788442338813695	0.0044115607758073	F	F	F
0.7500001695034015	0.5788442338813695	0.0044115607758073	F	F	F
0.2500001695034015	0.6711556923839126	0.0044115607758073	F	F	F
0.7500001695034015	0.6711556923839126	0.0044115607758073	F	F	F
0.2500001695034015	0.8288444033848066	0.0044115607758073	F	F	F
0.7500001695034015	0.8288444033848066	0.0044115607758073	F	F	F
0.2500001695034015	0.9211558618873497	0.0044115607758073	F	F	F
0.7500001695034015	0.9211558618873497	0.0044115607758073	F	F	F
0.5894972742763988	0.2322466987419627	0.4592040468610948	T	T	T
0.5039079249689943	0.3304980044684103	0.3931892760346294	T	T	T
0.6867661009132336	0.2925157077003054	0.4351053766983978	T	T	T
0.6031261121227829	0.3672971396270091	0.3532450919857845	T	T	T
0.6250723905513190	0.2625335106788894	0.4210251927052976	T	T	T
0.5702689169320201	0.3142463870055157	0.3779050726167186	T	T	T

Ethylene sublayer mode: E(PBE-D3) = -659.94526 eV, E(HSE06-D3) = -763.02194 eV

1.000000000000000

15.3244190216000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 15.3244190216000007 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.6720008849999992

Si H C

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Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0438344616013850	F	F	F
0.5000000000000000	0.0000000000000000	0.0438344616013850	F	F	F
0.0000000000000000	0.2500001695033731	0.0438344616013850	F	F	F
0.5000000000000000	0.2500001695033731	0.0438344616013850	F	F	F
0.2500001695034015	0.0000000000000000	0.0438344616013850	F	F	F
0.7500001695034015	0.0000000000000000	0.0438344616013850	F	F	F
0.0000000000000000	0.5000000319229088	0.0438344616013850	F	F	F
0.5000000000000000	0.5000000319229088	0.0438344616013850	F	F	F
0.2500001695034015	0.2500001695033731	0.0438344616013850	F	F	F
0.7500001695034015	0.2500001695033731	0.0438344616013850	F	F	F
0.0000000000000000	0.7500002014262819	0.0438344616013850	F	F	F
0.5000000000000000	0.7500002014262819	0.0438344616013850	F	F	F
0.2500001695034015	0.5000000319229088	0.0438344616013850	F	F	F
0.7500001695034015	0.5000000319229088	0.0438344616013850	F	F	F
0.2500001695034015	0.7500002014262819	0.0438344616013850	F	F	F
0.7500001695034015	0.7500002014262819	0.0438344616013850	F	F	F
0.1249999139362856	0.0000000000000000	0.1063344564968744	F	F	F
0.6249999139362927	0.0000000000000000	0.1063344564968744	F	F	F
0.1249999139362856	0.2500001695033731	0.1063344564968744	F	F	F
0.6249999139362927	0.2500001695033731	0.1063344564968744	F	F	F
0.3750000834396943	0.0000000000000000	0.1063344564968744	F	F	F
0.8750000834396942	0.0000000000000000	0.1063344564968744	F	F	F
0.1249999139362856	0.5000000319229088	0.1063344564968744	F	F	F
0.6249999139362927	0.5000000319229088	0.1063344564968744	F	F	F
0.3750000834396943	0.2500001695033731	0.1063344564968744	F	F	F
0.8750000834396942	0.2500001695033731	0.1063344564968744	F	F	F
0.1249999139362856	0.7500002014262819	0.1063344564968744	F	F	F
0.6249999139362927	0.7500002014262819	0.1063344564968744	F	F	F
0.3750000834396943	0.5000000319229088	0.1063344564968744	F	F	F
0.8750000834396942	0.5000000319229088	0.1063344564968744	F	F	F
0.3750000834396943	0.7500002014262819	0.1063344564968744	F	F	F
0.8750000834396942	0.7500002014262819	0.1063344564968744	F	F	F
0.1266123537315544	0.1242894396801080	0.1657442365324046	T	T	T
0.6252972549083148	0.1250654171662662	0.1666677822816232	T	T	T
0.3821917233921854	0.1266841651677858	0.1688709671352213	T	T	T
0.8778891720085057	0.1249978295030671	0.1655943954012523	T	T	T
0.3701249014225846	0.3758305429111863	0.1693643500709217	T	T	T
0.8720945243675250	0.3743245081035910	0.1722909198498551	T	T	T
0.1224656082794222	0.3749153569692494	0.1728774615850621	T	T	T
0.6226166152998424	0.3748790212176853	0.1728301872555904	T	T	T
0.3745822769550101	0.6245952629655617	0.1657691897578946	T	T	T
0.8748994592868730	0.6241923808959979	0.1659780201814916	T	T	T
0.1248132919475203	0.6255423460966199	0.1659912209108088	T	T	T
0.6251878150403644	0.6256468277437987	0.1658241331121500	T	T	T
0.1260775324446069	0.8747552318796201	0.1713167878875373	T	T	T
0.6256852894886055	0.8747754861087792	0.1712354423327258	T	T	T
0.3763039776319874	0.8752682560858686	0.1729367580591672	T	T	T
0.8770803441599490	0.8742190164592162	0.1718278181252864	T	T	T
0.0022324456217484	0.1236630827225593	0.2274316940289820	T	T	T
0.5071956236632124	0.1333828163382193	0.2351488359510898	T	T	T

0.2528144938574158	0.1242507449301615	0.2249523746465998	T	T	T
0.7524355047002689	0.1211845193140483	0.2238389565478325	T	T	T
0.4923019806727926	0.3793622711263541	0.2331699973569475	T	T	T
0.9963624446218771	0.3736103024522140	0.2380246748920258	T	T	T
0.2480584157400258	0.3755866945134420	0.2368173238018259	T	T	T
0.7472072928780433	0.3713930927588231	0.2389293820975111	T	T	T
0.4998238126577558	0.6283229254917679	0.2260007783744146	T	T	T
0.9998082268787885	0.6239049115133739	0.2267897450975970	T	T	T
0.2498170707627273	0.6250290498252075	0.2266519005094657	T	T	T
0.7499828735089680	0.6225607666266267	0.2267240852902616	T	T	T
0.0023600312892051	0.8736760010629976	0.2371586981012242	T	T	T
0.5025052587343466	0.8781472234714724	0.2380485518387931	T	T	T
0.2501533205880423	0.8747389695060043	0.2368931427598594	T	T	T
0.7516327327178363	0.8706964174658487	0.2347484232140714	T	T	T
0.2457302880084035	0.0058797775252469	0.2948260563377074	T	T	T
0.7483075522003131	0.0003914974269834	0.2918051361921297	T	T	T
0.0128100564716839	0.0031357494258918	0.2971952360998654	T	T	T
0.5155227588637773	0.0076772497079138	0.2997597958594538	T	T	T
0.4858804884293887	0.2598891081064186	0.3012766134565065	T	T	T
0.9871818302116590	0.2430174128334725	0.2982496172752252	T	T	T
0.2511688380869534	0.2432035124533494	0.2933365608139644	T	T	T
0.7546436571534344	0.2351094589359495	0.2939466225274921	T	T	T
0.4892559841114563	0.5082461783594836	0.2943088836825868	T	T	T
0.9904281547038990	0.5046219803436156	0.2969584142851325	T	T	T
0.2570229840084301	0.5058054758725755	0.2962207665925096	T	T	T
0.7560575587838488	0.5034164450728169	0.2969365205089767	T	T	T
0.0084746474612885	0.7432058936943383	0.2965990517434316	T	T	T
0.5085350148670709	0.7466894703127007	0.2966382196215124	T	T	T
0.2421622446096865	0.7444254934240675	0.2961862802731054	T	T	T
0.7423382878443154	0.7423534316184747	0.2958429589969359	T	T	T
0.1295118830746683	0.0388026280927791	0.3653589014086818	T	T	T
0.6382830611300969	0.0150476590713413	0.3687191334661851	T	T	T
0.3788533988820837	0.0621820762867923	0.3299438104072813	T	T	T
0.8793262339113304	0.0589726476276203	0.3295293906794378	T	T	T
0.1199362298297804	0.1855111627666763	0.3305266389000920	T	T	T
0.6492313497538177	0.1663579667905606	0.3566673486114105	T	T	T
0.3668061903485492	0.2075441472365611	0.3605628766123466	T	T	T
0.8707503537084370	0.2046345400110611	0.3663734200371271	T	T	T
0.3743036026699201	0.5411308330392720	0.3647666955851140	T	T	T
0.8733934176327907	0.5394807068717077	0.3653029848733259	T	T	T
0.1237731282241953	0.5618280964343957	0.3309152816927552	T	T	T
0.6228837746762946	0.5623369210591761	0.3300163258746343	T	T	T
0.3754315858055020	0.6885096561147906	0.3307048116710500	T	T	T
0.8751666914519362	0.6865056085784765	0.3309741640086308	T	T	T
0.1254348901886498	0.7088475374610324	0.3650626424971848	T	T	T
0.6251688307159612	0.7093894947241172	0.3648662718653766	T	T	T
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0.2500001695034015	0.9211558618873497	0.0044115607758073	F	F	F
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0.5424261024048758	0.2108266970304702	0.4372244671992777	T	T	T
0.5119510458400307	0.3564767683687484	0.3872080154812584	T	T	T
0.6404374598097669	0.2729423544303159	0.4455409140777058	T	T	T
0.6112422796182877	0.3492926904909387	0.3448492174954626	T	T	T
0.5950097548742039	0.2441688373188841	0.4118015060296786	T	T	T
0.5584595690848200	0.3102502599780887	0.3656655327059736	T	T	T