

Supporting Information

Contents

1. Conformational Analysis of Stable States of THF on Si(001)	2
1.1. Intermediate	2
1.2. Final State of Reaction A	3
1.3. Final State of Reaction B	4
1.4. Final State of Reaction C	6
2. Reactions from the THF/Si(001) Datively Bonded Intermediate (DB).....	7
2.1. DB To Final State A	7
2.2. DB To Final State B.....	8
2.3. DB To Final State C.....	9
3. The σ^* (C-O) Orbital in the Intermediate	13
4. Accuracy of Computed Energy Differences	14
5. Diethylether on Si(001).....	15
6. The Dative Bond in the Transition State Structure.....	18
7. References.....	18
8. Cartesian Coordinates and Total Energies.....	19
8.1. THF Molecule.....	19
8.2. Slab Configurations	19
8.3. Intermediate Configurations	28
8.4. Final State A Configurations	49
8.5. Final State B Configurations.....	57
8.6. Final State C Configurations.....	100
8.7. Transition States of Reaction A	107
8.8. Transition States of Reaction B	111
8.9. Transition States of Reaction C	116
8.10. Diethylether on Si(001).....	122

1. Conformational Analysis of Stable States of THF on Si(001)

Since for each adsorption state, at least two different conformations were found, we optimized every stable conformation and the transition states (TS) between them in order to be able to determine which conformation is the most stable and if transitions between them are possible at a given temperature. All barriers for conformational change were found to be lower than 50 kJ mol^{-1} and since the lowest reaction barrier was determined to be 53 kJ mol^{-1} , we assumed that in any temperature regime where the reaction takes place at an experimental time scale, the minimum conformation of each state can be expected.

An abbreviation scheme is introduced at this point for brevity in the SI. The dative bond (DB) intermediate structure is labeled with the letter *I*, while the products of the nucleophilic substitution reaction via surface atoms **A**, **B** and **C** are labeled with *A*, *B* and *C*, respectively. Since the conformations often resembled the chair, boat and twist structures of cyclohexane, a lowercase *c*, *b* or *t* is introduced. As an example, *Ib* denotes the intermediate in boat conformation, while *Ac* denotes the product of reaction A in chair conformation. All energies in the SI are calculated at PBE-D3/PAW(400 eV) if not stated otherwise.

1.1. Intermediate

Two conformations were found for the intermediate, *Ib* and *Ic* (Figure S1), of which the *Ib* structure is slightly more stable by 2 kJ mol^{-1} . There are three different ways of changing the conformation (Figure S1(b,c)): Ring inversion (*invert*), tilting of the molecule over the Si-Si dimer bond (*tilt*) and rotation around the O-Si axis (*rotate*). While the rotation has the highest energy barrier at 18 kJ mol^{-1} , the other two are very similar with the inversion having the lowest one (8 kJ mol^{-1}). This is in line with the finding for gas phase ring inversion of THF known to occur via a pseudorotation motion with energy differences and barriers below 1 kJ mol^{-1} .^[1]

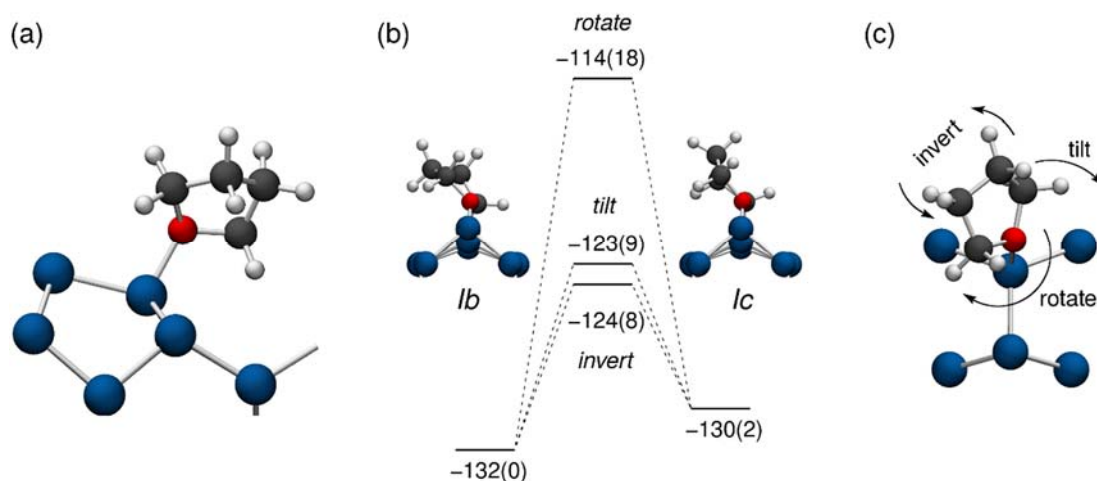


Figure S1 (a) Side view of the *lb* conformation. (b) Energy diagram for the three different types of conformational change. (c) Depiction of the three different types of motion. Bonding energies between surface and molecule given in kJ mol⁻¹, relative energies (in parentheses) given with respect to the lowest energy conformation.

1.2. Final State of Reaction A

The product of reaction A features three different conformations (Figure S2), where *Ac* is the most stable one with a bonding energy of -309 kJ mol⁻¹.

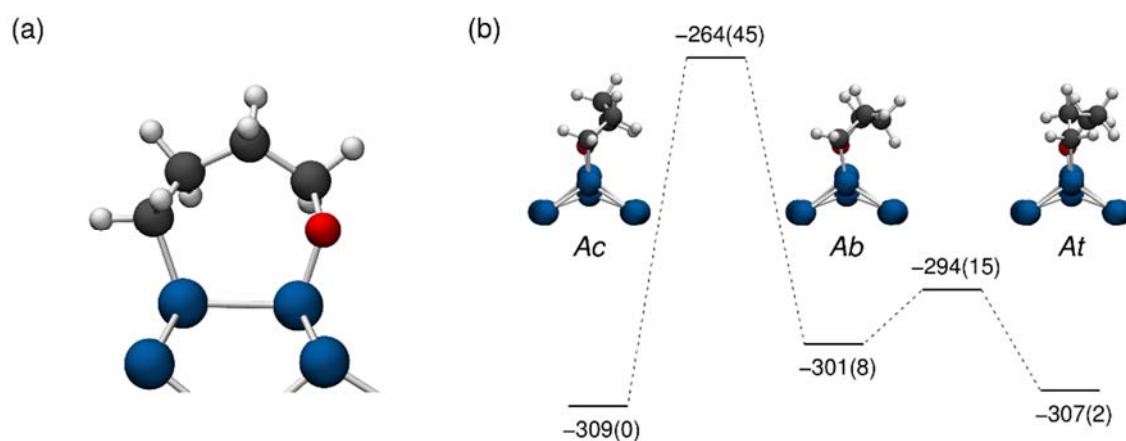


Figure S2 (a) Side view of the *Ac* conformation. (b) Energy diagram for conformational change of A. Bonding energies between surface and molecule given in kJ mol⁻¹, relative energies (in parentheses) given with respect to the lowest energy conformation.

1.3. Final State of Reaction B

In this case, eight different conformations were found in total. Since the qualitative differentiation is far more complicated than in the other cases, the conformations are simply numbered *B1*, *B2*, etc. with *B1* set to the conformation of lowest energy (see Figure S3). Two other conformations, *B4* and *B6*, are close in energy to *B1* albeit with considerable barriers towards conversion. Furthermore, the low barrier of 1 kJ mol⁻¹ for conversion from *B5* to *B4* could only be an artifact of the computational method and in reality, *B5* might not be a minimum structure at all.

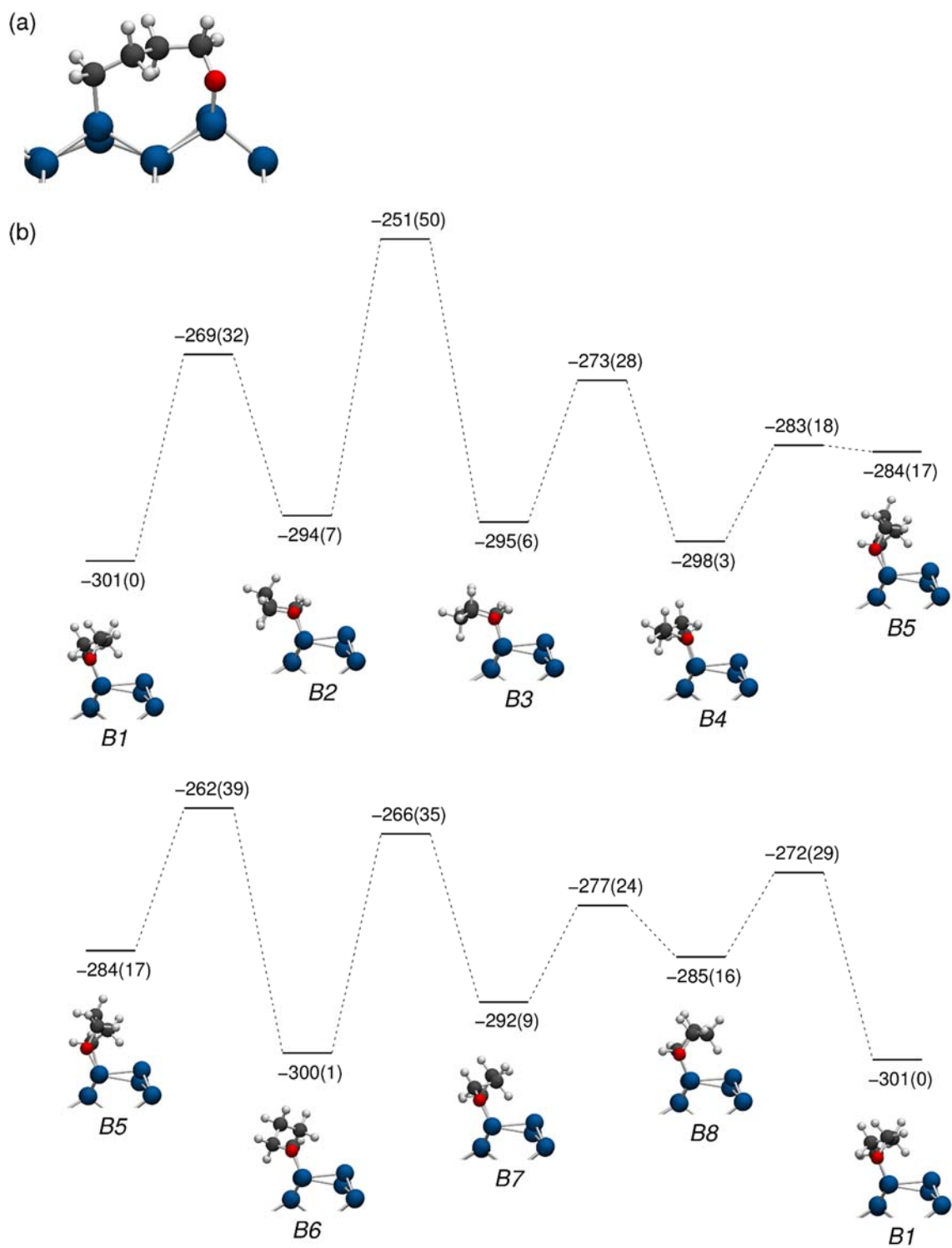


Figure S3 (a) Side view of the *B1* conformation. (b) Energy diagram for conformational change of *B*. Bonding energies between surface and molecule given in kJ mol^{-1} , relative energies (in parentheses) given with respect to the lowest energy conformation.

1.4. Final State of Reaction C

The product of reaction C only features a chair-type (*Cc*) and boat-type (*Cb*) conformation, of which the *Cb* structure is more stable by 5 kJ mol⁻¹.

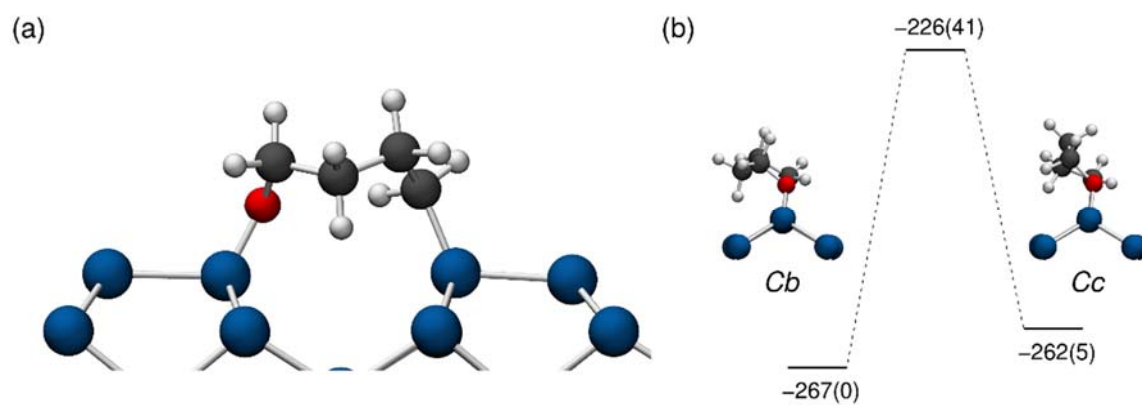


Figure S4 (a) Side view of the *Cb* conformation. (b) Energy diagram for conformational change of C. Bonding energies between surface and molecule given in kJ mol⁻¹, relative energies (in parentheses) given with respect to the lowest energy conformation.

2. Reactions from the THF/Si(001) Datively Bonded Intermediate (DB)

Since there are different transition states for each reaction, depending on the conformation of the initial and final state, all found reactions are listed here and the reader is given an explanation for the choice of the numbers that are given in the main text (Table 2).

2.1. DB To Final State A

There are two possible reactions from *I* to final state *A* (Figure S5): One from conformation *Ib* to product conformation *Ac* (a) and one from *Ic* to *At* (b). The lowest energy barrier is reached at the reaction *Ib*→*Ac*, which also leads to the lowest energy conformation product, so these are the numbers that are given in the main article.

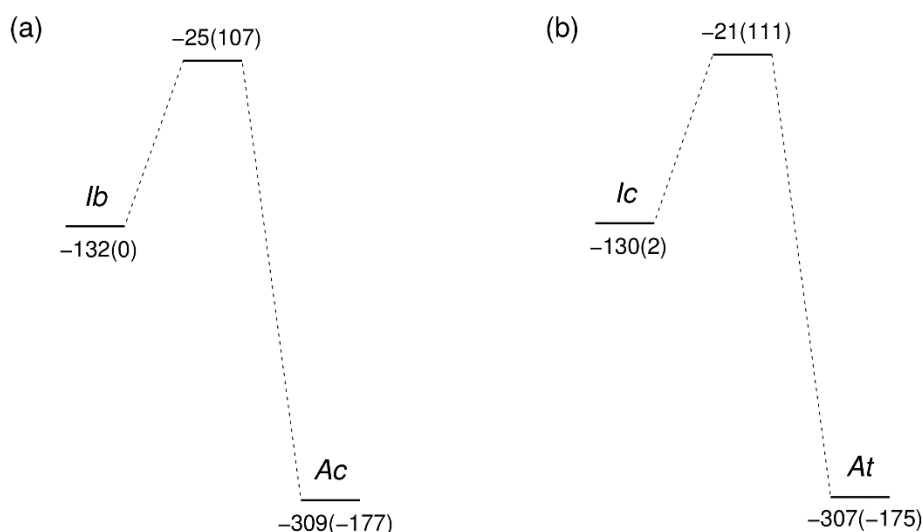


Figure S5 Reaction energy profiles for the attack of surface atom **A** in two different conformations of the intermediate, leading to two different conformations of product **A**. Bonding energies between surface and molecule given in kJ mol⁻¹, relative energies (in parentheses) given with respect to the energy of the minimum intermediate structure *Ib*. See also Figures S1 and S2.

2.2. DB To Final State B

Although there are eight conformations of final state B, only two are directly accessible from the intermediate (Figure S6). The lowest energy barrier is reached at the reaction $Ib \rightarrow B2$, from which the system can easily convert to the lowest energy conformation, $B1$, by overcoming an energy barrier of 25 kJ mol^{-1} (Figure S3). Hence, the energies given in Table 2 of the main article are the activation energy of Figure S6(a) and the reaction energy to the $B1$ state (Figure S3). Differences in Ib and Ic energies compared to the values given in Figures S1 and S5 can be attributed to the fact that these calculations had to be done in a 4×4 cell compared to the smaller 4×2 cell used for the other reactions, resulting in slightly different bonding energies for the same states.

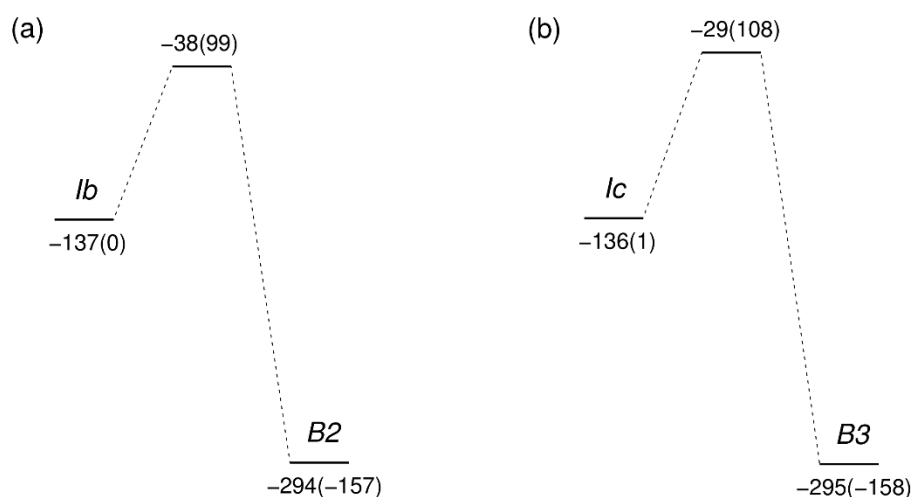


Figure S6 Reaction energy profiles for the attack of surface atom **B** in two different conformations of the intermediate, leading to two different conformations of product *B*. Bonding energies between surface and molecule given in kJ mol^{-1} , relative energies (in parentheses) given with respect to the energy of the minimum intermediate structure *Ib*. See also Figures S1 and S3.

2.3. DB To Final State C

Since this reaction involves two surface dimer rows whereas the previous two reactions occur on a single row (see main article, Scheme 3), the surface reconstruction becomes important. This is particularly evident in the reaction energy barriers (Figure S7), which drop from 75-76 kJ mol⁻¹ for a 4×2 reconstruction to 53-56 kJ mol⁻¹ for a 2×2 reconstruction. This reconstruction is only 2 kJ mol⁻¹ higher in energy than 4×2 (Figure S8) and when the activation energy of 30 kJ mol⁻¹ can be overcome, a significant percentage of the surface will be present as 2×2. The presence of a THF molecule in the intermediate structure has only minor effects on the energy barrier for flipping the dimers on the opposing row (Figure S8(b)), so it can be expected that most of the reactions will take place with the dimer flipping as an intermediate step.

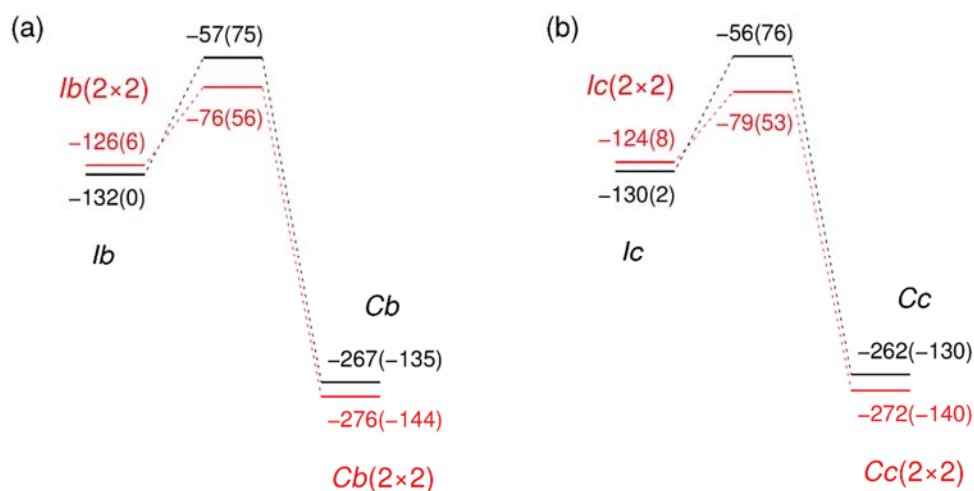


Figure S7 Reaction energy profiles for the attack of surface atom C in two different conformations of the intermediate and also two different kinds of surface reconstructions (4×2: black, 2×2: red). Bonding energies between surface and molecule given in kJ mol⁻¹, relative energies (in parentheses) given with respect to the energy of the minimum intermediate structure *lb*. See also Figures S1, S4 and S8.

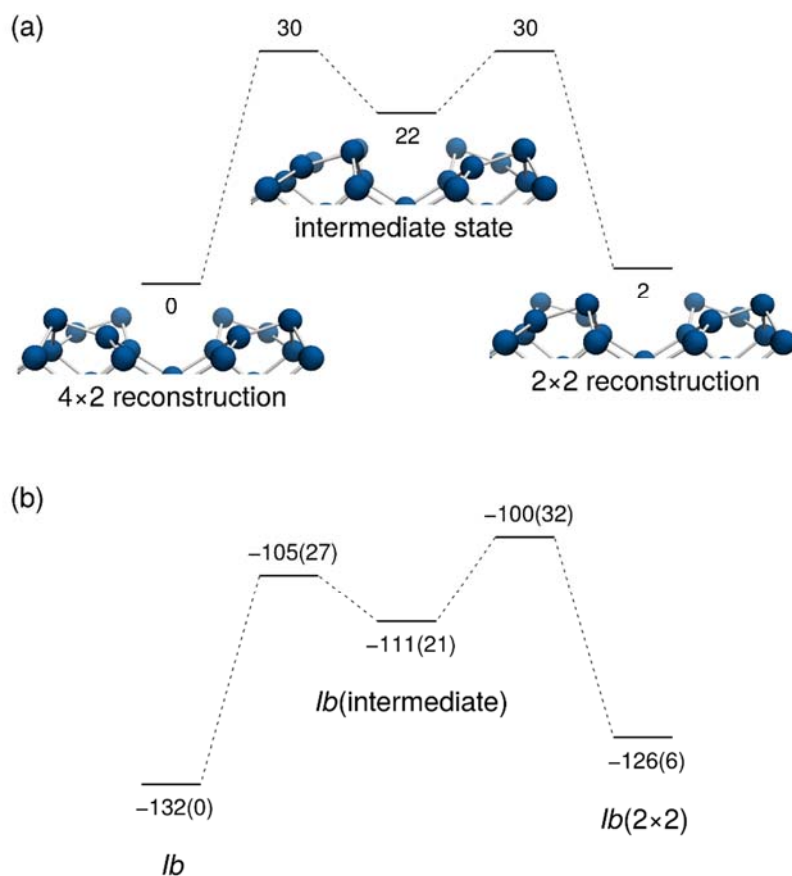


Figure S8 (a) Energy diagram for the change of the surface slab from 4×2 to 2×2 reconstruction. (b) Energy diagram for the same change if a THF molecule is present in the intermediate *lb* structure and the reconstruction change is occurring on the opposing dimer row. Bonding energies in (b) between surface and molecule given in kJ mol^{-1} , relative energies (in parentheses) given with respect to the energy of the minimum intermediate structure *lb*.

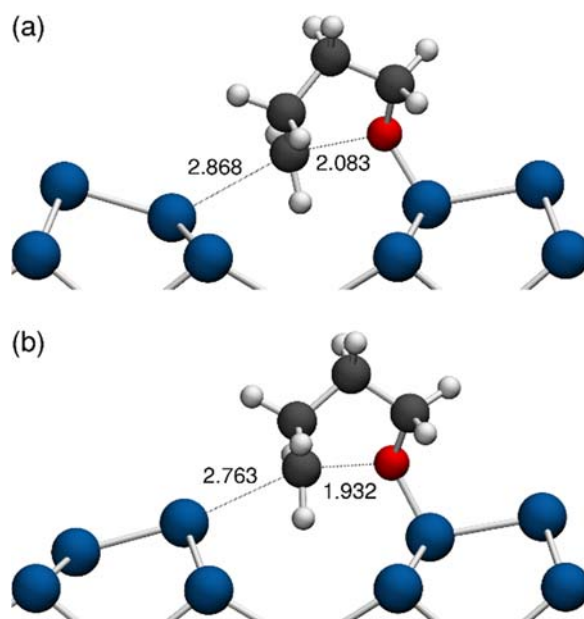


Figure S9 Comparison of the C-Si and C-O bond lengths at the transition state of the $Ic \rightarrow Cc$ reaction between (a) 4×2 and (b) 2×2 surface reconstruction.

The reason for the lowered energy barrier is exemplified by the transition state bond lengths of the C-Si and C-O bond (Figure S9): Due to the increased distance of the opposing Si atom, the C-O bond has to elongate significantly more (2.083 Å) than in the 2×2 reconstructed cell (1.932 Å) in order to reach the transition state. The reaction in the cell with 4×2 reconstruction can therefore be interpreted as the reaction in the 2×2 reconstructed cell plus an additional dimer flipping motion (Figure S8). This is underlined by the difference in activation energies between the two reconstructions, 19-23 kJ mol⁻¹, which is close to the energy needed to flip the opposing dimer, 30 kJ mol⁻¹.

The total reaction from the minimum intermediate structure *Ib* to the minimum structure of state C, *Cb*(2×2), therefore occurs in four steps (Figure S10): First, the surface reconstruction changes from 4×2 to 2×2 , in the second step, the intermediate changes to the chair conformation *Ic*, in the third step, the actual reaction takes place and in the fourth and final step, the product changes its conformation to the minimum. For this minimum energy reaction pathway, the numbers were given in the main article in Table 2.

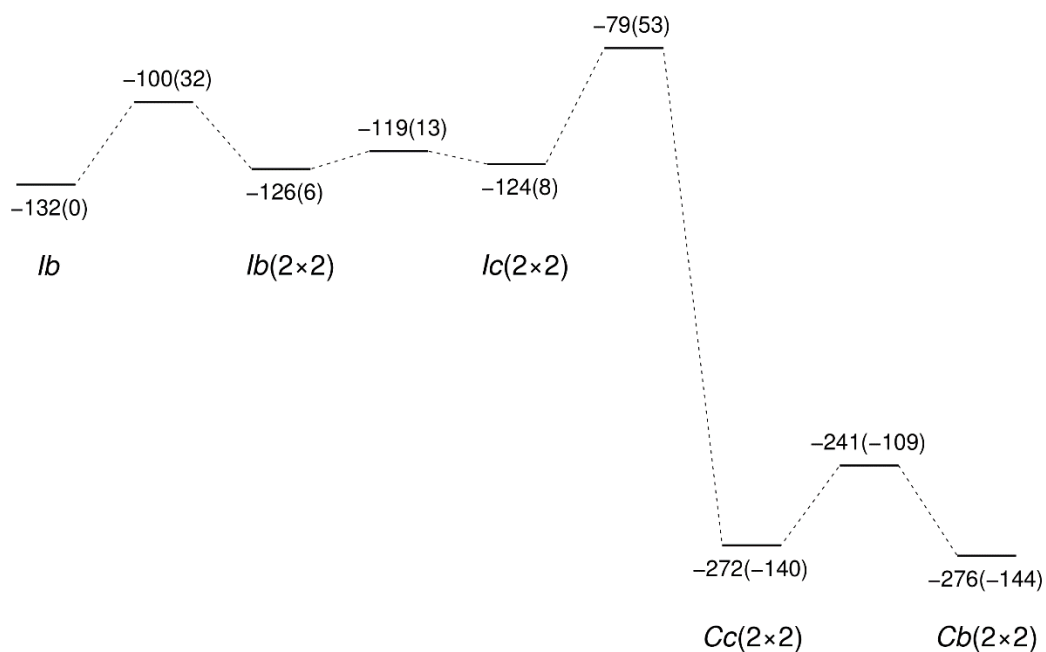


Figure S10 The full reaction path leading from the lowest energy intermediate structure (*lb*) to the lowest energy product structure (*Cb*(2×2)), including surface reconstruction change (step 1), conformation change (step 2), the actual reaction (step 3) and product conformation change (step 4). Bonding energies between surface and molecule given in kJ mol⁻¹, relative energies (in parentheses) given with respect to the energy of the minimum intermediate structure *lb*. See also Figures S1, S4, S7 and S8.

3. The $\sigma^*(\text{C-O})$ Orbital in the Intermediate

In order to rule out an electron-transfer promoted mechanism of the ether cleavage, selected crystal orbitals (COs) of the intermediate structure *Ib* are displayed in Figure S16. To promote such a reaction, electrons have to be transferred from the occupied orbitals at the Si_{up} atoms of the opposing row to any orbital weakening the C-O bond. The highest occupied Si_{up} orbital of this row is found in the HOCO-4 (Figure S11, top) at -4.25 eV, while the lowest unoccupied orbital with a $\sigma^*(\text{C-O})$ contribution is found in the LUCO+6 (Figure S11, bottom) at -2.50 eV. The energy difference between these two orbitals, i.e. the estimated energy required for an electron transfer, is 1.75 eV or 169 kJ mol^{-1} , which is much higher than the 53 kJ mol^{-1} of the thermally promoted nucleophilic substitution process (Figure S10). Therefore, we concluded that an electron-transfer promoted process is highly unlikely.

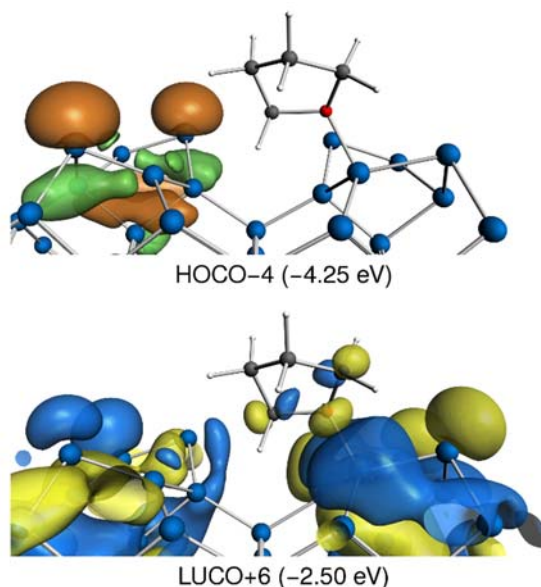


Figure S11 Two selected crystal orbitals of the *Ib* intermediate structure of THF on Si(001) shown at the Γ point in k space, calculated using PBE/TZ2P.

4. Accuracy of Computed Energy Differences

To check the accuracy of the GGA-type PBE functional, the reaction and activation energies from the dative bond structure (main article, Table 2) were also calculated using the HSE06-D3 range-separated hybrid functional. The results (Table S1) show that while the difference between reaction energies is higher and also activation energies are higher by 30-44%, the overall qualitative picture stays the same, i.e. the reaction via surface atom **C** is the most favored one and an anti-Bell-Evans-Polanyi behavior is observed.

Table S1 Reaction energies E_{react} and activation energies E_{a} for the nucleophilic attack of surface atom **A**, **B** or **C** (see main article, Scheme 3), calculated using both PBE-D3(PAW) and HSE06-D3(PAW).^[a]

Reaction via	$E_{\text{react}}(\text{PBE-D3})$	$E_{\text{a}}(\text{PBE-D3})$	$E_{\text{react}}(\text{HSE06-D3})$	$E_{\text{a}}(\text{HSE06-D3})$
A	-177	107	-188	144
B	-163	100	-168	130
C	-144	53	-134	76

[a] All energies given relative to *lb* in kJ mol^{-1} .

5. Diethylether on Si(001)

To rule out any influence of the ring strain in THF on the observed reactivity, selected calculations were performed with diethylether (**2**). Since experiments showed reaction via **C** to be the predominant feature as well,^[2] only this reaction was considered (Figure S12). Again, the influence of the surface reconstruction is of major importance (compare Section S2.3) and the lowest energy barrier is reached in a cell of 2×2 reconstruction. While the intermediate (*I*) is more weakly bound by 16 kJ mol⁻¹, the activation energy is slightly higher at 61 kJ mol⁻¹ compared to 53 kJ mol⁻¹ in THF. The final state, however has a very similar bonding energy, -274 kJ mol⁻¹, compared to -276 kJ mol⁻¹ in THF (see also Figures S7, S10).

pEDA results (Table S2) show a very similar picture in comparison to THF (main article, Table 1). With the exception of dispersion interaction, all pEDA terms are slightly smaller in the intermediate, leading to an interaction energy that is weaker by about 5 kJ mol⁻¹ for diethylether. The second contribution leading to a slightly weaker bonding energy in this system is the increased preparation energy of 33 kJ mol⁻¹ compared to 22 kJ mol⁻¹ in THF, which can be attributed to the need of rotation of the ethylene groups for an ideal exposure of the oxygen atom.

The results for the transition state structure yield similar results again with the exception that the interaction is slightly stronger than in THF, which is reflected in an interaction energy of -248 kJ mol⁻¹ (THF: -235 kJ mol⁻¹). This, however, is again overcompensated by a higher preparation energy of 192 kJ mol⁻¹ (THF: 157 kJ mol⁻¹) which leads to a higher energy barrier in general for diethylether.

The two most important NOCV deformation densities (Figure S13) show no qualitative and only minor numerical difference to the ones of THF (main article, Figure 1).

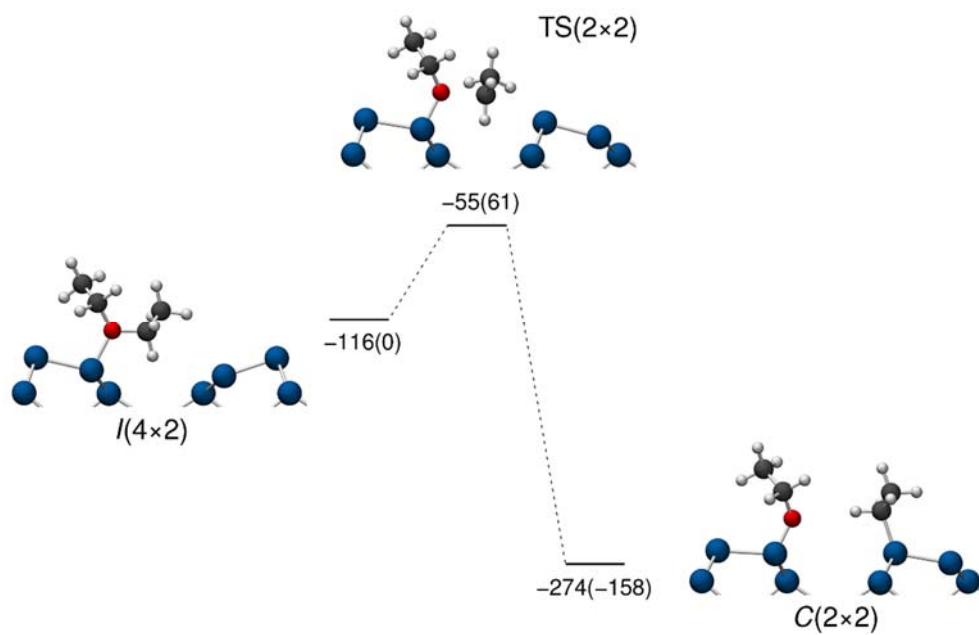


Figure S12 Reaction energy profile for the attack of surface atom **C** at a diethylether molecule on Si(001). The reaction also includes a change of the surface reconstruction from 4x2 to 2x2, which can be expected to occur similarly to the THF system (Figure S10) and is omitted in this diagram.

Table S1 Bonding analysis (pEDA) of the molecule-surface interaction between diethylether and Si(001) at the *I* and TS structures (See also Figure S12).^[a]

	<i>I</i> (4×2 surface)	TS(2×2 surface)
ΔE_{int}	-151	-248
$\Delta E_{\text{int}}(\text{disp})^{[b]}$	-54 (37%)	-58 (23%)
$\Delta E_{\text{int}}(\text{elec})^{[b]}$	-97 (63%)	-190 (77%)
ΔE_{Pauli}	645	1001
$\Delta E_{\text{elstat}}^{[c]}$	-409 (55%)	-611 (51%)
$\Delta E_{\text{orb}}^{[c]}$	-334 (45%)	-580 (49%)
$\Delta E_{\text{orb}}(\text{dative})^{[d]}$	-284 (85%)	-402 (69%)
$\Delta E_{\text{orb}}(\text{S}_N)^{[d]}$	0	-117 (20%)
ΔE_{prep}	33	192
$E_{\text{bond}}^{[e]}$	-118 (-116)	-56 (-55)

[a] All values in kJ mol^{-1} , calculated using PBE-D3/TZ2P. [b] Percentage values: Relative contributions of dispersion and electronic effects to the interaction energy ΔE_{int} . [c] Percentage values: Relative contributions between the attractive pEDA terms ΔE_{elstat} and ΔE_{orb} . [d] Percentage values: Relative contributions to the orbital interaction ΔE_{orb} . [e] PBE-D3/PAW values calculated in VASP given for comparison (in parentheses).

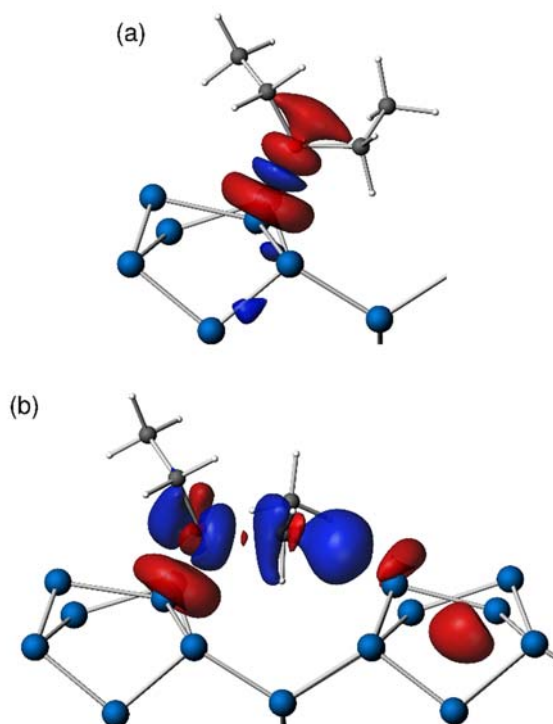


Figure S13 a) pEDA deformation densities $\Delta\rho_1$ at the *P*(4×2) structure of diethylether on Si(001). $\Delta E_1 = -202 \text{ kJ mol}^{-1}$, $v_1 = \pm 0.74 \text{ q}_e$. b) Deformation density $\Delta\rho_2$ at the TS(2×2) structure. $\Delta E_2 = -117 \text{ kJ mol}^{-1}$, $v_2 = \pm 0.72 \text{ q}_e$.

6. The Dative Bond in the Transition State Structure

The NOCV deformation densities, energies and eigenvalues at the transition state structures TS(DB→C) (THF) and TS(2×2) (diethylether) are given here to show that the dative bond between the oxygen atom and the surface is still the dominating contribution to the orbital energy. The difference of ΔE_1 (THF) to the value of -397 kJ mol^{-1} mentioned in the main article arises from additional minor contributions of σ and π symmetry that are not shown here.

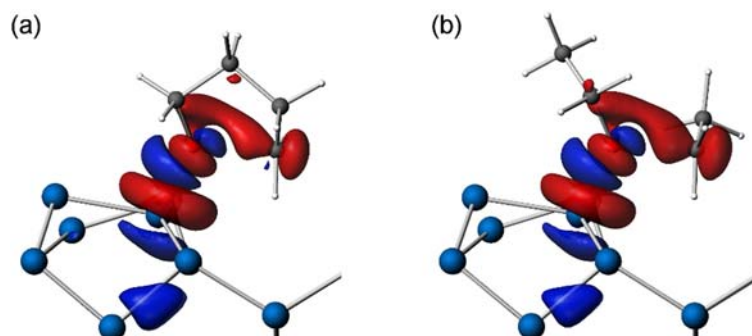


Figure S14 pEDA deformation densities $\Delta\rho_1$ of a) the TS(DB→C) structure of THF on ($\Delta E_1 = -263 \text{ kJ mol}^{-1}$, $v_1 = \pm 1.00 \text{ q}_e$) and b) the TS(2×2) structure of diethylether ($\Delta E_1 = -256 \text{ kJ mol}^{-1}$, $v_1 = \pm 0.96 \text{ q}_e$)

7. References

- [1] V. M. Rayón, J. A. Sordo, *J. Chem. Phys.* **2005**, *122*, 204303.
- [2] a) M. Reutzel, G. Mette, P. Stromberger, U. Koert, M. Dürr, U. Höfer, *J. Phys. Chem. C* **2015**, *119*, 6018.; b) M. Reutzel, M. Lipponer, M. Dürr, U. Höfer, *J. Phys. Chem. Lett.* **2015**, *6*, 3971.

8. Cartesian Coordinates and Total Energies

8.1. THF Molecule

Molecule(4x2), E(PBE-D3/PAW) = -72.258583 eV, E(HSE06-D3/PAW) = -84.482333 eV, E(PBE-D3/TZ2P) = -72.2240 eV

```
1.0000000000000000
 7.6621999740000000  0.0000000000000000  0.0000000000000000
-0.0000006700000000  15.3243999479999999  0.0000000000000000
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O C H
 1  4  8
```

Direct

```
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0.4477372206593573  0.2221834726808309  0.3734601807383408
0.4825422779647897  0.3008834549682003  0.4068656170906052
0.4748036469100440  0.3756269236357915  0.3688753000584534
0.3282276542868693  0.3455628149840293  0.3340775151864024
0.3890554454513212  0.1663869196302598  0.3931420542173253
0.5694262747279585  0.1998739391581523  0.3551523569148410
0.3779054111997033  0.3078154908406263  0.4347742172370820
0.6078830050947910  0.2966494474050164  0.4266274923408809
0.4483701865321350  0.4395963431694099  0.3857817290669660
0.5992038880571301  0.3800727211057968  0.3483955235409401
0.1998108561888148  0.3703032069325131  0.3465693462100117
0.3480809482674512  0.3658921645156351  0.2950320801232018
```

Molecule(4x4), E(PBE-D3) = -72.239426 eV, E(HSE06-D3) = -84.429373 eV

```
1.0000000000000000
 15.3243999479999999  0.0000000000000000  0.0000000000000000
-0.0000006700000000  15.3243999479999999  0.0000000000000000
-0.0000007340000000 -0.0000007340000000  26.7875003810000010
O C H
 1  4  8
```

Direct

```
0.1631470172187455  0.2514422802965737  0.3360388692265114
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0.2373093154678405  0.3757157777546197  0.3688770707442474
0.1641289547621470  0.3455616680584556  0.3340332809930538
0.1940139441820521  0.1666306739360828  0.3932483524527034
0.2845899797903025  0.1992459344544793  0.3553549879640346
0.1893734251819932  0.3078378409145855  0.4348733324036980
0.3042802888404489  0.2967141228978107  0.4264251334789905
0.2238128429373217  0.4395215310695346  0.3859119338772624
0.2994527129543408  0.3805607420158971  0.3484234473978778
0.0998531794629957  0.3700243147689384  0.3464820419120507
0.1741260503965827  0.3660246606880388  0.2950128948250205
```

8.2. Slab Configurations

Slab(4x2), E(PBE-D3/PAW) = -312.95109 eV, E(HSE06-D3/PAW) = -361.89223 eV, E(PBE-D3/TZ2P) = -300.5073 eV

```
1.0000000000000000
 7.6621999740000000  0.0000000000000000  0.0000000000000000
-0.0000006700000000  15.3243999479999999  0.0000000000000000
-0.0000007340000000 -0.0000007340000000  26.7875003810000010
```

Si H

48 16

Selective dynamics

Direct

0.0982437263469365	0.0000000011734684	0.0289689852776363	F	F	F
0.0982437493469206	0.2500002971734435	0.0289689852776363	F	F	F
0.5982443673469362	0.0000000011734684	0.0289689852776363	F	F	F
0.0982437713469366	0.5000005951734678	0.0289689852776363	F	F	F
0.5982443673469362	0.2500002971734435	0.0289689852776363	F	F	F
0.0982437933469313	0.7500008931734712	0.0289689852776363	F	F	F
0.5982444273469341	0.5000005951734678	0.0289689852776363	F	F	F
0.5982444273469341	0.7500008931734712	0.0289689852776363	F	F	F
0.3481889148011417	0.9995021537363799	0.0796618693222372	F	F	F
0.3482099635546240	0.2528227589216172	0.0806418874415160	F	F	F
0.8482098579642852	0.9984169186223468	0.0807822717142629	F	F	F
0.3481536313615905	0.4981877663151130	0.0807373416799068	F	F	F
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0.3481955688589979	0.7531385895576663	0.0800458566958044	F	F	F
0.8482115512265977	0.4972844060945221	0.0801440306302298	F	F	F
0.8483293512468748	0.7520680719318023	0.0806932257095598	F	F	F
0.3482452675029934	0.1251004238746446	0.1275471158914763	T	T	T
0.3483382692561421	0.3754777563813113	0.1351315574451415	T	T	T
0.8481866574948842	0.1261124092904691	0.1276989741549491	T	T	T
0.3482485564674023	0.6265254470756314	0.1273274117842609	T	T	T
0.8483152901988628	0.3748430460443980	0.1338326896986701	T	T	T
0.3482698751788421	0.8763846139589699	0.1333286907690024	T	T	T
0.8482770359495876	0.6239381942901114	0.1274051521164516	T	T	T
0.8482921676874977	0.8752391876038002	0.1349588305726151	T	T	T
0.0983802921106297	0.1254308811044516	0.1769281737236092	T	T	T
0.0963231249181274	0.3753458642540878	0.1869137072951158	T	T	T
0.5981179714456956	0.1254314130599190	0.1769633819152540	T	T	T
0.0983620555961361	0.6253072521821881	0.1767126937836923	T	T	T
0.6003802737832332	0.3753436644933943	0.1869234022744372	T	T	T
0.1006568651576241	0.8755272957196403	0.1866069156838874	T	T	T
0.5981594816023952	0.6253329080866930	0.1767027973981689	T	T	T
0.5959084615999249	0.8755327716686776	0.1866092098246192	T	T	T
0.1147251266053734	0.0066338954285029	0.2338425167468802	T	T	T
0.0821229036782827	0.2440767748380425	0.2339696942915065	T	T	T
0.5816357293730854	0.0066061311607045	0.2338898631069561	T	T	T
0.0819072996659449	0.5067687441501081	0.2338503437889156	T	T	T
0.6147893080048497	0.2441148283957964	0.2340180959535952	T	T	T
0.1149489843112100	0.7441925009320358	0.2336242216000530	T	T	T
0.6148989005879525	0.5067835886730351	0.2338427874251450	T	T	T
0.5815076513628684	0.7442008988550494	0.2336291752586209	T	T	T
0.3481402933053184	0.0409101981200769	0.2895982573257729	T	T	T
0.3484605941186931	0.1876718252506319	0.2618478024201706	T	T	T
0.8482065199803631	0.0628862349875234	0.2616912883257702	T	T	T
0.3483962464049266	0.5630585088520100	0.2616427001029201	T	T	T
0.8485023574565390	0.2095648413444039	0.2895926527396326	T	T	T
0.3482411225576066	0.7098451330013261	0.2893949235108441	T	T	T
0.8483863061764839	0.5415256138979073	0.2894564672926087	T	T	T
0.8482360307146520	0.6881407009668493	0.2614237677939841	T	T	T
0.0982437210000029	0.9179475529999266	0.0000000000000000	F	F	F
0.0982437879999907	0.0820524620000000	0.0000000162939813	F	F	F
0.0982437429999905	0.1679478439999969	0.0000000000000000	F	F	F
0.0982438099999853	0.3320527369999980	0.0000000162939813	F	F	F
0.5982443090000018	0.0820524470000024	0.0000000000000000	F	F	F

0.5982443089999313 0.9179475379999005 0.0000000162939813 F F F
0.0982437660000031 0.4179481569999628 0.0000000000000000 F F F
0.0982438329999979 0.5820530649999256 0.0000000162939813 F F F
0.5982443089999165 0.3320527079999994 0.0000000000000000 F F F
0.5982443090000018 0.1679478289999992 0.0000000162939813 F F F
0.0982437950000019 0.6679484840000008 0.0000000000000000 F F F
0.0982438469999920 0.8320534229999055 0.0000000162939813 F F F
0.5982443689999997 0.5820530060000032 0.0000000000000000 F F F
0.5982443690000008 0.4179481269999958 0.0000000162939813 F F F
0.5982443690000001 0.8320533629999289 0.0000000000000000 F F F
0.5982443689999155 0.6679484249999206 0.0000000162939813 F F F

TS Slab(4x2) Slab(intermediate), E = -312.64393 eV

1.0000000000000000
7.6621999740000000 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si H

48 16

Selective dynamics

Direct

0.0982437263469365 0.0000000011734684 0.0289689852776365 F F F
0.0982437493469206 0.2500002971734435 0.0289689852776365 F F F
0.5982443673469362 0.0000000011734684 0.0289689852776365 F F F
0.0982437713469366 0.5000005951734678 0.0289689852776365 F F F
0.5982443673469362 0.2500002971734435 0.0289689852776365 F F F
0.0982437933469313 0.7500008931734712 0.0289689852776365 F F F
0.5982444273469341 0.5000005951734678 0.0289689852776365 F F F
0.5982444273469341 0.7500008931734712 0.0289689852776365 F F F
0.3481889148011417 0.9995021537363799 0.0796618693222380 F F F
0.3482099635546240 0.2528227589216172 0.0806418874415167 F F F
0.8482098579642852 0.9984169186223468 0.0807822717142637 F F F
0.3481536313615905 0.4981877663151135 0.0807373416799076 F F F
0.8482139166746969 0.2521299693376946 0.0802085390540564 F F F
0.3481955688589979 0.7531385895576725 0.0800458566958052 F F F
0.8482115512265977 0.4972844060945221 0.0801440306302306 F F F
0.8483293512468748 0.7520680719318023 0.0806932257095606 F F F
0.3482405329430827 0.1251274304633818 0.1275406587638201 T T T
0.3482415541236394 0.3754329460674183 0.1352735289634206 T T T
0.8482374967567790 0.1260505712859223 0.1278420282201067 T T T
0.3482475209306790 0.6262321916570127 0.1282838190633502 T T T
0.8482485592103269 0.3747407674612334 0.1338562004893184 T T T
0.3482640388613976 0.8758944090689156 0.1334521426639664 T T T
0.8483162260931075 0.6245420651578086 0.1266225024222843 T T T
0.8482968986794930 0.8754369208833513 0.1344258194478700 T T T
0.0986666750133292 0.1253406836963083 0.1769583909869403 T T T
0.0955244771026381 0.3752184471448871 0.1870378254053903 T T T
0.5978138051516267 0.1253117127434494 0.1769646335943913 T T T
0.0957294895977383 0.6220655857173686 0.1767293443112003 T T T
0.6009831447296697 0.3752275791364961 0.1870268911223131 T T T
0.0991575051464944 0.8772471135873037 0.1863613303200887 T T T
0.6008384394981826 0.6220651881621435 0.1767020467115725 T T T
0.5973896074637378 0.8772309984229629 0.1863491792561389 T T T
0.1148473066049595 0.0072864207983131 0.2342824711943710 T T T
0.0824304958367420 0.2439585355469590 0.2339099203964094 T T T
0.5817427041635646 0.0072519761894319 0.2342887840131151 T T T

0.0809062896274570	0.5062505163182734	0.2342453371822336	T	T	T
0.6140468262241031	0.2439623191353928	0.2338920463987321	T	T	T
0.0973840626076512	0.7449875664148655	0.2326076989165895	T	T	T
0.6156752880404280	0.5062622832478915	0.2342263450538528	T	T	T
0.5992321873525905	0.7449694983907827	0.2325835798654723	T	T	T
0.3482820579634544	0.0406233129412551	0.2902810684144497	T	T	T
0.3482586078853507	0.1875444893217332	0.2619292327420242	T	T	T
0.8482835364033146	0.0634700107198317	0.2618198366278498	T	T	T
0.3483058871505121	0.5396147197248995	0.2724052974869536	T	T	T
0.8482133682165450	0.2099060414151895	0.2893735624119701	T	T	T
0.3483099198697995	0.6860305993933182	0.2665804392137713	T	T	T
0.8482762480674019	0.5312101217613233	0.2917431080332856	T	T	T
0.8483040759604625	0.6784621508164105	0.2644720745242810	T	T	T
0.0982437210000029	0.9179475529999266	0.0000000000000000	F	F	F
0.0982437879999907	0.0820524620000000	0.0000000162939813	F	F	F
0.0982437429999905	0.1679478439999969	0.0000000000000000	F	F	F
0.0982438099999853	0.3320527369999980	0.0000000162939813	F	F	F
0.5982443090000018	0.0820524470000024	0.0000000000000000	F	F	F
0.5982443089999313	0.9179475379999005	0.0000000162939813	F	F	F
0.0982437660000031	0.4179481569999628	0.0000000000000000	F	F	F
0.0982438329999979	0.5820530649999256	0.0000000162939813	F	F	F
0.5982443089999165	0.3320527079999994	0.0000000000000000	F	F	F
0.5982443090000018	0.1679478289999992	0.0000000162939813	F	F	F
0.0982437950000019	0.6679484840000008	0.0000000000000000	F	F	F
0.0982438469999920	0.8320534229999055	0.0000000162939813	F	F	F
0.5982443689999997	0.5820530060000032	0.0000000000000000	F	F	F
0.5982443690000008	0.4179481269999958	0.0000000162939813	F	F	F
0.5982443690000001	0.8320533629999289	0.0000000000000000	F	F	F
0.5982443689999161	0.6679484249999206	0.0000000162939813	F	F	F

Slab(intermediate), E = -312.71955 eV

1.0000000000000000		
7.6621999740000000	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000
-0.0000007340000000	-0.0000007340000000	26.7875003810000010

Si H

48 16

Selective dynamics

Direct

0.0982437263469365	0.0000000011734684	0.0289689852776365	F	F	F
0.0982437493469206	0.2500002971734435	0.0289689852776365	F	F	F
0.5982443673469362	0.0000000011734684	0.0289689852776365	F	F	F
0.0982437713469366	0.5000005951734678	0.0289689852776365	F	F	F
0.5982443673469362	0.2500002971734435	0.0289689852776365	F	F	F
0.0982437933469313	0.7500008931734712	0.0289689852776365	F	F	F
0.5982444273469341	0.5000005951734678	0.0289689852776365	F	F	F
0.5982444273469341	0.7500008931734712	0.0289689852776365	F	F	F
0.3481889148011417	0.9995021537363799	0.0796618693222378	F	F	F
0.3482099635546240	0.2528227589216172	0.0806418874415165	F	F	F
0.8482098579642852	0.9984169186223468	0.0807822717142635	F	F	F
0.3481536313615905	0.4981877663151135	0.0807373416799074	F	F	F
0.8482139166746969	0.2521299693376946	0.0802085390540562	F	F	F
0.3481955688589979	0.7531385895576709	0.0800458566958049	F	F	F
0.8482115512265977	0.4972844060945221	0.0801440306302304	F	F	F
0.8483293512468748	0.7520680719318023	0.0806932257095603	F	F	F
0.3482523910536106	0.1250554263610869	0.1274672018179608	T	T	T

0.3482298996032550	0.3750739347564855	0.1351702539355217	T	T	T
0.8482549606206610	0.1260530776418136	0.1278040391568668	T	T	T
0.3481757371874489	0.6262350740082087	0.1273765959639606	T	T	T
0.8482701818721006	0.3750182789882067	0.1343799924963752	T	T	T
0.3482555221131728	0.8757803692853080	0.1333326772712285	T	T	T
0.8482226470921028	0.6248069220144289	0.1273923216301426	T	T	T
0.8483014278972441	0.8752173976791502	0.1344811852246384	T	T	T
0.0987860170724903	0.1250394358409244	0.1769520400646945	T	T	T
0.0970962589496211	0.3758905006222303	0.1873281322410018	T	T	T
0.5977279684945552	0.1250331452516816	0.1769515206844922	T	T	T
0.0982224773411855	0.6202464167698867	0.1764472303351345	T	T	T
0.5994115786053813	0.3758994235986350	0.1873130087524075	T	T	T
0.0998239561206819	0.8763161789420122	0.1863266591359346	T	T	T
0.5981612640446513	0.6202519517008771	0.1764273948074705	T	T	T
0.5967401182739098	0.8763169882237105	0.1863118184917329	T	T	T
0.1150061798634977	0.0066678602255079	0.2341688578176577	T	T	T
0.0829509075138557	0.2439592325851231	0.2338592587558800	T	T	T
0.5816241082305795	0.0066630468789879	0.2341670548621601	T	T	T
0.0976526732609839	0.5067755237325831	0.2350745332384823	T	T	T
0.6135821466087337	0.2439694098815910	0.2338436556923544	T	T	T
0.0992855944887619	0.7438248328979419	0.2328020065704315	T	T	T
0.5988218029816502	0.5067852151961927	0.2350556981163019	T	T	T
0.5973405403300950	0.7438191302113308	0.2327814053804551	T	T	T
0.3483140344151157	0.0398024111147537	0.2902317481746312	T	T	T
0.3482864388966648	0.1869410667134321	0.2621082768199159	T	T	T
0.8483204624013160	0.0630865092782762	0.2617839622785962	T	T	T
0.3482638108381384	0.5288238236346271	0.2869994992334623	T	T	T
0.8482500291032267	0.2095881508744807	0.2891466495204867	T	T	T
0.3483298122232762	0.6733957953151387	0.2625319881486604	T	T	T
0.8482227523440744	0.5303958760003933	0.2871434861515112	T	T	T
0.8483104061285649	0.6748291956264784	0.2622333720189413	T	T	T
0.0982437210000029	0.9179475529999266	0.0000000000000000	F	F	F
0.0982437879999907	0.0820524620000000	0.0000000162939813	F	F	F
0.0982437429999905	0.1679478439999969	0.0000000000000000	F	F	F
0.0982438099999853	0.3320527369999980	0.0000000162939813	F	F	F
0.5982443090000018	0.0820524470000024	0.0000000000000000	F	F	F
0.5982443089999313	0.9179475379999005	0.0000000162939813	F	F	F
0.0982437660000031	0.4179481569999628	0.0000000000000000	F	F	F
0.0982438329999979	0.5820530649999256	0.0000000162939813	F	F	F
0.5982443089999165	0.3320527079999994	0.0000000000000000	F	F	F
0.5982443090000018	0.1679478289999992	0.0000000162939813	F	F	F
0.0982437950000019	0.6679484840000008	0.0000000000000000	F	F	F
0.0982438469999920	0.8320534229999055	0.0000000162939813	F	F	F
0.5982443689999997	0.5820530060000032	0.0000000000000000	F	F	F
0.5982443690000008	0.4179481269999958	0.0000000162939813	F	F	F
0.5982443690000001	0.8320533629999289	0.0000000000000000	F	F	F
0.5982443689999161	0.6679484249999206	0.0000000162939813	F	F	F

TS Slab(intermediate) Slab(2x2), E = -312.63744 eV

1.0000000000000000		
7.6621999740000000	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000
-0.0000007340000000	-0.0000007340000000	26.7875003810000010

Si H

48 16

Selective dynamics

Direct

0.0982437263469365 0.0000000011734684 0.0289689852776366 F F F
0.0982437493469206 0.2500002971734435 0.0289689852776366 F F F
0.5982443673469362 0.0000000011734684 0.0289689852776366 F F F
0.0982437713469366 0.5000005951734678 0.0289689852776366 F F F
0.5982443673469362 0.2500002971734435 0.0289689852776366 F F F
0.0982437933469313 0.7500008931734712 0.0289689852776366 F F F
0.5982444273469341 0.5000005951734678 0.0289689852776366 F F F
0.5982444273469341 0.7500008931734712 0.0289689852776366 F F F
0.3481889148011417 0.9995021537363799 0.0796618693222381 F F F
0.3482099635546240 0.2528227589216172 0.0806418874415169 F F F
0.8482098579642852 0.9984169186223468 0.0807822717142639 F F F
0.3481536313615905 0.4981877663151135 0.0807373416799077 F F F
0.8482139166746969 0.2521299693376946 0.0802085390540565 F F F
0.3481955688589979 0.7531385895576739 0.0800458566958053 F F F
0.8482115512265977 0.4972844060945221 0.0801440306302308 F F F
0.8483293512468748 0.7520680719318023 0.0806932257095607 F F F
0.3482292241775022 0.1251355818241631 0.1275695076798189 T T T
0.3482648578014200 0.3747806172112778 0.1346375320212317 T T T
0.8482255068209532 0.1260232906480301 0.1278294074502063 T T T
0.3482480696846827 0.6259505221195347 0.1266695127352054 T T T
0.8482777342536759 0.3753895367171213 0.1344896914417982 T T T
0.3482773031132844 0.8760230020477590 0.1332643985033324 T T T
0.8482569394580820 0.6247894806061790 0.1283329116604008 T T T
0.8483098329986959 0.8753609738141784 0.1345654047478006 T T T
0.0986254391313559 0.1253651494324449 0.1769520159308823 T T T
0.0988043441282653 0.3751508651139361 0.1870610021404265 T T T
0.5978348810712584 0.1253419554044088 0.1769556924169633 T T T
0.1007171743512317 0.6222381945771169 0.1768241924418489 T T T
0.5977464392576008 0.3751580881096366 0.1870559572264771 T T T
0.1003533061834857 0.8774399193802176 0.1863041997591171 T T T
0.5957989044484376 0.6222373906476800 0.1768216313092837 T T T
0.5962398081314688 0.8774199860347304 0.1862956369954972 T T T
0.1147576483080974 0.0073967969410905 0.2342706906532217 T T T
0.0832202401837641 0.2439146958362361 0.2339855863493953 T T T
0.5818413038982601 0.0073659534083923 0.2342723089768084 T T T
0.1147919878644280 0.5061264975674059 0.2342567134984792 T T T
0.6133371078627043 0.2439165164942323 0.2339753815853412 T T T
0.1012779117125567 0.7452557462984014 0.2325672108100112 T T T
0.5817349188798990 0.5061261457302987 0.2342568181205882 T T T
0.5953066322222348 0.7452512724282394 0.2325723677434510 T T T
0.3482956466148720 0.0400505748100441 0.2903161673369450 T T T
0.3482941530691957 0.1869038574219033 0.2620523844677091 T T T
0.8482934980676623 0.0637476550171973 0.2617701685712224 T T T
0.3482685397035091 0.5300132887460987 0.2916637798057586 T T T
0.8482573237607358 0.2102930933804148 0.2894063892590346 T T T
0.3482879880108695 0.6774897032411330 0.2648357444896783 T T T
0.8482603262221644 0.5412986999214292 0.2721872188379010 T T T
0.8482990119726835 0.6878782374814582 0.2661435447531798 T T T
0.0982437210000029 0.9179475529999266 0.0000000000000000 F F F
0.0982437879999907 0.0820524620000000 0.0000000162939813 F F F
0.0982437429999905 0.1679478439999969 0.0000000000000000 F F F
0.0982438099999853 0.3320527369999980 0.0000000162939813 F F F
0.5982443090000018 0.0820524470000024 0.0000000000000000 F F F
0.5982443089999313 0.9179475379999005 0.0000000162939813 F F F
0.0982437660000031 0.4179481569999628 0.0000000000000000 F F F
0.0982438329999979 0.5820530649999256 0.0000000162939813 F F F

0.5982443089999165 0.3320527079999994 0.0000000000000000 F F F
0.5982443090000018 0.1679478289999992 0.0000000162939813 F F F
0.0982437950000019 0.6679484840000008 0.0000000000000000 F F F
0.0982438469999920 0.8320534229999055 0.0000000162939813 F F F
0.5982443689999997 0.5820530060000032 0.0000000000000000 F F F
0.5982443690000008 0.4179481269999958 0.0000000162939813 F F F
0.5982443690000001 0.8320533629999289 0.0000000000000000 F F F
0.5982443689999161 0.6679484249999206 0.0000000162939813 F F F

Slab(2x2), E = -312.92831 eV

1.0000000000000000
7.6621999740000000 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si H

48 16

Selective dynamics

Direct

0.0982437263469365 0.0000000011734684 0.0289689852776364 F F F
0.0982437493469206 0.2500002971734435 0.0289689852776364 F F F
0.5982443673469362 0.0000000011734684 0.0289689852776364 F F F
0.0982437713469366 0.5000005951734678 0.0289689852776364 F F F
0.5982443673469362 0.2500002971734435 0.0289689852776364 F F F
0.0982437933469313 0.7500008931734712 0.0289689852776364 F F F
0.5982444273469341 0.5000005951734678 0.0289689852776364 F F F
0.5982444273469341 0.7500008931734712 0.0289689852776364 F F F
0.3481889148011417 0.9995021537363799 0.0796618693222376 F F F
0.3482099635546240 0.2528227589216172 0.0806418874415163 F F F
0.8482098579642852 0.9984169186223468 0.0807822717142633 F F F
0.3481536313615905 0.4981877663151135 0.0807373416799071 F F F
0.8482139166746969 0.2521299693376946 0.0802085390540559 F F F
0.3481955688589979 0.7531385895576690 0.0800458566958047 F F F
0.8482115512265977 0.4972844060945221 0.0801440306302302 F F F
0.8483293512468748 0.7520680719318023 0.0806932257095601 F F F
0.3482610512327142 0.1250829143035687 0.1275231269249318 T T T
0.3482954457946968 0.3748933135160734 0.1346485999611293 T T T
0.8482612281337502 0.1260993688243797 0.1276729270611678 T T T
0.3482036427409839 0.6253581320681496 0.1272956539378057 T T T
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0.3482374808745495 0.8757958057521774 0.1338275466631351 T T T
0.8482309894190743 0.6250935478867572 0.1273622144105588 T T T
0.8482791863306273 0.8758163653448678 0.1344628908579316 T T T
0.0983957758772580 0.1253370994180272 0.1769184279618493 T T T
0.0980193152285158 0.3752878698198909 0.1869491092628520 T T T
0.5981272295323423 0.1253335327259294 0.1769230253578880 T T T
0.0983039462298774 0.6252773293964708 0.1766731338321280 T T T
0.5985996031412886 0.3752858718585765 0.1869451745295790 T T T
0.0988453563400043 0.8754676551242737 0.1866413154021795 T T T
0.5981375346942499 0.6252738231596584 0.1766633122199461 T T T
0.5976780052686576 0.8754744481419046 0.1866286588845949 T T T
0.1138615740509787 0.0065774059522672 0.2339196348832528 T T T
0.0829223451779630 0.2439580400725771 0.2340356265966584 T T T
0.5827200654161495 0.0065757831885422 0.2339295668666158 T T T
0.1138141247785465 0.5067809604958399 0.2338910158465622 T T T
0.6137615489022338 0.2439620292118859 0.2340414964388869 T T T
0.0830574334595131 0.7440786497936207 0.2336799418925582 T T T

0.5829082746433751 0.5067828922225267 0.2338826014074499 T T T
0.6135189965606408 0.7440918554483303 0.2336640101420422 T T T
0.3482788245300967 0.0397240197354525 0.2896045083258232 T T T
0.3483498905227554 0.1866025497712949 0.2620124829581897 T T T
0.8483002151846282 0.0638014290476766 0.2618959452347274 T T T
0.3483663928774697 0.5398385570670602 0.2895655933678090 T T T
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0.3483118402436269 0.6866128598515028 0.2617619925706662 T T T
0.8483597969907837 0.5643214916971746 0.2618034799691711 T T T
0.8482695375911962 0.7112381264425091 0.2893170736475098 T T T
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0.0982437879999907 0.0820524620000000 0.0000000162939813 F F F
0.0982437429999905 0.1679478439999969 0.0000000000000000 F F F
0.0982438099999853 0.3320527369999980 0.0000000162939813 F F F
0.5982443090000018 0.0820524470000024 0.0000000000000000 F F F
0.5982443089999313 0.9179475379999005 0.0000000162939813 F F F
0.0982437660000031 0.4179481569999628 0.0000000000000000 F F F
0.0982438329999979 0.5820530649999256 0.0000000162939813 F F F
0.5982443089999165 0.3320527079999994 0.0000000000000000 F F F
0.5982443090000018 0.1679478289999992 0.0000000162939813 F F F
0.0982437950000019 0.6679484840000008 0.0000000000000000 F F F
0.0982438469999920 0.8320534229999055 0.0000000162939813 F F F
0.5982443689999997 0.5820530060000032 0.0000000000000000 F F F
0.5982443690000008 0.4179481269999958 0.0000000162939813 F F F
0.5982443690000001 0.8320533629999289 0.0000000000000000 F F F
0.5982443689999161 0.6679484249999206 0.0000000162939813 F F F

Slab(4x4), E(PBE-D3) = -627.20971 eV, E(HSE06-D3) = -725.27251 eV

1.0000000000000000
15.3243999479999999 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si H

96 32

Selective dynamics

Direct

0.0000000016986164 0.0000000016986164 0.0354635925893945 F F F
0.5000006559493571 0.0000000016986164 0.0354635925893945 F F F
0.0000000126289095 0.2500003288239867 0.0354635925893945 F F F
0.5000006668796502 0.2500003288239867 0.0354635925893945 F F F
0.2500003288239867 0.0000000016986164 0.0354635925893945 F F F
0.7500009830747274 0.0000000016986164 0.0354635925893945 F F F
0.0000000235592097 0.5000006559493571 0.0354635925893945 F F F
0.5000006778099504 0.5000006559493571 0.0354635925893945 F F F
0.2500003397542798 0.2500003288239867 0.0354635925893945 F F F
0.7500009940050276 0.2500003288239867 0.0354635925893945 F F F
0.0000000344895028 0.7500009830747274 0.0354635925893945 F F F
0.5000006887402435 0.7500009830747274 0.0354635925893945 F F F
0.2500003506845800 0.5000006559493571 0.0354635925893945 F F F
0.7500010049353207 0.5000006559493571 0.0354635925893945 F F F
0.2500003616148732 0.7500009830747274 0.0354635925893945 F F F
0.7500010158656139 0.7500009830747274 0.0354635925893945 F F F
0.1250001350555152 0.0000000041205368 0.0860282208949457 F F F
0.6250007893062559 0.0000000041205368 0.0860282208949457 F F F
0.1250001459858083 0.2500003312459071 0.0860282208949457 F F F
0.6250008002365490 0.2500003312459071 0.0860282208949457 F F F

0.3750004621808856 0.0000000041205368 0.0860282208949457 F F F
0.8750011164316192 0.0000000041205368 0.0860282208949457 F F F
0.1250001569161086 0.5000006583712775 0.0860282208949457 F F F
0.6250008111668492 0.5000006583712775 0.0860282208949457 F F F
0.3750004731111787 0.2500003312459071 0.0860282208949457 F F F
0.8750011273619194 0.2500003312459071 0.0860282208949457 F F F
0.1250001678464017 0.7500009854966478 0.0860282208949457 F F F
0.6250008220971424 0.7500009854966478 0.0860282208949457 F F F
0.3750004840414789 0.5000006583712775 0.0860282208949457 F F F
0.8750011382922125 0.5000006583712775 0.0860282208949457 F F F
0.3750004949717720 0.7500009854966478 0.0860282208949457 F F F
0.8750011492225056 0.7500009854966478 0.0860282208949457 F F F
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0.1251004585060400 0.3750089798923568 0.1398369913139206 T T T
0.3749504026574684 0.1256084567210536 0.1342341065089698 T T T
0.1250446198438979 0.6255965472997360 0.1342441033860098 T T T
0.3750673457671354 0.3750173600009319 0.1387743159758656 T T T
0.1250134633415030 0.8750007214723112 0.1387674996497310 T T T
0.3750274371755964 0.6244103036040585 0.1342471648945178 T T T
0.3750325141225304 0.8749934955947083 0.1398215197764117 T T T
0.9999854064316622 0.1250522814989026 0.1833390515455662 T T T
0.4991363896534224 0.3750345574204417 0.1919834543538457 T T T
0.2499914506471370 0.1250205479604887 0.1833753626201400 T T T
0.0000460201307959 0.6250526143296398 0.1833683457558166 T T T
0.2510708676211593 0.3749793413991469 0.1920255896413963 T T T
0.0009745887450165 0.8750404820700197 0.1919914062687624 T T T
0.2500331937603590 0.6249913587572777 0.1833692133004590 T T T
0.2490859692428202 0.8749906106337164 0.1919894147255334 T T T
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0.2418618800748291 0.0056633004172753 0.2397935219802889 T T T
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0.2585242307832658 0.2443507687754192 0.2398583550951372 T T T
0.0082425529507972 0.7443800506746214 0.2398031074499514 T T T
0.2582573728988535 0.5056816575536587 0.2398118892936552 T T T
0.2418818023499654 0.7443222538469456 0.2397963866147421 T T T
0.1250089657197364 0.0407296105061690 0.2953028952913641 T T T
0.1253174531178516 0.1877250240382011 0.2676227562045597 T T T
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0.1250941202998348 0.5623363571208060 0.2676697343195116 T T T
0.3754086092314139 0.2093325877738152 0.2953591335967758 T T T
0.1250748375733934 0.7093348355147313 0.2953580062784340 T T T
0.3750746518002259 0.5407397963510334 0.2953464226309990 T T T
0.3750857678733013 0.6877237917454337 0.2676475652360679 T T T
0.6250197234598716 0.1244012293057963 0.1342430932905998 T T T
0.6250959189686753 0.3750089172804678 0.1398422698418500 T T T
0.8749719294919416 0.1256077244860521 0.1342400413878195 T T T
0.6250214941663543 0.6255942795300129 0.1342329080289062 T T T
0.8750865600762197 0.3750013814013897 0.1387675648148914 T T T
0.6250415267329714 0.8750078537953314 0.1387766427814086 T T T
0.8750446099290059 0.6244184377477424 0.1342372262158023 T T T
0.8750143073640899 0.8750084064220474 0.1398402615844603 T T T
0.4999705461135235 0.1249973857293227 0.1833286977329749 T T T
0.9991697412106575 0.3750662222726362 0.1919919358202478 T T T
0.7500095174546004 0.1250490194602065 0.1833970899640249 T T T
0.5000381217121941 0.6249801176354168 0.1833663451563368 T T T
0.7510660632030763 0.3750199588885366 0.1920134154752162 T T T

0.5009834005004450	0.8749822069377728	0.1919864051111375	T	T	T
0.7500336467000750	0.6250411069905724	0.1833528476594211	T	T	T
0.7490794265467358	0.8750485887388280	0.1920188574367430	T	T	T
0.5081272967171557	0.0056805304434349	0.2397571846240254	T	T	T
0.9921183508766305	0.2443657238118035	0.2397523695510131	T	T	T
0.7418244703566543	0.0057157772822123	0.2398471755113363	T	T	T
0.9919202832004785	0.5057252281103857	0.2397955545905930	T	T	T
0.7585046926661505	0.2443936804320614	0.2398632021355809	T	T	T
0.5082668249568485	0.7443105990350958	0.2397876470570068	T	T	T
0.7582644207090965	0.5057207099256260	0.2397966116633654	T	T	T
0.7418724244796522	0.7443478094317584	0.2397969952442196	T	T	T
0.6249285126588049	0.0407191224571548	0.2953389878241666	T	T	T
0.6253378400149572	0.1877275898938677	0.2676634841670307	T	T	T
0.8750219602073699	0.0623549601541100	0.2676745609741857	T	T	T
0.6250762453358476	0.5623093345105019	0.2676539492084729	T	T	T
0.8753679480048717	0.2093615748646513	0.2953675452665010	T	T	T
0.6250596828484163	0.7093135442278538	0.2953585013835038	T	T	T
0.8750842664443397	0.5407761032981000	0.2953539979618469	T	T	T
0.8750726405223404	0.6877600699838382	0.2676494697703902	T	T	T
0.0000000076540800	0.1711559350786800	0.0035690153482122	F	F	F
0.5000006619048207	0.1711559350786800	0.0035690153482122	F	F	F
0.0000000145484051	0.3288447195139526	0.0035690153482122	F	F	F
0.5000006687991458	0.3288447195139526	0.0035690153482122	F	F	F
0.0000000185843732	0.4211562622040503	0.0035690153482122	F	F	F
0.5000006728351138	0.4211562622040503	0.0035690153482122	F	F	F
0.0000000036181120	0.0788443923885822	0.0035690153482122	F	F	F
0.5000006578688527	0.0788443923885822	0.0035690153482122	F	F	F
0.2500003307434824	0.0788443923885822	0.0035690153482122	F	F	F
0.7500009849942231	0.0788443923885822	0.0035690153482122	F	F	F
0.2500003347794504	0.1711559350786800	0.0035690153482122	F	F	F
0.7500009890301911	0.1711559350786800	0.0035690153482122	F	F	F
0.2500003416737755	0.3288447195139526	0.0035690153482122	F	F	F
0.7500009959245233	0.3288447195139526	0.0035690153482122	F	F	F
0.2500003457097435	0.4211562622040503	0.0035690153482122	F	F	F
0.7500009999604842	0.4211562622040503	0.0035690153482122	F	F	F
0.0000000295146663	0.6711565893294207	0.0035690153482122	F	F	F
0.5000006837654070	0.6711565893294207	0.0035690153482122	F	F	F
0.0000000364089985	0.8288453737646861	0.0035690153482122	F	F	F
0.5000006906597392	0.8288453737646861	0.0035690153482122	F	F	F
0.0000000404449665	0.9211569164547910	0.0035690153482122	F	F	F
0.5000006946957072	0.9211569164547910	0.0035690153482122	F	F	F
0.0000000254787054	0.5788450466393158	0.0035690153482122	F	F	F
0.5000006797294461	0.5788450466393158	0.0035690153482122	F	F	F
0.2500003526040757	0.5788450466393158	0.0035690153482122	F	F	F
0.7500010068548164	0.5788450466393158	0.0035690153482122	F	F	F
0.2500003566400366	0.6711565893294207	0.0035690153482122	F	F	F
0.7500010108907773	0.6711565893294207	0.0035690153482122	F	F	F
0.2500003635343688	0.8288453737646861	0.0035690153482122	F	F	F
0.7500010177851095	0.8288453737646861	0.0035690153482122	F	F	F
0.2500003675703368	0.9211569164547910	0.0035690153482122	F	F	F
0.7500010218210775	0.9211569164547910	0.0035690153482122	F	F	F

8.3. Intermediate Configurations

Ib(4x2), E(PBE-D3/PAW) = -386.57855 eV, E(HSE06-D3/PAW) = -447.89821 eV, E(PBE-D3/TZ2P) = -374.1200 eV

1.0000000000000000

7.6621999740000000 0.0000000000000000 0.0000000000000000

-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si H C O

48 24 4 1

Selective dynamics

Direct

0.0982437263469365 0.0000000011734684 0.0289689852776363 F F F
0.0982437493469206 0.2500002971734503 0.0289689852776363 F F F
0.5982443673469362 0.0000000011734684 0.0289689852776363 F F F
0.0982437713469366 0.5000005951734463 0.0289689852776363 F F F
0.5982443673469362 0.2500002971734503 0.0289689852776363 F F F
0.0982437933469384 0.7500008931734712 0.0289689852776363 F F F
0.5982444273469341 0.5000005951734463 0.0289689852776363 F F F
0.5982444273469341 0.7500008931734712 0.0289689852776363 F F F
0.3481889148011276 0.9995021537364084 0.0796618693222371 F F F
0.3482099635546093 0.2528227589216314 0.0806418874415229 F F F
0.8482098579643209 0.9984169186223255 0.0807822717142628 F F F
0.3481536313616118 0.4981877663151266 0.0807373416799067 F F F
0.8482139166747305 0.2521299693376946 0.0802085390540555 F F F
0.3481955688590048 0.7531385895576650 0.0800458566958042 F F F
0.8482115512265838 0.4972844060945292 0.0801440306302297 F F F
0.8483293512469317 0.7520680719318165 0.0806932257095596 F F F
0.3478477086888165 0.1251126358877488 0.1274003650645306 T T T
0.3480008335909495 0.3756716467422268 0.1349608171164759 T T T
0.8488253452249541 0.1255986921337340 0.1279060974004354 T T T
0.3484598470040761 0.6265559871474987 0.1274102805682031 T T T
0.8483646485739739 0.3748421684988479 0.1337844873021601 T T T
0.3482594589070990 0.8764496658029072 0.1335087276586805 T T T
0.8486050250223730 0.6239309385608475 0.1272586830811661 T T T
0.8483597095383429 0.8754686148463288 0.1350985634773049 T T T
0.0989480817754591 0.1258096851779633 0.1769289856104914 T T T
0.0963849126775352 0.3745161011814708 0.1868445928515229 T T T
0.5977433008762398 0.1249851678690198 0.1763367240706173 T T T
0.0981831501676584 0.6257062306328661 0.1767653951202605 T T T
0.5999149899338618 0.3747445677370186 0.1865858092648716 T T T
0.1006206328921827 0.8771270090448439 0.1869344847650521 T T T
0.5989746213690927 0.6256885098378724 0.1766708470282757 T T T
0.5959928261544093 0.8769362508002486 0.1868705153944880 T T T
0.1169867085076799 0.0083109610228873 0.2345264235795415 T T T
0.0866541497703246 0.2426348015844638 0.2332619623738889 T T T
0.5795323943115747 0.0081308587120825 0.2343524939545844 T T T
0.0817173038242662 0.5063490990420805 0.2335384491571601 T T T
0.6086761410471171 0.2420323314100443 0.2320482234643693 T T T
0.1141103061844963 0.7449751345061180 0.2336104394875504 T T T
0.6151747856114559 0.5064915634282366 0.2334104964702918 T T T
0.5827061108252338 0.7448498919686223 0.2335669724625917 T T T
0.3485594859597617 0.0414937792154032 0.2913683153008222 T T T
0.3490915926112846 0.1946456630831877 0.2704024857728364 T T T
0.8480270230706964 0.0636503585852691 0.2610494715176399 T T T
0.3484684967245006 0.5636211695010017 0.2609692352196084 T T T
0.8453524346358868 0.2106692122231596 0.2868443319057520 T T T
0.3484173159713271 0.7098121853191992 0.2888962526893658 T T T
0.8484198319037494 0.5405410483193454 0.2895292006704808 T T T
0.8484412876062258 0.6881450775942203 0.2618600078767990 T T T
0.0982437210000029 0.9179475529999410 0.0000000000000000 F F F
0.0982437879999978 0.0820524620000000 0.0000000162939813 F F F
0.0982437429999976 0.1679478439999969 0.0000000000000000 F F F

0.0982438099999854	0.3320527369999837	0.0000000162939813	F	F	F
0.5982443090000018	0.0820524470000024	0.0000000000000000	F	F	F
0.5982443089999381	0.9179475379999504	0.0000000162939813	F	F	F
0.0982437660000031	0.4179481569999766	0.0000000000000000	F	F	F
0.0982438329999979	0.5820530649999611	0.0000000162939813	F	F	F
0.5982443089999663	0.3320527079999992	0.0000000000000000	F	F	F
0.5982443089999736	0.1679478289999992	0.0000000162939813	F	F	F
0.0982437950000019	0.6679484840000003	0.0000000000000000	F	F	F
0.0982438469999991	0.8320534229999552	0.0000000162939813	F	F	F
0.5982443689999997	0.5820530060000026	0.0000000000000000	F	F	F
0.5982443689999715	0.4179481269999813	0.0000000162939813	F	F	F
0.5982443689999999	0.8320533629999434	0.0000000000000000	F	F	F
0.5982443689999288	0.6679484249999632	0.0000000162939813	F	F	F
0.3365605648994238	0.3731855524271370	0.2945209294650442	T	T	T
0.5382945868208537	0.3569630112979536	0.3278276815092300	T	T	T
0.3968434406917883	0.3863926908588763	0.4076192968559493	T	T	T
0.2681633182790631	0.4556465306128354	0.3687951485886927	T	T	T
0.0986398834373068	0.3299701417275435	0.4212527955269050	T	T	T
0.0463535248577946	0.3414517542581503	0.3567397840444601	T	T	T
0.2983838299180758	0.2078512980277023	0.4033700985685709	T	T	T
0.1327385728632393	0.1907438826403720	0.3564378511984589	T	T	T
0.3958707347082164	0.3497370772503413	0.3295142685339849	T	T	T
0.3081660797833873	0.3877084445517918	0.3753345834382067	T	T	T
0.1521609586650463	0.3265480568615471	0.3832823003733515	T	T	T
0.2272696267131112	0.2373161910871329	0.3720035477456168	T	T	T
0.3603130598061876	0.2542818653026228	0.3325850379392432	T	T	T

TS Ib(4x2) Ib(intermediate), E = -386.29339 eV

1.0000000000000000		
7.6621999740000000	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000
-0.0000007340000000	-0.0000007340000000	26.7875003810000010

Si O C H
48 1 4 24

Selective dynamics

Direct

0.0982437263469365	0.0000000011734684	0.0289689852776374	F	F	F
0.0982437493469206	0.2500002971734362	0.0289689852776374	F	F	F
0.5982443673469362	0.0000000011734684	0.0289689852776374	F	F	F
0.0982437713469366	0.5000005951734678	0.0289689852776374	F	F	F
0.5982443673469362	0.2500002971734362	0.0289689852776374	F	F	F
0.0982437933469313	0.7500008931734712	0.0289689852776374	F	F	F
0.5982444273469341	0.5000005951734678	0.0289689852776374	F	F	F
0.5982444273469341	0.7500008931734712	0.0289689852776374	F	F	F
0.3481889148011417	0.9995021537363588	0.0796618693222408	F	F	F
0.3482099635546240	0.2528227589216101	0.0806418874415196	F	F	F
0.8482098579642641	0.9984169186223468	0.0807822717142666	F	F	F
0.3481536313615763	0.4981877663150990	0.0807373416799104	F	F	F
0.8482139166746706	0.2521299693376946	0.0802085390540592	F	F	F
0.3481955688589979	0.7531385895576951	0.0800458566958080	F	F	F
0.8482115512265977	0.4972844060945010	0.0801440306302335	F	F	F
0.8483293512468535	0.7520680719317809	0.0806932257095634	F	F	F
0.3481488832247407	0.1251312887380104	0.1273892163791018	T	T	T
0.3480052750215110	0.3755869109048150	0.1352274181091551	T	T	T
0.8493473440532353	0.1256358665940309	0.1280141149206463	T	T	T
0.3482133079926371	0.6262495879022359	0.1283573891547965	T	T	T

0.8484287670282247 0.3746665583478124 0.1340858949490280 T T T
0.3483054447180783 0.8759336296201855 0.1335387964919592 T T T
0.8482627682230094 0.6245970686533119 0.1264856929576210 T T T
0.8483813304003980 0.8756233510781104 0.1343202277260225 T T T
0.0996613231103361 0.1261029625837280 0.1770941661519283 T T T
0.0961567015133700 0.3745310334033997 0.1873607927685327 T T T
0.5979786119105096 0.1250354016036580 0.1763537815891688 T T T
0.0951069888981612 0.6224113141815786 0.1767063425555964 T T T
0.6002436475618103 0.3747089532179309 0.1870751429777403 T T T
0.0987733587301996 0.8785444615582635 0.1863738212434844 T T T
0.6013746518201927 0.6223013483803208 0.1766799172497912 T T T
0.5979187892376457 0.8783084520646606 0.1863291200755276 T T T
0.1167669205667742 0.0084840226358237 0.234555537648769 T T T
0.0885983006126471 0.2425334450018261 0.2338240138067300 T T T
0.5803493124659482 0.0083110038598427 0.2343820772676513 T T T
0.0809649155327810 0.5063145261863866 0.2340403180261006 T T T
0.6082945950930283 0.2416785887864537 0.2323616482276714 T T T
0.0959258246391358 0.7458517409109895 0.2323605032365262 T T T
0.6153970365473982 0.5063019809582943 0.2340746169676240 T T T
0.6002079379283276 0.7456917072240248 0.2323458303159305 T T T
0.3488549254615863 0.0393568524468820 0.2913847317095948 T T T
0.3500957449316786 0.1928379799649551 0.2711509554154070 T T T
0.8483874277687886 0.0639822504048987 0.2613131842619242 T T T
0.3481034848433172 0.5424929213034867 0.2718466375774325 T T T
0.8459107623334319 0.2107674102643099 0.2868924787138067 T T T
0.3479925778689907 0.6884448022459683 0.2664273374739442 T T T
0.8483173531053260 0.5306307380157662 0.2917496361645854 T T T
0.8480995895268229 0.6788384265648776 0.2649079974829999 T T T
0.3637166993517970 0.2463732223546190 0.3346851970774367 T T T
0.4133619018196363 0.3404129389844759 0.3358738175227169 T T T
0.3272916981078578 0.3756528074235661 0.3825986911147368 T T T
0.1623852262361589 0.3194487809439667 0.3870389187748494 T T T
0.2264039929079070 0.2293479240217600 0.3728836101104340 T T T
0.0982437210000029 0.9179475529999053 0.0000000000000000 F F F
0.0982437879999907 0.0820524620000000 0.0000000162939813 F F F
0.0982437429999905 0.1679478439999969 0.0000000000000000 F F F
0.0982438099999853 0.3320527369999980 0.0000000162939813 F F F
0.5982443090000018 0.0820524470000024 0.0000000000000000 F F F
0.5982443089999103 0.9179475379998721 0.0000000162939813 F F F
0.0982437660000031 0.4179481569999628 0.0000000000000000 F F F
0.0982438329999979 0.5820530649999043 0.0000000162939813 F F F
0.5982443089998952 0.3320527079999994 0.0000000000000000 F F F
0.5982443090000018 0.1679478289999992 0.0000000162939813 F F F
0.0982437950000019 0.6679484840000008 0.0000000000000000 F F F
0.0982438469999920 0.8320534229998771 0.0000000162939813 F F F
0.5982443689999997 0.5820530060000032 0.0000000000000000 F F F
0.5982443690000008 0.4179481269999958 0.0000000162939813 F F F
0.5982443690000001 0.8320533629999076 0.0000000000000000 F F F
0.5982443689999003 0.6679484249998993 0.0000000162939813 F F F
0.3602777854127183 0.3705232634666735 0.3017612650330704 T T T
0.5565233400322069 0.3425761448567509 0.3351539470765828 T T T
0.4124418414036424 0.3672074875071680 0.4153080824397767 T T T
0.2983832950122604 0.4455157670406628 0.3782536705043859 T T T
0.1054668249243850 0.3202808870919557 0.4246483424053502 T T T
0.0617698521444300 0.3411590468349158 0.3603821959016889 T T T
0.2916792122270900 0.1943168119570214 0.4034119669316263 T T T
0.1271384305048913 0.1876867785077638 0.3553087767340687 T T T

Ib(intermediate), E = -386.36110 eV

1.0000000000000000
7.6621999740000000 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H
48 1 4 24

Selective dynamics

Direct

0.0982437263469365 0.0000000011734684 0.0289689852776378 F F F
0.0982437493469206 0.2500002971734435 0.0289689852776378 F F F
0.5982443673469362 0.0000000011734684 0.0289689852776378 F F F
0.0982437713469366 0.5000005951734678 0.0289689852776378 F F F
0.5982443673469362 0.2500002971734435 0.0289689852776378 F F F
0.0982437933469313 0.7500008931734712 0.0289689852776378 F F F
0.5982444273469341 0.5000005951734678 0.0289689852776378 F F F
0.5982444273469341 0.7500008931734712 0.0289689852776378 F F F
0.3481889148011417 0.9995021537364011 0.0796618693222421 F F F
0.3482099635546240 0.2528227589216172 0.0806418874415209 F F F
0.8482098579643065 0.9984169186223468 0.0807822717142678 F F F
0.3481536313615976 0.4981877663151266 0.0807373416799117 F F F
0.8482139166747206 0.2521299693376946 0.0802085390540605 F F F
0.3481955688589979 0.7531385895577054 0.0800458566958093 F F F
0.8482115512265977 0.4972844060945292 0.0801440306302347 F F F
0.8483293512468961 0.7520680719318094 0.0806932257095647 F F F
0.3481956985618672 0.1250790394647956 0.1274023856648990 T T T
0.3479521161553811 0.3752208436696773 0.1351740133148009 T T T
0.8495748530511591 0.1256616684042640 0.1280772549809322 T T T
0.3478189914615925 0.6262551613491797 0.1274400259026862 T T T
0.8484355793416980 0.3748502634747069 0.1346310281213167 T T T
0.3481594310214768 0.8758103082105592 0.1333709588116389 T T T
0.8477952790903136 0.6248532681841402 0.1272292092691291 T T T
0.8481677386087294 0.8754317828003730 0.1342131393875250 T T T
0.1000071443845752 0.1259930586778953 0.1772226152970526 T T T
0.0976630138895625 0.3748049433980438 0.1877280533290454 T T T
0.5979871961651488 0.1248097075676025 0.1763818813027891 T T T
0.0973176771365823 0.6205124780550962 0.1764302201520803 T T T
0.5986577864001933 0.3750388302861977 0.1874237297786386 T T T
0.0988405142096772 0.8779124196613812 0.1860955571682638 T T T
0.5981565660826390 0.6204107548563719 0.1764426111161298 T T T
0.5974093285179850 0.8776965931862407 0.1860879267359459 T T T
0.1164663355822858 0.0077531631857363 0.2343159207053590 T T T
0.0901386653511298 0.2423902417211100 0.2341376440297304 T T T
0.5802437752016472 0.0076578996589972 0.2341744616909564 T T T
0.0958362264776787 0.5066314909504763 0.2347666977001589 T T T
0.6079278201822772 0.2414564330959069 0.2324741060063442 T T T
0.0964019887631415 0.7451473708875715 0.2322957611432737 T T T
0.5990653848370562 0.5066331770199811 0.2348699780940574 T T T
0.5989454621300537 0.7449802136726188 0.2323175920305545 T T T
0.3485604110195483 0.0379300806350618 0.2910901131926190 T T T
0.3508983763349486 0.1917747461047233 0.2716325384080847 T T T
0.8482907745366501 0.0632933868677125 0.2611611677523691 T T T
0.3469803481047531 0.5333016731008440 0.2854769114148230 T T T
0.8463722261276677 0.2100657729735420 0.2866485758012230 T T T
0.3474988241643245 0.6771830072269922 0.2615828894068403 T T T

0.8476386025385999	0.5295412125340174	0.2876449089951495	T	T	T
0.8477162514915738	0.6747091408481309	0.2626096752579685	T	T	T
0.3671191355758603	0.2404346266089436	0.3361551177208092	T	T	T
0.4408936979467428	0.3296991569225683	0.3426538201903176	T	T	T
0.3579025523996724	0.3633048133111946	0.3902235837355096	T	T	T
0.1805540872203410	0.3168332427884668	0.3909295040092192	T	T	T
0.2254170534969814	0.2257929706541615	0.3732387443569617	T	T	T
0.0982437210000029	0.9179475529999339	0.0000000000000000	F	F	F
0.0982437879999907	0.0820524620000000	0.0000000162939813	F	F	F
0.0982437429999905	0.1679478439999969	0.0000000000000000	F	F	F
0.0982438099999853	0.3320527369999980	0.0000000162939813	F	F	F
0.5982443090000018	0.0820524470000024	0.0000000000000000	F	F	F
0.5982443089999392	0.9179475379999147	0.0000000162939813	F	F	F
0.0982437660000031	0.4179481569999695	0.0000000000000000	F	F	F
0.0982438329999979	0.5820530649999327	0.0000000162939813	F	F	F
0.5982443089999316	0.3320527079999994	0.0000000000000000	F	F	F
0.5982443090000018	0.1679478289999992	0.0000000162939813	F	F	F
0.0982437950000019	0.6679484840000008	0.0000000000000000	F	F	F
0.0982438469999920	0.8320534229999197	0.0000000162939813	F	F	F
0.5982443689999997	0.5820530060000032	0.0000000000000000	F	F	F
0.5982443690000008	0.4179481269999958	0.0000000162939813	F	F	F
0.5982443690000001	0.8320533629999444	0.0000000000000000	F	F	F
0.5982443689999293	0.6679484249999348	0.0000000162939813	F	F	F
0.4012588146339470	0.3682424947131077	0.3098473406499359	T	T	T
0.5833796502680784	0.3221821992006643	0.3432895411721635	T	T	T
0.4363302571390741	0.3454721859152594	0.4230713858803533	T	T	T
0.3457553113949917	0.4347373932313564	0.3886714909949436	T	T	T
0.1197551093226595	0.3160622128555318	0.4280412457865179	T	T	T
0.0890869785338896	0.3478676619470730	0.3645975327593552	T	T	T
0.2812734991845498	0.1837744095180130	0.4023929162200673	T	T	T
0.1187419514171545	0.1919694270940457	0.3537673775488702	T	T	T

TS lb(intermediate) Pb(2x2), E = -386.24168 eV

1.0000000000000000		
7.6621999740000000	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000
-0.0000007340000000	-0.0000007340000000	26.7875003810000010

Si O C H
48 1 4 24

Selective dynamics

Direct

0.0982437263469365	0.0000000011734684	0.0289689852776370	F	F	F
0.0982437493469206	0.2500002971734435	0.0289689852776370	F	F	F
0.5982443673469362	0.0000000011734684	0.0289689852776370	F	F	F
0.0982437713469366	0.5000005951734678	0.0289689852776370	F	F	F
0.5982443673469362	0.2500002971734435	0.0289689852776370	F	F	F
0.0982437933469313	0.7500008931734712	0.0289689852776370	F	F	F
0.5982444273469341	0.5000005951734678	0.0289689852776370	F	F	F
0.5982444273469341	0.7500008931734712	0.0289689852776370	F	F	F
0.3481889148011417	0.9995021537363940	0.0796618693222395	F	F	F
0.3482099635546240	0.2528227589216172	0.0806418874415182	F	F	F
0.8482098579643009	0.9984169186223468	0.0807822717142652	F	F	F
0.3481536313615976	0.4981877663151266	0.0807373416799091	F	F	F
0.8482139166747127	0.2521299693376946	0.0802085390540579	F	F	F
0.3481955688589979	0.7531385895576844	0.0800458566958066	F	F	F
0.8482115512265977	0.4972844060945292	0.0801440306302321	F	F	F

0.8483293512468961 0.7520680719318165 0.0806932257095620 F F F
0.3481198981790168 0.1251511987853042 0.1274819279730673 T T T
0.3479477821454796 0.3749190458188981 0.1347247978596518 T T T
0.8492159346459260 0.1257112313873795 0.1280046554700865 T T T
0.3480866892578562 0.6259424465389497 0.1265048541941940 T T T
0.8483019807099621 0.3752518904434313 0.1349434905834798 T T T
0.3482030509129933 0.8760470332063600 0.1332738057775721 T T T
0.8480382370999615 0.6248259729048311 0.1283457194425828 T T T
0.8482327806765961 0.8755223111515743 0.1341708036680102 T T T
0.0994285673305214 0.1263086013336783 0.1771396704685278 T T T
0.0995645703475767 0.3742910064043918 0.1877125266058742 T T T
0.5980451729201048 0.1254094312753833 0.1764747885454550 T T T
0.1009869331743850 0.6225571074644065 0.1767169770586714 T T T
0.5966121173375715 0.3745182956714541 0.1874909618820907 T T T
0.0992548210484030 0.8785740557894359 0.1859666343767125 T T T
0.5950824165784798 0.6224087379533677 0.1767500696729646 T T T
0.5971533216869951 0.8783597970310304 0.1859376857282424 T T T
0.1160075232608673 0.0081141845717005 0.2341528936484702 T T T
0.0897777474073772 0.2421852056909100 0.2343895243599385 T T T
0.5810659752009331 0.0080186621171501 0.2339799270166206 T T T
0.1151332121832075 0.5064695722980261 0.2341703528238905 T T T
0.6072249739624361 0.2414692316718049 0.2330716202752079 T T T
0.0981127304852241 0.7463237566985157 0.2319900736990036 T T T
0.5806188390140414 0.5064426251708759 0.2343085942776438 T T T
0.5975415426729919 0.7461538736083303 0.2319991246943735 T T T
0.3488309533196649 0.0367309535293166 0.2907679230624234 T T T
0.3500218360145947 0.1902806880236758 0.2716276525595598 T T T
0.8483949531381868 0.0640465891821743 0.2613788167557684 T T T
0.3475507384639540 0.5354756993974539 0.2911095795508464 T T T
0.8462665492596045 0.2109279584999380 0.2874140463618506 T T T
0.3476602097666361 0.6819669845835089 0.2640005947058610 T T T
0.8480197972805340 0.5423835089419990 0.2715928559796240 T T T
0.8478900644751957 0.6890961253520163 0.2675447170589406 T T T
0.3633081882370532 0.2372133558821825 0.3365673973002181 T T T
0.4185479959673259 0.3296013158083395 0.3427432416557893 T T T
0.3433790438977057 0.3562052490303388 0.3927293916106814 T T T
0.1746990073345159 0.3025030895186471 0.3955821392759455 T T T
0.2288582547391616 0.2148005720209600 0.3746823282910054 T T T
0.0982437210000029 0.9179475529999339 0.0000000000000000 F F F
0.0982437879999978 0.0820524620000000 0.0000000162939813 F F F
0.0982437429999976 0.1679478439999969 0.0000000000000000 F F F
0.0982438099999853 0.3320527369999980 0.0000000162939813 F F F
0.5982443090000018 0.0820524470000024 0.0000000000000000 F F F
0.5982443089999450 0.9179475379999076 0.0000000162939813 F F F
0.0982437660000031 0.4179481569999695 0.0000000000000000 F F F
0.0982438329999979 0.5820530649999327 0.0000000162939813 F F F
0.5982443089999316 0.3320527079999994 0.0000000000000000 F F F
0.5982443090000018 0.1679478289999992 0.0000000162939813 F F F
0.0982437950000019 0.6679484840000008 0.0000000000000000 F F F
0.0982438469999920 0.8320534229999197 0.0000000162939813 F F F
0.5982443689999997 0.5820530060000032 0.0000000000000000 F F F
0.5982443690000008 0.4179481269999958 0.0000000162939813 F F F
0.5982443690000001 0.8320533629999444 0.0000000000000000 F F F
0.5982443689999293 0.6679484249999348 0.0000000162939813 F F F
0.3610355171521606 0.3669743185081874 0.3116992561309174 T T T
0.5614870319151566 0.3299940340080947 0.3398632396042804 T T T
0.4328200437579819 0.3389210586008799 0.4233062092260280 T T T

0.3203843413300792 0.4269579035151995 0.3935606228580069 T T T
0.1233263938717976 0.2965279733888422 0.4336933354173152 T T T
0.0724122870597749 0.3312966923833723 0.3718251803398873 T T T
0.2941981950043151 0.1720756924820544 0.4017970779680853 T T T
0.1239421967645388 0.1793696014143716 0.3553971149075820 T T T

Ib(2x2), E = -386.52065 eV

1.0000000000000000
7.6621999740000000 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H
48 1 4 24

Selective dynamics

Direct

0.0982437263469365 0.0000000011734684 0.0289689852776368 F F F
0.0982437493469206 0.2500002971734503 0.0289689852776368 F F F
0.5982443673469362 0.0000000011734684 0.0289689852776368 F F F
0.0982437713469366 0.5000005951734678 0.0289689852776368 F F F
0.5982443673469362 0.2500002971734503 0.0289689852776368 F F F
0.0982437933469313 0.7500008931734712 0.0289689852776368 F F F
0.5982444273469341 0.5000005951734678 0.0289689852776368 F F F
0.5982444273469341 0.7500008931734712 0.0289689852776368 F F F
0.3481889148011417 0.9995021537364087 0.0796618693222389 F F F
0.3482099635546240 0.2528227589216243 0.0806418874415176 F F F
0.8482098579643140 0.9984169186223468 0.0807822717142646 F F F
0.3481536313615976 0.4981877663151266 0.0807373416799084 F F F
0.8482139166747232 0.2521299693376946 0.0802085390540572 F F F
0.3481955688589979 0.7531385895576793 0.0800458566958060 F F F
0.8482115512265977 0.4972844060945292 0.0801440306302315 F F F
0.8483293512469032 0.7520680719318165 0.0806932257095614 F F F
0.3480246294872927 0.1251691918345114 0.1275063335019690 T T T
0.3478860587847477 0.3750201957528463 0.1346254103189756 T T T
0.8490586206038323 0.1257164830550284 0.1279189217714928 T T T
0.3481668505756934 0.6253457962451916 0.1272539350510113 T T T
0.8482387064500447 0.3753032198928281 0.1346276056014747 T T T
0.3481474234760817 0.8758773740964285 0.1338246280192521 T T T
0.8481330366208736 0.6251178563691204 0.1273635955433081 T T T
0.8482280493182435 0.8759632097072778 0.1341600657306376 T T T
0.0990328524371323 0.1262440675095849 0.1770745559928073 T T T
0.0985984624629673 0.3742591967878630 0.1873314114440745 T T T
0.5981661250130044 0.1254090789412051 0.1764481976657818 T T T
0.0983146407543739 0.6257101950746417 0.1766838729780578 T T T
0.5974420043779972 0.3744324657313065 0.1871141925145093 T T T
0.0979618216752535 0.8770356733856248 0.1863708482591023 T T T
0.5979596314764901 0.6255508407613536 0.1767174174913035 T T T
0.5983820373452076 0.8768245654414519 0.1863210665640022 T T T
0.1152402263820200 0.0076606063581097 0.2339656950651025 T T T
0.0888921527623578 0.2423128537736021 0.2341733279991414 T T T
0.5818407466968354 0.0075450543841540 0.2337711998974180 T T T
0.1133354632214889 0.5067471737887310 0.2336487922057835 T T T
0.6076367744897982 0.2416271789332191 0.2329508121065465 T T T
0.0816267411542720 0.7455055184658683 0.2331765688714647 T T T
0.5824903644478635 0.5066468120757870 0.2337713474182755 T T T
0.6142257254812489 0.7453530557527853 0.2331760447188224 T T T
0.3489008856607991 0.0372736435039266 0.2903000145154717 T T T

0.3496645957661097	0.1907073411857792	0.2711461885834854	T	T	T
0.8483637167292164	0.0642342858250284	0.2613766609471849	T	T	T
0.3477666161059997	0.5439068121085391	0.288650006225612	T	T	T
0.8461421520835873	0.2113715411055833	0.2875556459547028	T	T	T
0.3478178411685161	0.6901184396254415	0.2611057447539028	T	T	T
0.8479597926762992	0.5643388248701099	0.2615506262382061	T	T	T
0.8479418723668429	0.7113157710595700	0.2889567704001072	T	T	T
0.3619362915718602	0.2397287993913783	0.3357118932252557	T	T	T
0.4061082881335575	0.3338706175149519	0.3400300587890824	T	T	T
0.3335088345282466	0.3603022515896164	0.3903571211795304	T	T	T
0.1711470591547666	0.3023433932065143	0.3952507813232117	T	T	T
0.2319468647596610	0.2154237929025103	0.3747219708979937	T	T	T
0.0982437210000029	0.9179475529999418	0.0000000000000000	F	F	F
0.0982437879999907	0.0820524620000000	0.0000000162939813	F	F	F
0.0982437429999976	0.1679478439999969	0.0000000000000000	F	F	F
0.0982438099999853	0.3320527369999980	0.0000000162939813	F	F	F
0.5982443090000018	0.0820524470000024	0.0000000000000000	F	F	F
0.5982443089999450	0.9179475379999218	0.0000000162939813	F	F	F
0.0982437660000031	0.4179481569999766	0.0000000000000000	F	F	F
0.0982438329999979	0.5820530649999399	0.0000000162939813	F	F	F
0.5982443089999379	0.3320527079999994	0.0000000000000000	F	F	F
0.5982443090000018	0.1679478289999992	0.0000000162939813	F	F	F
0.0982437950000019	0.6679484840000008	0.0000000000000000	F	F	F
0.0982438469999920	0.8320534229999268	0.0000000162939813	F	F	F
0.5982443689999997	0.5820530060000032	0.0000000000000000	F	F	F
0.5982443690000008	0.4179481269999958	0.0000000162939813	F	F	F
0.5982443690000001	0.8320533629999444	0.0000000000000000	F	F	F
0.5982443689999372	0.6679484249999419	0.0000000162939813	F	F	F
0.3409144879100741	0.3680084568579450	0.3090176716443552	T	T	T
0.5483214981336996	0.3384330514295817	0.3358330021908267	T	T	T
0.4278152005415672	0.3463762564475094	0.4202925692208734	T	T	T
0.3035333261332074	0.4304032188168604	0.3907234369321807	T	T	T
0.1245839233974469	0.2963039487370260	0.4338573183430332	T	T	T
0.0634192109739101	0.3275196000340955	0.3721278857587572	T	T	T
0.3027123630827234	0.1748589364882032	0.4017915359600214	T	T	T
0.1291177682074084	0.1772100234586376	0.3562973240706048	T	T	T

Ib(4x4), E(PBE-D3) = -700.87167 eV, E(HSE06-D3) = -811.30005 eV

1.0000000000000000		
15.3244190216000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.3244190216000007	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7875003810000010

Si O C H
96 1 4 40

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0354635925893945	F	F	F
0.5000000319229088	0.0000000000000000	0.0354635925893945	F	F	F
0.0000000000000000	0.2500000159614544	0.0354635925893945	F	F	F
0.5000000319229088	0.2500000159614544	0.0354635925893945	F	F	F
0.2500000159614544	0.0000000000000000	0.0354635925893945	F	F	F
0.7500000478843631	0.0000000000000000	0.0354635925893945	F	F	F
0.0000000000000000	0.5000000319229088	0.0354635925893945	F	F	F
0.5000000319229088	0.5000000319229088	0.0354635925893945	F	F	F
0.2500000159614544	0.2500000159614544	0.0354635925893945	F	F	F
0.7500000478843631	0.2500000159614544	0.0354635925893945	F	F	F

0.0000000000000000 0.7500000478843631 0.0354635925893945 F F F
0.5000000319229088 0.7500000478843631 0.0354635925893945 F F F
0.2500000159614544 0.5000000319229088 0.0354635925893945 F F F
0.7500000478843631 0.5000000319229088 0.0354635925893945 F F F
0.2500000159614544 0.7500000478843631 0.0354635925893945 F F F
0.7500000478843631 0.7500000478843631 0.0354635925893945 F F F
0.1249999753530631 0.0000000000000000 0.0860282208949456 F F F
0.6250000072759718 0.0000000000000000 0.0860282208949456 F F F
0.1249999753530631 0.2500000159614544 0.0860282208949456 F F F
0.6250000072759718 0.2500000159614544 0.0860282208949456 F F F
0.3749999913145174 0.0000000000000000 0.0860282208949456 F F F
0.8750000232374191 0.0000000000000000 0.0860282208949456 F F F
0.1249999753530631 0.5000000319229088 0.0860282208949456 F F F
0.6250000072759718 0.5000000319229088 0.0860282208949456 F F F
0.3749999913145174 0.2500000159614544 0.0860282208949456 F F F
0.8750000232374191 0.2500000159614544 0.0860282208949456 F F F
0.1249999753530631 0.7500000478843631 0.0860282208949456 F F F
0.6250000072759718 0.7500000478843631 0.0860282208949456 F F F
0.3749999913145174 0.5000000319229088 0.0860282208949456 F F F
0.8750000232374191 0.5000000319229088 0.0860282208949456 F F F
0.3749999913145174 0.7500000478843631 0.0860282208949456 F F F
0.8750000232374191 0.7500000478843631 0.0860282208949456 F F F
0.1249068543638109 0.1243564122149312 0.1340890692172093 T T T
0.1249182480611025 0.3751548256907802 0.1397194183374973 T T T
0.3746976587600014 0.1253242155709644 0.1342732196180904 T T T
0.1250139980696419 0.6256399482985114 0.1341970505340463 T T T
0.3748661879506476 0.3750208533090144 0.1387318348623121 T T T
0.1250063886799553 0.8750700973226507 0.1388678707132608 T T T
0.3752288499597530 0.6244236124047924 0.1341541440080274 T T T
0.3747482551752250 0.8751379118218141 0.1399139488468210 T T T
0.0004007489947845 0.1254644809242890 0.1833940852435588 T T T
0.4988768805872550 0.3749163614521869 0.1919690301878116 T T T
0.2497870005434981 0.1248337811984978 0.1829563423738567 T T T
0.9999567039552177 0.6254877439468312 0.1832971044142690 T T T
0.2507343087055932 0.3744011254090581 0.1918380610873118 T T T
0.0010933719870265 0.8763077649019196 0.1922552682137444 T T T
0.2501851700309135 0.6255449577092035 0.1831683986118952 T T T
0.2489213418258913 0.8762751740732100 0.1922555636336958 T T T
0.0097688148427007 0.0069803133192393 0.2403277420302868 T T T
0.4909132992779033 0.2445862426959222 0.2399697598785688 T T T
0.2406134953143358 0.0069996078824886 0.2402826223949777 T T T
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0.2581325847493326 0.5057382112539677 0.2392410699610086 T T T
0.2420502377905751 0.7449590689261812 0.2396700027243658 T T T
0.1252159243893305 0.0412850569968936 0.2971805566341853 T T T
0.1256891642051510 0.1949931243479765 0.2764888239248050 T T T
0.3740957363186905 0.0632700862947393 0.2675043516870779 T T T
0.1249643527294352 0.5631433406004029 0.2669932395300124 T T T
0.3727896567911801 0.2103260092581810 0.2944514135976449 T T T
0.1250005576456284 0.7096112049660452 0.2950292936024710 T T T
0.3744978264286076 0.5403996172520957 0.2952914952303546 T T T
0.3748461307131682 0.6878102394485899 0.2678011065333360 T T T
0.6248578956477723 0.1245052758786035 0.1342628534184161 T T T
0.6248416604506926 0.3750658351666552 0.1397770029250002 T T T
0.8756275866281956 0.1253947041923617 0.1343820438340551 T T T

0.6250947205249692 0.6255937868545189 0.1343400658158405 T T T
0.8750778076336100 0.3750055997646066 0.1387617893169574 T T T
0.6249299226209184 0.8750323010807977 0.1388689167734750 T T T
0.8749658610748490 0.6243959313690154 0.1341781550539076 T T T
0.8752272730544878 0.8751335642731000 0.1399180247993687 T T T
0.4998617497268780 0.1252645202552607 0.1833571634417550 T T T
0.9991361772042120 0.3744142161170088 0.1919876563085545 T T T
0.7500576778577487 0.1250379029734202 0.1830821376138205 T T T
0.4999947302678276 0.6250575559245717 0.1834696606445877 T T T
0.7508397430672834 0.3751655404740031 0.1918158376553201 T T T
0.5007539480608565 0.8754986157930317 0.1921043279818795 T T T
0.7502024653884650 0.6249930296844830 0.1834794943257261 T T T
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0.5075937917761326 0.0063125717060838 0.2399616803301355 T T T
0.9946352517311065 0.2429331872770998 0.2390440035520117 T T T
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0.7571918288723112 0.2444765871139466 0.2393405415462024 T T T
0.5079351816809810 0.7445788589171682 0.2398185548490075 T T T
0.7581870302795545 0.5055410423870170 0.2398595651072098 T T T
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0.6249634072508172 0.0411605927915093 0.2951041456598887 T T T
0.6241682438600394 0.1879837824380737 0.2676153164065171 T T T
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0.6248751856069918 0.5621887028433572 0.2676319859975496 T T T
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0.6249799307961585 0.7091455286028312 0.2951426694587948 T T T
0.8752971556267840 0.5402716391183428 0.2954633625889173 T T T
0.8751261803326125 0.6877928997341285 0.2678953789954276 T T T
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0.1494115507827389 0.3493634456970492 0.3361431249629054 T T T
0.1055462413524828 0.3867368677197488 0.3821331063190981 T T T
0.0275777690266498 0.3254558126582502 0.3899736854674637 T T T
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0.0000000000000000 0.1711557218778097 0.0035690153482122 F F F
0.5000000319229088 0.1711557218778097 0.0035690153482122 F F F
0.0000000000000000 0.3288443100450991 0.0035690153482122 F F F
0.5000000319229088 0.3288443100450991 0.0035690153482122 F F F
0.0000000000000000 0.4211557378392641 0.0035690153482122 F F F
0.5000000319229088 0.4211557378392641 0.0035690153482122 F F F
0.0000000000000000 0.0788442940836447 0.0035690153482122 F F F
0.5000000319229088 0.0788442940836447 0.0035690153482122 F F F
0.2500000159614544 0.0788442940836447 0.0035690153482122 F F F
0.7500000478843631 0.0788442940836447 0.0035690153482122 F F F
0.2500000159614544 0.1711557218778097 0.0035690153482122 F F F
0.7500000478843631 0.1711557218778097 0.0035690153482122 F F F
0.2500000159614544 0.3288443100450991 0.0035690153482122 F F F
0.7500000478843631 0.3288443100450991 0.0035690153482122 F F F
0.2500000159614544 0.4211557378392641 0.0035690153482122 F F F
0.7500000478843631 0.4211557378392641 0.0035690153482122 F F F
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0.5000000319229088 0.6711557538007185 0.0035690153482122 F F F
0.0000000000000000 0.8288443419680007 0.0035690153482122 F F F
0.5000000319229088 0.8288443419680007 0.0035690153482122 F F F
0.0000000000000000 0.9211557697621728 0.0035690153482122 F F F
0.5000000319229088 0.9211557697621728 0.0035690153482122 F F F
0.0000000000000000 0.5788443260065463 0.0035690153482122 F F F

0.5000000319229088 0.5788443260065463 0.0035690153482122 F F F
0.2500000159614544 0.5788443260065463 0.0035690153482122 F F F
0.7500000478843631 0.5788443260065463 0.0035690153482122 F F F
0.2500000159614544 0.6711557538007185 0.0035690153482122 F F F
0.7500000478843631 0.6711557538007185 0.0035690153482122 F F F
0.2500000159614544 0.8288443419680007 0.0035690153482122 F F F
0.7500000478843631 0.8288443419680007 0.0035690153482122 F F F
0.2500000159614544 0.9211557697621728 0.0035690153482122 F F F
0.7500000478843631 0.9211557697621728 0.0035690153482122 F F F
0.1200794017695138 0.3734936754752400 0.3012131632114565 T T T
0.2206805017004840 0.3562279495540943 0.3346887679223416 T T T
0.1499697051494027 0.3851470902602024 0.4143629949692966 T T T
0.0854282949055967 0.4547191526639649 0.3758675275130043 T T T
0.0010075148322384 0.3284766391784444 0.4279941142206735 T T T
0.9744813662021259 0.3406222493284264 0.3636139751282541 T T T
0.1013407788205879 0.2069043476433197 0.4094927413741182 T T T
0.0179223726338795 0.1897440198003537 0.3629082984018084 T T T

Ic(4x2), E = -386.55667 eV

1.0000000000000000
7.6621999740000000 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H
48 1 4 24

Selective dynamics

Direct

0.0982437263469365 0.0000000011734684 0.0289689852776368 F F F
0.0982437493469206 0.2500002971734435 0.0289689852776368 F F F
0.5982443673469362 0.0000000011734684 0.0289689852776368 F F F
0.0982437713469366 0.5000005951734678 0.0289689852776368 F F F
0.5982443673469362 0.2500002971734435 0.0289689852776368 F F F
0.0982437933469313 0.7500008931734712 0.0289689852776368 F F F
0.5982444273469341 0.5000005951734678 0.0289689852776368 F F F
0.5982444273469341 0.7500008931734712 0.0289689852776368 F F F
0.3481889148011417 0.9995021537363799 0.0796618693222388 F F F
0.3482099635546240 0.2528227589216172 0.0806418874415176 F F F
0.8482098579642852 0.9984169186223468 0.0807822717142645 F F F
0.3481536313615905 0.4981877663151135 0.0807373416799084 F F F
0.8482139166746969 0.2521299693376946 0.0802085390540572 F F F
0.3481955688589979 0.7531385895576791 0.0800458566958060 F F F
0.8482115512265977 0.4972844060945221 0.0801440306302314 F F F
0.8483293512468748 0.7520680719317955 0.0806932257095614 F F F
0.3481064799572325 0.1251348317794909 0.1274566339846488 T T T
0.3478835057188761 0.3756469106591145 0.1349717207322348 T T T
0.8487924492987751 0.1256182941332659 0.1278880960097566 T T T
0.3482862465239915 0.6265602091166621 0.1273851486782513 T T T
0.8482930323651824 0.3748159208955864 0.1338293822479784 T T T
0.3482830208990995 0.8764771704240475 0.1334895363199646 T T T
0.8484311187346640 0.6239282008488524 0.1272770562672345 T T T
0.8484114665555148 0.8754393114380160 0.1350427508793285 T T T
0.0989465388029175 0.1258188471500084 0.1768854743133219 T T T
0.0963511205790533 0.3744916983690630 0.1869211911751882 T T T
0.5980387453331649 0.1253202932794174 0.1764601050378006 T T T
0.0980652836112672 0.6256869129086691 0.1767637983738380 T T T
0.5997342971485281 0.3746787097681147 0.1866469105569006 T T T

0.1005764967544640 0.8770914235498657 0.1868768085837669 T T T
0.5986582117589829 0.6257193813479929 0.1766615467592831 T T T
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0.1169665485611711 0.0082200852645597 0.2344774515391710 T T T
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0.6090204629052286 0.2422142839609402 0.2324243238398638 T T T
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0.8485243247967765 0.0638860408083418 0.2612190110820808 T T T
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0.3583093596665629 0.2517567123927084 0.3330607207793298 T T T
0.3716410594686862 0.3486538118641969 0.3323458831665831 T T T
0.2253990451897130 0.3788799291627423 0.3662105064220839 T T T
0.2154245382059746 0.3056918799604663 0.4052175317588144 T T T
0.2397386786463369 0.2237708234427842 0.3741805024369789 T T T
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Ic(2x2), E = -386.49737 eV

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Si O C H
48 1 4 24

Selective dynamics

Direct

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 0.8482098579642930 0.9984169186223468 0.0807822717142645 F F F
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 0.8482139166747048 0.2521299693376946 0.0802085390540572 F F F
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 0.8482115512265977 0.4972844060945221 0.0801440306302314 F F F
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0.0982438099999783 0.3320527369999980 0.0000000162939813 F F F
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0.0982437660000031 0.4179481569999695 0.0000000000000000 F F F
0.0982438329999979 0.5820530649999256 0.0000000162939813 F F F
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0.5982443690000008 0.4179481269999958 0.0000000162939813 F F F
0.5982443690000001 0.8320533629999289 0.0000000000000000 F F F
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Ic(4x4), E = -700.85390 eV

1.0000000000000000
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0.0000000000000000 15.3244190216000007 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.7875003810000010

Si O C H
96 1 4 40

Selective dynamics

Direct

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0.0000000000000000 0.2500000159614544 0.0354635925893937 F F F
0.5000000319229088 0.2500000159614544 0.0354635925893937 F F F
0.2500000159614544 0.0000000000000000 0.0354635925893937 F F F
0.7500000478843631 0.0000000000000000 0.0354635925893937 F F F
0.0000000000000000 0.5000000319229088 0.0354635925893937 F F F
0.5000000319229088 0.5000000319229088 0.0354635925893937 F F F
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0.7500000478843631 0.2500000159614544 0.0354635925893937 F F F
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0.7500000478843631 0.5000000319229088 0.0354635925893937 F F F
0.2500000159614544 0.7500000478843631 0.0354635925893937 F F F
0.7500000478843631 0.7500000478843631 0.0354635925893937 F F F
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0.6250000072759718 0.0000000000000000 0.0860282208949446 F F F
0.1249999753530631 0.2500000159614544 0.0860282208949446 F F F
0.6250000072759718 0.2500000159614544 0.0860282208949446 F F F
0.3749999913145174 0.0000000000000000 0.0860282208949446 F F F
0.8750000232374191 0.0000000000000000 0.0860282208949446 F F F
0.1249999753530631 0.5000000319229088 0.0860282208949446 F F F
0.6250000072759718 0.5000000319229088 0.0860282208949446 F F F

0.3749999913145174 0.2500000159614544 0.0860282208949446 F F F
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0.8750000232374191 0.5000000319229088 0.0860282208949446 F F F
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0.8750000232374191 0.7500000478843631 0.0860282208949446 F F F
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0.7500000478843631 0.3288443100450991 0.0035690153482121 F F F
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0.5000000319229088 0.8288443419680007 0.0035690153482121 F F F
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0.2500000159614544 0.5788443260065463 0.0035690153482121 F F F
0.7500000478843631 0.5788443260065463 0.0035690153482121 F F F
0.2500000159614544 0.6711557538007185 0.0035690153482121 F F F
0.7500000478843631 0.6711557538007185 0.0035690153482121 F F F
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0.1301459203286109 0.3690294425917870 0.3000926862486921 T T T
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0.0754782192091342 0.4408817808079014 0.3894404582680089 T T T
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0.1055754149315184 0.1674390167989729 0.3989896957278264 T T T
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TS Ib Ic invert, E = -386.49620 eV

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-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H

48 1 4 24

Selective dynamics

Direct

0.0982437263469365 0.0000000011734684 0.0289689852776368 F F F
0.0982437493469206 0.2500002971734290 0.0289689852776368 F F F
0.5982443673469362 0.0000000011734684 0.0289689852776368 F F F
0.0982437713469366 0.5000005951734678 0.0289689852776368 F F F
0.5982443673469362 0.2500002971734290 0.0289689852776368 F F F
0.0982437933469313 0.7500008931734712 0.0289689852776368 F F F
0.5982444273469341 0.5000005951734678 0.0289689852776368 F F F
0.5982444273469341 0.7500008931734712 0.0289689852776368 F F F
0.3481889148011417 0.9995021537363513 0.0796618693222389 F F F
0.3482099635546240 0.2528227589216031 0.0806418874415176 F F F
0.8482098579642510 0.9984169186223468 0.0807822717142646 F F F
0.3481536313615763 0.4981877663151056 0.0807373416799085 F F F
0.8482139166746706 0.2521299693376946 0.0802085390540573 F F F
0.3481955688589979 0.7531385895576795 0.0800458566958060 F F F
0.8482115512265977 0.4972844060945155 0.0801440306302315 F F F
0.8483293512468464 0.7520680719317809 0.0806932257095614 F F F
0.3478412776386227 0.1251479106685832 0.1274520700625801 T T T
0.3481190081598192 0.3756150207556724 0.1350021437427691 T T T
0.8489494459607217 0.1256606031699725 0.1279169660666865 T T T
0.3481382028303435 0.6265703981032530 0.1273663956279890 T T T
0.8487504052718282 0.3747949458970776 0.1337966096216795 T T T
0.3482092454772465 0.8764308853591690 0.1334424939687081 T T T
0.8481008267082238 0.6239490302274137 0.1272421720961653 T T T
0.8482821107607660 0.8754340720565426 0.1350450595168541 T T T
0.0989998022468720 0.1261390289852379 0.1770459911185601 T T T
0.0965934381607443 0.3744759734683191 0.1869431904642535 T T T
0.5978386808746528 0.1250746874266735 0.1763871246067595 T T T
0.0977789387230023 0.6258217896125335 0.1766404244386678 T T T
0.6002713488656891 0.3745852610285478 0.1865769473810741 T T T
0.1005803967364038 0.8770029331475879 0.1868216173012243 T T T
0.5984278753172367 0.6256130594146796 0.1766832290560268 T T T
0.5958672067585693 0.8767674110804645 0.1867919545656533 T T T
0.1166512614717898 0.0081616642050304 0.2343460131069064 T T T
0.0865843174786142 0.2428563216761833 0.2336182567207613 T T T
0.5797269029414981 0.0079501877107261 0.2342392374194682 T T T
0.0820052418893155 0.5065424818018883 0.2332643266006174 T T T
0.6094321708232624 0.2419947612695917 0.2322819159951213 T T T
0.1142851952366923 0.7449420042728626 0.2335305257114391 T T T
0.6153761859803355 0.5063529861126432 0.2334286232426837 T T T
0.5824004289472781 0.7447754747856163 0.2335600076838243 T T T
0.3482713212197301 0.0415420698283429 0.2909252662780630 T T T
0.3491477608346926 0.1949351156193460 0.2704025512992907 T T T
0.8480244447173600 0.0633555950403866 0.2610259725725360 T T T

0.3486064315258534	0.5633491222459661	0.2609990257132288	T	T	T
0.8457866955341768	0.2100801354641137	0.2871472171645760	T	T	T
0.3482848746119154	0.7096971934131359	0.2889368796877738	T	T	T
0.8488214277910699	0.5407521893169084	0.2893097838159326	T	T	T
0.8484489552104142	0.6882595995447861	0.2616907084305620	T	T	T
0.3661686555755075	0.2507460481610027	0.3338850953846642	T	T	T
0.4072528068196852	0.3447123122293923	0.3372805319243935	T	T	T
0.2496527071499994	0.3866529423360675	0.3626629475300258	T	T	T
0.1428366239633931	0.3102074063659505	0.3850172268254159	T	T	T
0.2530647226566684	0.2289685583150983	0.376656069833845	T	T	T
0.0982437210000029	0.9179475529998982	0.0000000000000000	F	F	F
0.0982437879999907	0.0820524620000000	0.0000000162939813	F	F	F
0.0982437429999905	0.1679478439999969	0.0000000000000000	F	F	F
0.0982438099999853	0.3320527369999980	0.0000000162939813	F	F	F
0.5982443090000018	0.0820524470000024	0.0000000000000000	F	F	F
0.5982443089999103	0.9179475379998649	0.0000000162939813	F	F	F
0.0982437660000031	0.4179481569999552	0.0000000000000000	F	F	F
0.0982438329999979	0.5820530649998972	0.0000000162939813	F	F	F
0.5982443089998817	0.3320527079999994	0.0000000000000000	F	F	F
0.5982443090000018	0.1679478289999992	0.0000000162939813	F	F	F
0.0982437950000019	0.6679484840000008	0.0000000000000000	F	F	F
0.0982438469999920	0.8320534229998700	0.0000000162939813	F	F	F
0.5982443689999997	0.5820530060000032	0.0000000000000000	F	F	F
0.5982443690000008	0.4179481269999958	0.0000000162939813	F	F	F
0.5982443690000001	0.8320533629999076	0.0000000000000000	F	F	F
0.5982443689998872	0.6679484249998853	0.0000000162939813	F	F	F
0.4309415814316129	0.3672491347920251	0.2989530356173275	T	T	T
0.5287913075518044	0.3497003427591857	0.3588858064367621	T	T	T
0.2927639161866352	0.4331135329364744	0.3913118575381074	T	T	T
0.1699682679048889	0.4229927870518149	0.3355547747326798	T	T	T
0.1153295158783345	0.3193903989896313	0.4248920064733249	T	T	T
0.0176752265692320	0.3032338053653824	0.3652391724912031	T	T	T
0.3411517555110259	0.2137137805468161	0.4078842690888877	T	T	T
0.1796507685260695	0.1703411478353686	0.3659611543795614	T	T	T

TS Ib Ic tilt, E = -386.48131 eV

1.0000000000000000		
7.6621999740000000	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000
-0.0000007340000000	-0.0000007340000000	26.7875003810000010

Si O C H

48 1 4 24

Selective dynamics

Direct

0.0982437263469365	0.0000000011734684	0.0289689852776397	F	F	F
0.0982437493469206	0.2500002971734362	0.0289689852776397	F	F	F
0.5982443673469362	0.0000000011734684	0.0289689852776397	F	F	F
0.0982437713469366	0.5000005951734678	0.0289689852776397	F	F	F
0.5982443673469362	0.2500002971734362	0.0289689852776397	F	F	F
0.0982437933469313	0.7500008931734712	0.0289689852776397	F	F	F
0.5982444273469341	0.5000005951734678	0.0289689852776397	F	F	F
0.5982444273469341	0.7500008931734712	0.0289689852776397	F	F	F
0.3481889148011417	0.9995021537363877	0.0796618693222480	F	F	F
0.3482099635546240	0.2528227589216101	0.0806418874415267	F	F	F
0.8482098579642930	0.9984169186223468	0.0807822717142737	F	F	F
0.3481536313615905	0.4981877663151135	0.0807373416799176	F	F	F

0.8482139166747048 0.2521299693376946 0.0802085390540664 F F F
0.3481955688589979 0.7531385895577521 0.0800458566958152 F F F
0.8482115512265977 0.4972844060945221 0.0801440306302406 F F F
0.8483293512468819 0.7520680719318094 0.0806932257095705 F F F
0.3483025759763476 0.1251894858175325 0.1275373231492938 T T T
0.3484007802956045 0.3756019125188977 0.1350465411262526 T T T
0.8479519545677168 0.1255812457042286 0.1277986486076776 T T T
0.3482204464401643 0.6265555576650421 0.1273553918343200 T T T
0.8483046267195804 0.3748609691597640 0.1337998886201766 T T T
0.3482843601258621 0.8764831139048394 0.1334692941882188 T T T
0.8482327022428174 0.6239218638630583 0.1272683099644672 T T T
0.8482883774133884 0.8754421622849536 0.1350112112471794 T T T
0.0981743672410090 0.1256483568294619 0.1765558587391403 T T T
0.0964468252555465 0.3744730681158389 0.1867532383357443 T T T
0.5980374830096002 0.1259252710934794 0.1767740319074944 T T T
0.0979661954389299 0.6257062653018114 0.1766801883497159 T T T
0.6003382106270068 0.3744952121375987 0.1868460354790816 T T T
0.1005039114764595 0.8769564240824795 0.1867922260678011 T T T
0.5985053653380409 0.6257184427114142 0.1766970888985504 T T T
0.5961162942107860 0.8770171000659975 0.1868128254251765 T T T
0.1159975854623972 0.0082549705472369 0.2341891727909519 T T T
0.0860544910670476 0.2422296555751802 0.2328127888257038 T T T
0.5806652049837011 0.0082678977207647 0.2343000959795121 T T T
0.0824114186095662 0.5064421810698702 0.2334019947151076 T T T
0.6103711692932183 0.2425005317940796 0.2332060123209425 T T T
0.1142831004951867 0.7449597429883358 0.2335133912815446 T T T
0.6156320677015567 0.5064347768063934 0.2335020577538796 T T T
0.5825365298866466 0.7449747687151845 0.2335360482748189 T T T
0.3481485429138105 0.0412884081840340 0.2906774015012629 T T T
0.3480152103053363 0.1944849900740212 0.2699785764600914 T T T
0.8483971215437536 0.0642436693862816 0.2613905764229337 T T T
0.3489616906980666 0.5636049648587633 0.2610072854973001 T T T
0.8486292978769185 0.2111692792490243 0.2881484246460191 T T T
0.3484293323756914 0.7099367641711116 0.2889022531840379 T T T
0.8490782532173116 0.5408958228382794 0.2893920931220983 T T T
0.8484797593480693 0.6883040670492548 0.2616832271274090 T T T
0.3453433237443302 0.2532164735041678 0.3318177050566090 T T T
0.3196995322856858 0.3488455027326872 0.3331664307752074 T T T
0.3441969725787385 0.3719075122754562 0.3877600835664206 T T T
0.2775624141437426 0.2898943314452945 0.4146674358002310 T T T
0.3483049292455097 0.2160876091002610 0.3827788323782519 T T T
0.0982437210000029 0.9179475529999339 0.0000000000000000 F F F
0.0982437879999978 0.0820524620000000 0.0000000162939813 F F F
0.0982437429999976 0.1679478439999969 0.0000000000000000 F F F
0.0982438099999853 0.3320527369999980 0.0000000162939813 F F F
0.5982443090000018 0.0820524470000024 0.0000000000000000 F F F
0.5982443089999392 0.9179475379999005 0.0000000162939813 F F F
0.0982437660000031 0.4179481569999628 0.0000000000000000 F F F
0.0982438329999979 0.5820530649999327 0.0000000162939813 F F F
0.5982443089999094 0.3320527079999994 0.0000000000000000 F F F
0.5982443090000018 0.1679478289999992 0.0000000162939813 F F F
0.0982437950000019 0.6679484840000008 0.0000000000000000 F F F
0.0982438469999920 0.8320534229999055 0.0000000162939813 F F F
0.5982443689999997 0.5820530060000032 0.0000000000000000 F F F
0.5982443690000008 0.4179481269999958 0.0000000162939813 F F F
0.5982443690000001 0.8320533629999365 0.0000000000000000 F F F
0.5982443689999161 0.6679484249999348 0.0000000162939813 F F F

0.1867381953905659 0.3616595805820295 0.3193738322715876 T T T
0.4159795909003341 0.3775763232191874 0.3075746699638745 T T T
0.4830667107719905 0.3832219241297808 0.3959455438459995 T T T
0.2708747889014572 0.4309644547959864 0.3976863465897242 T T T
0.3238107802278765 0.2852210926230377 0.4533661569907593 T T T
0.1339941342271770 0.2884768509404309 0.4147473498243276 T T T
0.4849956913416076 0.1995091248477484 0.3909900930185995 T T T
0.2688169901013296 0.1565965167956179 0.3817913648461613 T T T

TS Ib Ic rotate, E = -386.38989 eV

1.0000000000000000
7.6621999740000000 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H

48 1 4 24

Selective dynamics

Direct

0.0982433274800485 0.0000000013875479 0.0289691083140594 F F F
0.0982433493406134 0.2500000022358651 0.0289691083140594 F F F
0.5982446342848898 0.0000000013875479 0.0289691083140594 F F F
0.0982433712012352 0.5000006556382885 0.0289691083140594 F F F
0.5982446561454542 0.2500000022358651 0.0289691083140594 F F F
0.0982433930617930 0.7500006564866055 0.0289691083140594 F F F
0.5982446780060757 0.5000006556382885 0.0289691083140594 F F F
0.5982446998666333 0.7500006564866055 0.0289691083140594 F F F
0.3481886060388885 0.9995021084313791 0.0796617814148032 F F F
0.3482094225726087 0.2528229537429070 0.0806417160718848 F F F
0.8482094894791755 0.9984169110185107 0.0807824533540650 F F F
0.3481533243845121 0.4981878628309879 0.0807372830327292 F F F
0.8482133394917644 0.2521299412690823 0.0802086782805670 F F F
0.3481951100741014 0.7531387915948997 0.0800459158003800 F F F
0.8482120558142654 0.4972847279296115 0.0801440959203074 F F F
0.8483295378834946 0.7520679503495344 0.0806932326367157 F F F
0.3484658170444908 0.1250025408394420 0.1271451376781614 T T T
0.3483179334670605 0.3757285669900073 0.1349128759305434 T T T
0.8480295243492509 0.1256000632992384 0.1281270569900214 T T T
0.3482278825150165 0.6265128212045653 0.1275044360297338 T T T
0.8482245984682916 0.3749593354557278 0.1335191317088568 T T T
0.3482800026986223 0.8763241230072321 0.1334442598207615 T T T
0.8483474185825144 0.6238821241594132 0.1273100446247626 T T T
0.8482767726740442 0.8756400846233225 0.1354300734495846 T T T
0.0999755109392793 0.1245236763008746 0.1765060047238910 T T T
0.0959971366809044 0.3748994778350379 0.1864080685535796 T T T
0.5965233074574284 0.1249253353081788 0.1767531142272546 T T T
0.0978654085576256 0.6254290264114265 0.1768853696301012 T T T
0.6005623675185283 0.3748592561506366 0.1864478971653416 T T T
0.1017252468585700 0.8770249851269234 0.1871511747837005 T T T
0.5987226678087872 0.6255313141181444 0.1768089838025601 T T T
0.5948375447546219 0.8771004109416666 0.1871602642149963 T T T
0.1198525094075782 0.0082328248506114 0.2348846924964196 T T T
0.0873767727364355 0.2423039911411367 0.2316451979712118 T T T
0.5765408190623629 0.0083003555614687 0.2349407542648466 T T T
0.0811841421895070 0.5059739672509279 0.2336535779755738 T T T
0.6093528990007918 0.2426334266710908 0.2320832218201133 T T T
0.1141940373744488 0.7446432496007058 0.2337432179635491 T T T

0.6150978980108344	0.5061066971243028	0.2335099774414697	T	T	T
0.5824158731571942	0.7446638231242151	0.2337210577075167	T	T	T
0.3481015427814408	0.0454899887624042	0.2926079532516789	T	T	T
0.3479138488187863	0.2003350951138493	0.2712651841993713	T	T	T
0.8482374537444407	0.0612107625020046	0.2599077991404948	T	T	T
0.3481641712896779	0.5623288360077515	0.2612207715670576	T	T	T
0.8488775827941796	0.2073595800896570	0.2848102538796025	T	T	T
0.3483125221011810	0.7086935885601187	0.2889106255646360	T	T	T
0.8480175227919139	0.5402632762718433	0.2896977347232085	T	T	T
0.8482947358732115	0.6880292054312755	0.2619699774155071	T	T	T
0.3477684006013298	0.2682426722584659	0.3321543623384168	T	T	T
0.5075557431664972	0.3133295422644783	0.3496752047755399	T	T	T
0.4468258060485375	0.3636519909843852	0.3949906900843264	T	T	T
0.2633829272508129	0.3930448571382062	0.3794927924043870	T	T	T
0.1911187013736726	0.3148819860125059	0.3514687973321389	T	T	T
0.0982434049723793	0.9179478509914460	0.0000000000000000	F	F	F
0.0982433318797860	0.0820521524018362	0.0000000000000000	F	F	F
0.0982433393906987	0.1679478484464812	0.0000000000000000	F	F	F
0.0982433537404006	0.3320528058042603	0.0000000000000000	F	F	F
0.5982446386846195	0.0820521524018362	0.0000000000000000	F	F	F
0.5982447117772196	0.9179478509914460	0.0000000000000000	F	F	F
0.0982433612512565	0.4179478492948050	0.0000000000000000	F	F	F
0.0982433756009655	0.5820528066525767	0.0000000000000000	F	F	F
0.5982446605452409	0.3320528058042603	0.0000000000000000	F	F	F
0.5982446461955330	0.1679478484464812	0.0000000000000000	F	F	F
0.0982433831118783	0.6679485026972226	0.0000000000000000	F	F	F
0.0982433974615802	0.8320534600549934	0.0000000000000000	F	F	F
0.5982446824058059	0.5820528066525767	0.0000000000000000	F	F	F
0.5982446680560973	0.4179478492948050	0.0000000000000000	F	F	F
0.5982447042664205	0.8320534600549934	0.0000000000000000	F	F	F
0.5982446899167189	0.6679485026972226	0.0000000000000000	F	F	F
0.5523404211384165	0.3565979209542793	0.3193839094715545	T	T	T
0.6062761712644366	0.2627250908442852	0.3562656581926442	T	T	T
0.4417415107273420	0.3209632701043394	0.4279880167505536	T	T	T
0.5343446552476326	0.4186566200442860	0.4029910677980960	T	T	T
0.1801336321175683	0.4105526135713680	0.4112938287715673	T	T	T
0.2707492938476337	0.4500678131500290	0.3545289562833123	T	T	T
0.1210759403521013	0.2677138404399153	0.3749423759416200	T	T	T
0.1092664191542944	0.3320302806610874	0.3193189956934484	T	T	T

8.4. Final State A Configurations

Ac, E(PBE-D3) = -388.41297 eV, E(HSE06-D3) = -449.84266 eV

1.0000000000000000		
7.6621999740000000	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000
-0.0000007340000000	-0.0000007340000000	26.7875003810000010

Si O C H
48 1 4 24

Selective dynamics

Direct

0.0982437263469294	0.0000000016016131	0.0289689852776363	F	F	F
0.0982437493469277	0.2500002971734433	0.0289689852776363	F	F	F
0.5982443673469362	0.0000000016016131	0.0289689852776363	F	F	F
0.0982437713469366	0.5000005951734678	0.0289689852776363	F	F	F
0.5982443673469362	0.2500002971734433	0.0289689852776363	F	F	F
0.0982437933469313	0.7500008931734712	0.0289689852776363	F	F	F

0.5982444273469341 0.5000005951734678 0.0289689852776363 F F F
0.5982444273469341 0.7500008931734712 0.0289689852776363 F F F
0.3480383385581050 0.9981421732642418 0.0800122532992163 F F F
0.3480377191238091 0.2523206682297641 0.0807251537912919 F F F
0.8480882003325192 0.9990134760524754 0.0809062178506253 F F F
0.3480599805555897 0.4977572267302294 0.0807011518149352 F F F
0.8481536924994943 0.2521531409645092 0.0801095804747902 F F F
0.3479654336356290 0.7518208992697737 0.0800015227840163 F F F
0.8482636818747196 0.4982203957225907 0.0800102540313006 F F F
0.8484488576981448 0.7510569402139282 0.0809839353321493 F F F
0.3483836654120207 0.1244148837622736 0.1271711990178072 T T T
0.3487111986125573 0.3753433283081714 0.1351913841582473 T T T
0.8472114416568830 0.1261291439762796 0.1287920809182290 T T T
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0.8481891861380408 0.3753946116842103 0.1336071481519215 T T T
0.3482422348911159 0.8751967297471973 0.1334208975259660 T T T
0.8483401216114821 0.6237009154884288 0.1279957599935357 T T T
0.8479992334005785 0.8747676543658622 0.1341990416203145 T T T
0.1004734427796647 0.1276031318209394 0.1767799735580901 T T T
0.0960544012043793 0.3752947105214480 0.1866796352387010 T T T
0.5949505323178926 0.1279298748212093 0.1775267774220363 T T T
0.0989390581157842 0.6250767734358029 0.1770738641430721 T T T
0.6010093893426932 0.3748603692044058 0.1870242665990990 T T T
0.0990241423360434 0.8741839192611002 0.1860339023263764 T T T
0.5975301527661928 0.6251610748667200 0.1769758724441216 T T T
0.5972431681285456 0.8744653553401238 0.1862404935676711 T T T
0.1064000430990902 0.0061254639910097 0.2320574285853224 T T T
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0.5900587796382059 0.0061494668717246 0.2328226252470922 T T T
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0.6054216550251574 0.2441461013085210 0.2346212646990462 T T T
0.1149397793993205 0.7439713219461114 0.2338766414406196 T T T
0.6142674062995144 0.5063981579926443 0.2338967692764281 T T T
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0.3462651986321191 0.2083399870758909 0.2776709753592073 T T T
0.8487916928584168 0.0688018223449222 0.2617816666392758 T T T
0.3484958498356688 0.5630531793120963 0.2620750740324345 T T T
0.8510132846785586 0.2141952805090425 0.2868489426796547 T T T
0.3484914507923196 0.7104532207666896 0.2898304283409547 T T T
0.8483297974605104 0.5410797231945594 0.2893402995453824 T T T
0.8484298066702598 0.6875546262968850 0.2616031820794197 T T T
0.3274642650445725 0.2420893300427161 0.3366852479640649 T T T
0.3417030405587607 0.0116651820443712 0.3466428980046683 T T T
0.4740242710423737 0.0544338253041347 0.3822798880850373 T T T
0.4203449763825295 0.1425537241020672 0.4052146209845383 T T T
0.4540213614856899 0.2255007413855968 0.3751556469862486 T T T
0.0982437210000029 0.9179475529999410 0.0000000000000000 F F F
0.0982437879999907 0.0820524620000000 0.0000000162939813 F F F
0.0982437429999976 0.1679478439999969 0.0000000000000000 F F F
0.0982438099999854 0.3320527369999980 0.0000000162939813 F F F
0.5982443090000018 0.0820524470000024 0.0000000000000000 F F F
0.5982443089999450 0.9179475379999291 0.0000000162939813 F F F
0.0982437660000031 0.4179481569999695 0.0000000000000000 F F F
0.0982438329999979 0.5820530649999399 0.0000000162939813 F F F
0.5982443089999379 0.3320527079999992 0.0000000000000000 F F F
0.5982443090000018 0.1679478289999992 0.0000000162939813 F F F

0.0982437950000019 0.6679484840000003 0.0000000000000000 F F F
0.0982438469999920 0.8320534229999339 0.0000000162939813 F F F
0.5982443689999997 0.5820530060000026 0.0000000000000000 F F F
0.5982443689999999 0.4179481269999955 0.0000000162939813 F F F
0.5982443689999999 0.8320533629999576 0.0000000000000000 F F F
0.5982443689999359 0.6679484249999348 0.0000000162939813 F F F
0.2076031488112716 0.0217435340221742 0.3605339065177401 T T T
0.3620542756438817 -0.0595719863637000 0.3453288154440662 T T T
0.4965370862590636 0.0086304769198370 0.4133793465695290 T T T
0.6021788216952407 0.0617308453245797 0.3637335451026179 T T T
0.2814061180122356 0.1408870978785995 0.4160762977861889 T T T
0.4946446106633038 0.1507123169257836 0.4402101270506822 T T T
0.4473953412940332 0.2822301236934535 0.4003576741340824 T T T
0.5871548753338233 0.2239899102461276 0.3590707672788427 T T T

Ab, E = -388.33117 eV

1.0000000000000000
7.6621999740000000 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H

48 1 4 24

Selective dynamics

Direct

0.0982437263469365 0.0000000011734684 0.0289689852776363 F F F
0.0982437493469277 0.2500002971734574 0.0289689852776363 F F F
0.5982443673469362 0.0000000011734684 0.0289689852776363 F F F
0.0982437713469366 0.5000005951734678 0.0289689852776363 F F F
0.5982443673469362 0.2500002971734574 0.0289689852776363 F F F
0.0982437933469313 0.7500008931734712 0.0289689852776363 F F F
0.5982444273469341 0.5000005951734678 0.0289689852776363 F F F
0.5982444273469341 0.7500008931734712 0.0289689852776363 F F F
0.3480383385581050 0.9981421732642418 0.0800122532992163 F F F
0.3480377191238304 0.2523206682297783 0.0807251537912919 F F F
0.8480882003325476 0.9990134760524754 0.0809062178506253 F F F
0.3480599805555897 0.4977572267302436 0.0807011518149352 F F F
0.8481536924995225 0.2521531409645164 0.0801095804747902 F F F
0.3479654336356290 0.7518208992697737 0.0800015227840163 F F F
0.8482636818747480 0.4982203957225977 0.0800102540313006 F F F
0.8484488576981735 0.7510569402139640 0.0809839353321493 F F F
0.3490934134701953 0.1243880335747542 0.1271609028930430 T T T
0.3491361572453668 0.3753869875480558 0.1351474785653822 T T T
0.8456321439694179 0.1261368858989370 0.1288882037067426 T T T
0.3480404669414054 0.6257120095069498 0.1274383333011771 T T T
0.8482151657979397 0.3753782690711865 0.1335851034248496 T T T
0.3486028907134723 0.8751871635392120 0.1334397040527301 T T T
0.8483592323050237 0.6236953245265958 0.1279744807528702 T T T
0.8477658257142561 0.8747610855021969 0.1341818862268141 T T T
0.1002443367746481 0.1279317492569881 0.1761597515059455 T T T
0.0964514165613185 0.3755831455114130 0.1864689702241230 T T T
0.5941156575699056 0.1275102248552010 0.1783742982483739 T T T
0.0988548279895525 0.6251081858519917 0.1770751788083522 T T T
0.6012825232318330 0.3746713966077831 0.1871196359924977 T T T
0.0990179703132206 0.8739235170512643 0.1858101255144767 T T T
0.5975271202572466 0.6250549565551061 0.1769327241198854 T T T
0.5974076007839726 0.8745219208821896 0.1864713098531796 T T T

0.1068016946133182	0.0063783772840337	0.2310530680764795	T	T	T
0.0941986145962257	0.2442273937409347	0.2328385786324407	T	T	T
0.5909903927747887	0.00533557729448217	0.2340884422163459	T	T	T
0.0826226638743392	0.5063123333733045	0.2339766567039392	T	T	T
0.6059817155809923	0.2444036534255929	0.2352681264002052	T	T	T
0.1146714569191313	0.7439705735400786	0.2339032172558448	T	T	T
0.6143073752903928	0.5063239102972065	0.2338654444618858	T	T	T
0.5818114280952941	0.7437702527758507	0.2338049517092014	T	T	T
0.3452896893796576	0.0513546134086458	0.2792513477431939	T	T	T
0.3464235235829548	0.2075931458892178	0.2779790235703016	T	T	T
0.8509138471198044	0.0690749552257493	0.2616135110884851	T	T	T
0.3484641557792550	0.5629930663107279	0.2620051152834350	T	T	T
0.8543627133493390	0.2147449389322292	0.2863120547446966	T	T	T
0.3483656187733896	0.7103269654450114	0.2897856635456053	T	T	T
0.8483197434732223	0.5408866605544519	0.2893569630310501	T	T	T
0.8482827771747429	0.6874031383649434	0.2616447748066235	T	T	T
0.3145504967377057	0.2369285771254470	0.3373532072564197	T	T	T
0.3071589166331004	0.0226724602443961	0.3476711903155549	T	T	T
0.4487947252816900	0.0494419998549086	0.3851937415225172	T	T	T
0.5360328232431443	0.1384677641701441	0.3777323185446242	T	T	T
0.4252181579492721	0.2210838372677420	0.3796899294937716	T	T	T
0.0982437210000029	0.9179475529999763	0.0000000000000000	F	F	F
0.0982437879999978	0.0820524620000000	0.0000000162939813	F	F	F
0.0982437429999976	0.1679478439999969	0.0000000000000000	F	F	F
0.0982438099999925	0.3320527369999980	0.0000000162939813	F	F	F
0.5982443090000018	0.0820524470000024	0.0000000000000000	F	F	F
0.5982443089999807	0.9179475379999644	0.0000000162939813	F	F	F
0.0982437660000031	0.4179481569999838	0.0000000000000000	F	F	F
0.0982438329999979	0.5820530649999753	0.0000000162939813	F	F	F
0.5982443089999663	0.3320527079999992	0.0000000000000000	F	F	F
0.5982443090000018	0.1679478289999992	0.0000000162939813	F	F	F
0.0982437950000019	0.6679484840000003	0.0000000000000000	F	F	F
0.0982438469999920	0.8320534229999625	0.0000000162939813	F	F	F
0.5982443689999997	0.5820530060000026	0.0000000000000000	F	F	F
0.5982443689999999	0.4179481269999955	0.0000000162939813	F	F	F
0.5982443689999999	0.8320533629999787	0.0000000000000000	F	F	F
0.5982443689999644	0.6679484249999632	0.0000000162939813	F	F	F
0.1836540274084515	0.0571942153810000	0.3557236275499746	T	T	T
0.2788782551408880	-0.0475988926502000	0.3509815359910670	T	T	T
0.3930139272537305	0.0464751565434983	0.4231886093168521	T	T	T
0.5533090633699055	-0.0000424252597495	0.3843852060484566	T	T	T
0.6374847290472864	0.1460140880384548	0.4066568327398301	T	T	T
0.6098481014613646	0.1387528580441242	0.3422156436006008	T	T	T
0.3382055202013928	0.2200030945231747	0.4125175978944172	T	T	T
0.5132969129758880	0.2776940200614326	0.3836858388730945	T	T	T

At, E = -388.38793 eV

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7.6621999740000000	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000
-0.0000007340000000	-0.0000007340000000	26.7875003810000010

Si O C H

48 1 4 24

Selective dynamics

Direct

0.0982437263469365	0.0000000011734684	0.0289689852776363	F	F	F
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0.0982437493469064 0.2500002971733936 0.0289689852776363 F F F
0.5982443673469362 0.0000000011734684 0.0289689852776363 F F F
0.0982437713469366 0.5000005951734678 0.0289689852776363 F F F
0.5982443673469362 0.2500002971733936 0.0289689852776363 F F F
0.0982437933469171 0.7500008931734712 0.0289689852776363 F F F
0.5982444273469341 0.5000005951734678 0.0289689852776363 F F F
0.5982444273469341 0.7500008931734712 0.0289689852776363 F F F
0.3480649108361930 0.9983821698181290 0.0799504208326738 F F F
0.3480681151998014 0.2524092724694711 0.0807104597295592 F F F
0.8481096693262131 0.9989082012117054 0.0808843450030495 F F F
0.3480765071683224 0.4978332043040012 0.0807075382616774 F F F
0.8481643202950906 0.2521490518538485 0.0801270437534925 F F F
0.3480060457338183 0.7520534328499624 0.0800093464154870 F F F
0.8482544823484377 0.4980552210823533 0.0800338616663794 F F F
0.8484277683242427 0.7512353752229759 0.0809326336340704 F F F
0.3483794713224802 0.1245705643541631 0.1271063241505835 T T T
0.3485048229964277 0.3753900825971569 0.1351833584291794 T T T
0.8477667706029863 0.1259829626970933 0.1287396400537203 T T T
0.3480688066614451 0.6258697932899387 0.1274159304559152 T T T
0.8481516666679046 0.3753280444211857 0.1336098829195853 T T T
0.3482387026825626 0.8754562417597576 0.1334227402686334 T T T
0.8482607635885562 0.6237516813265422 0.1278805564426686 T T T
0.8482838634062781 0.8749248286665712 0.1343664664303789 T T T
0.1008694133893805 0.1275677406025196 0.1768602891088834 T T T
0.0958502240688200 0.3752173471143040 0.1867083921794837 T T T
0.5952335824358447 0.1278057749585969 0.1772527482703446 T T T
0.0987388620219793 0.6251329757821583 0.1770038995755740 T T T
0.6009040146191141 0.3748503432897386 0.1869340269278176 T T T
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0.5975733668603864 0.6252187008218458 0.1769160363340850 T T T
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0.6051933772109326 0.2438634076306365 0.2342496983203202 T T T
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0.6140797652206853 0.5063830121868782 0.2338080608720153 T T T
0.5817219480431919 0.7440214826742706 0.2337983111937849 T T T
0.3479836912471346 0.0511197211585597 0.2807475776812744 T T T
0.3466397272641615 0.2099344993636068 0.2779540165954140 T T T
0.8485689935632134 0.0688227346134636 0.2616965970425097 T T T
0.3482245151981963 0.5629385595615776 0.2619472071723623 T T T
0.8499026378108503 0.2141123994944028 0.2867574122139858 T T T
0.3483398049207564 0.7102119710827570 0.2897335389811596 T T T
0.8480538613949741 0.5410590137822694 0.2892889563012656 T T T
0.8482618499824889 0.6875947300070241 0.2615658198383712 T T T
0.3260119018465191 0.2538429366636385 0.3347316792612325 T T T
0.3450264955123478 0.0074964213195446 0.3478796738386570 T T T
0.3327792878096678 0.0812835261130445 0.3865919477444695 T T T
0.4886125963217995 0.1448928068520386 0.3842082539963723 T T T
0.4377326115824608 0.2401418560886998 0.3769743070147309 T T T
0.0982437210000029 0.9179475529998202 0.0000000000000000 F F F
0.0982437879999764 0.0820524620000000 0.0000000162939813 F F F
0.0982437429999834 0.1679478439999969 0.0000000000000000 F F F
0.0982438099999570 0.3320527369999980 0.0000000162939813 F F F
0.5982443090000018 0.0820524470000024 0.0000000000000000 F F F

0.5982443089998244 0.9179475379997513 0.0000000162939813 F F F
0.0982437660000031 0.4179481569999197 0.0000000000000000 F F F
0.0982438329999979 0.5820530649998190 0.0000000162939813 F F F
0.5982443089997889 0.3320527079999992 0.0000000000000000 F F F
0.5982443090000018 0.1679478289999992 0.0000000162939813 F F F
0.0982437950000019 0.6679484840000003 0.0000000000000000 F F F
0.0982438469999778 0.8320534229997847 0.0000000162939813 F F F
0.5982443689999997 0.5820530060000026 0.0000000000000000 F F F
0.5982443689999999 0.4179481269999955 0.0000000162939813 F F F
0.5982443689999999 0.8320533629998226 0.0000000000000000 F F F
0.5982443689998007 0.6679484249998069 0.0000000162939813 F F F
0.2345912449392246 -0.0380967364976000 0.3514435545535740 T T T
0.4645774901626458 -0.0311979887196000 0.3537368346422053 T T T
0.2104892330692034 0.1177210723716701 0.3805995763931790 T T T
0.3231756396378322 0.0526392460921998 0.4242333747110995 T T T
0.5691940970923611 0.1405747826193977 0.4181998055561350 T T T
0.5775023738509750 0.1263214275803364 0.3533982086610137 T T T
0.3641661963886322 0.2643226842148269 0.4095300113453892 T T T
0.5563601415711407 0.2804749061781064 0.3728500697999893 T T T

TS Ab Ac, E = -387.94706 eV

1.0000000000000000
7.6621999740000000 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H
48 1 4 24

Selective dynamics

Direct

0.0982437263469365 0.0000000013875407 0.0289689852776363 F F F
0.0982437493469135 0.2500002971734219 0.0289689852776363 F F F
0.5982443673469362 0.0000000013875407 0.0289689852776363 F F F
0.0982437713469366 0.5000005951734678 0.0289689852776363 F F F
0.5982443673469362 0.2500002971734219 0.0289689852776363 F F F
0.0982437933469242 0.7500008931734712 0.0289689852776363 F F F
0.5982444273469341 0.5000005951734678 0.0289689852776363 F F F
0.5982444273469341 0.7500008931734712 0.0289689852776363 F F F
0.3480383385581050 0.9981421732642418 0.0800122532992234 F F F
0.3480377191237736 0.2523206682297428 0.0807251537912991 F F F
0.8480882003324623 0.9990134760524754 0.0809062178506324 F F F
0.3480599805555897 0.4977572267302008 0.0807011518149424 F F F
0.8481536924994451 0.2521531409644879 0.0801095804747974 F F F
0.3479654336356290 0.7518208992697737 0.0800015227840235 F F F
0.8482636818746629 0.4982203957225622 0.0800102540313078 F F F
0.8484488576980951 0.7510569402138645 0.0809839353321565 F F F
0.3484162848326398 0.1243934429703328 0.1273198827034707 T T T
0.3490858794847875 0.3753557041811931 0.1351754204000823 T T T
0.8473424630102453 0.1261042724947706 0.1287824454340460 T T T
0.3481481728872598 0.6257138586762809 0.1274267029784560 T T T
0.8484615740262790 0.3754704393924391 0.1334932944915202 T T T
0.3480406107493627 0.8752217884371410 0.1334468675770983 T T T
0.8483005751581082 0.6236879721826235 0.1279647210521289 T T T
0.8476499407058764 0.8747550811469866 0.1341692339810492 T T T
0.1003750451717209 0.1275470920666007 0.1769775216531661 T T T
0.0962319937936796 0.3751325309896142 0.1864741822807804 T T T
0.5952807935745841 0.1284394550569367 0.1776371978512331 T T T

0.0988991646332677	0.6249694406169428	0.1770095344458133	T	T	T
0.6017407128709039	0.3748430579824368	0.1869560756212754	T	T	T
0.0984977870700597	0.8739147802633221	0.1859864466240114	T	T	T
0.5975483719511919	0.6252151883252663	0.1769634630494053	T	T	T
0.5970303612804777	0.8746183924526580	0.1862900071301223	T	T	T
0.1034028674185360	0.0055027891079976	0.2323141874126262	T	T	T
0.0940014668767181	0.2443056453464574	0.2333876631825616	T	T	T
0.5890696216973670	0.0063597716531259	0.2328774151763370	T	T	T
0.0828264677052422	0.5060929616540460	0.2338308472930143	T	T	T
0.6081506840717096	0.2446032469920978	0.2349391622755175	T	T	T
0.1146020709965911	0.7437626677998301	0.2338278049051030	T	T	T
0.6145572450616320	0.5063314114920051	0.2338239277548539	T	T	T
0.5816452582322605	0.7439960358081171	0.2338530973640411	T	T	T
0.3446226185021917	0.0524240034251207	0.2786729637413731	T	T	T
0.3489804985814416	0.2087649714455868	0.2779255295124551	T	T	T
0.8475625756048839	0.0698637509176182	0.2618324950537128	T	T	T
0.3486183264146718	0.5628289089544243	0.2619133566281399	T	T	T
0.8535515867856863	0.2154513371173229	0.2875810468422930	T	T	T
0.3481896437581486	0.7101511919096231	0.2897481429932030	T	T	T
0.8486482314109803	0.5409114610746114	0.2892317323308458	T	T	T
0.8481246232672386	0.6874368906087853	0.2615885567886858	T	T	T
0.3218640406119452	0.2421513061644872	0.3358159603863638	T	T	T
0.3563112262801868	0.0303453431369930	0.3484619712135038	T	T	T
0.5146198553799095	0.0809816312058005	0.3695471643228763	T	T	T
0.4761810335374796	0.1562269794891008	0.4054838337726255	T	T	T
0.3711532464557046	0.2367988220212717	0.3868551261420285	T	T	T
0.0982437210000029	0.9179475529998917	0.0000000000000000	F	F	F
0.0982437879999836	0.0820524620000000	0.0000000162939813	F	F	F
0.0982437429999905	0.1679478439999969	0.0000000000000000	F	F	F
0.0982438099999783	0.3320527369999980	0.0000000162939813	F	F	F
0.5982443090000018	0.0820524470000024	0.0000000000000000	F	F	F
0.5982443089998959	0.9179475379998649	0.0000000162939813	F	F	F
0.0982437660000031	0.4179481569999484	0.0000000000000000	F	F	F
0.0982438329999979	0.5820530649998901	0.0000000162939813	F	F	F
0.5982443089998668	0.3320527079999994	0.0000000000000000	F	F	F
0.5982443090000018	0.1679478289999992	0.0000000162939813	F	F	F
0.0982437950000019	0.6679484840000007	0.0000000000000000	F	F	F
0.0982438469999778	0.8320534229998628	0.0000000162939813	F	F	F
0.5982443689999997	0.5820530060000031	0.0000000000000000	F	F	F
0.5982443690000003	0.4179481269999957	0.0000000162939813	F	F	F
0.5982443690000001	0.8320533629998941	0.0000000000000000	F	F	F
0.5982443689998653	0.6679484249998853	0.0000000162939813	F	F	F
0.2327518183782790	0.0531977211631312	0.3649756071236379	T	T	T
0.3656021542902215	0.9599814967461054	0.3561211154048320	T	T	T
0.6011814658635721	0.0351544127013800	0.3893264097376618	T	T	T
0.5966227131854214	0.1068133487920556	0.3388900075515037	T	T	T
0.4074937365178026	0.1296507790486716	0.4382981587448706	T	T	T
0.6034117091559811	0.1797579731931214	0.4191071043756784	T	T	T
0.2479229090827795	0.2412262623088295	0.4079221189670213	T	T	T
0.4465703442681102	0.2962577739252983	0.3953852562454070	T	T	T

TS At Ab, E = -388.25340 eV

1.0000000000000000		
7.6621999740000000	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000
-0.0000007340000000	-0.0000007340000000	26.7875003810000010

Si O C H
48 1 4 24

Selective dynamics

Direct

0.0982437263469365	0.0000000011734684	0.0289689852776363	F	F	F
0.0982437493469206	0.2500002971734148	0.0289689852776363	F	F	F
0.5982443673469362	0.0000000011734684	0.0289689852776363	F	F	F
0.0982437713469366	0.5000005951734678	0.0289689852776363	F	F	F
0.5982443673469362	0.2500002971734148	0.0289689852776363	F	F	F
0.0982437933469242	0.7500008931734712	0.0289689852776363	F	F	F
0.5982444273469341	0.5000005951734678	0.0289689852776363	F	F	F
0.5982444273469341	0.7500008931734712	0.0289689852776363	F	F	F
0.3480516246971419	0.9982621715411714	0.0799813370659451	F	F	F
0.3480529171618088	0.2523649703496249	0.0807178067604255	F	F	F
0.8480989348293736	0.9989608386320654	0.0808952814268409	F	F	F
0.3480682438619453	0.4977952155171081	0.0807043450383063	F	F	F
0.8481590063973101	0.2521510964091860	0.0801183121141449	F	F	F
0.3479857396847025	0.7519371660598754	0.0800054345997481	F	F	F
0.8482590821115895	0.4981378084024757	0.0800220578488436	F	F	F
0.8484383130112008	0.7511461577184662	0.0809582844831099	F	F	F
0.3489212957712172	0.1244921081067365	0.1270741512281578	T	T	T
0.3488019380292308	0.3753869571742033	0.1351652242070724	T	T	T
0.8464859338751866	0.1260751493574803	0.1288443825026857	T	T	T
0.3480933808291212	0.6257863136395827	0.1274336570197142	T	T	T
0.8481506291471417	0.3753458221715859	0.1336162754266552	T	T	T
0.3485107634414331	0.8752826173193821	0.1333964067768036	T	T	T
0.8483886153294088	0.6237210183375591	0.1279435837661035	T	T	T
0.8475971574959918	0.8748453004789505	0.1342703106672178	T	T	T
0.1007227495768319	0.1279360416947037	0.1763726310341116	T	T	T
0.0961653104950687	0.3755094884717796	0.1866072601313276	T	T	T
0.5944153689965255	0.1272349673124669	0.1779248857026863	T	T	T
0.0988835606357705	0.6251562870817177	0.1770635487168549	T	T	T
0.6009818347112571	0.3747235800457324	0.1870507109924076	T	T	T
0.0991678997870468	0.8740904422142007	0.1858318373479790	T	T	T
0.5975872150456433	0.6250946254430604	0.1769286675895023	T	T	T
0.5969376046575016	0.8747557186605390	0.1865232487315739	T	T	T
0.1083182450630036	0.0063897134361475	0.2312549728589278	T	T	T
0.0924995164821458	0.2441996696586807	0.2331820958083073	T	T	T
0.5897857946183512	0.0059156916990562	0.2338990806855601	T	T	T
0.0824563026948807	0.5063963718563766	0.2339991365681600	T	T	T
0.6050057515508315	0.2439540956422870	0.2346931744216099	T	T	T
0.1147354381497211	0.7440519466899376	0.2338796450767387	T	T	T
0.6141271861801018	0.5063475009584685	0.2338628281121424	T	T	T
0.5816616511911696	0.7438658890720048	0.2337877877004569	T	T	T
0.3453861847799620	0.0516020676726210	0.2802895704471206	T	T	T
0.3459157144161688	0.2081421708489552	0.2777587828010760	T	T	T
0.8508825344235927	0.0685220139771730	0.2612897384434144	T	T	T
0.3483235018648062	0.5630419492713967	0.2620330796870124	T	T	T
0.8518803546427365	0.2138376594188711	0.2862685447123912	T	T	T
0.3483308467093098	0.7103855712906540	0.2898032157928447	T	T	T
0.8481342510853009	0.5410270144234282	0.2893499578370389	T	T	T
0.8482199747849914	0.6875497061023080	0.2616036455926719	T	T	T
0.3256964175160162	0.2409100452177458	0.3369952658802131	T	T	T
0.3106427067719972	0.0123221767563563	0.3472576405382751	T	T	T
0.3978744666958718	0.0619688410347973	0.3911618978889718	T	T	T
0.5282573730936297	0.1350963736291821	0.3787820953154672	T	T	T
0.4553097430568366	0.2274987631127783	0.3749428900573777	T	T	T


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0.0982437210000029 0.9179475529998701 0.0000000000000000 F F F
0.0982437879999836 0.0820524620000000 0.0000000162939813 F F F
0.0982437429999834 0.1679478439999969 0.0000000000000000 F F F
0.0982438099999783 0.3320527369999980 0.0000000162939813 F F F
0.5982443090000018 0.0820524470000024 0.0000000000000000 F F F
0.5982443089998739 0.9179475379998295 0.0000000162939813 F F F
0.0982437660000031 0.4179481569999410 0.0000000000000000 F F F
0.0982438329999979 0.5820530649998690 0.0000000162939813 F F F
0.5982443089998527 0.3320527079999993 0.0000000000000000 F F F
0.5982443090000018 0.1679478289999992 0.0000000162939813 F F F
0.0982437950000019 0.6679484840000004 0.0000000000000000 F F F
0.0982438469999849 0.8320534229998486 0.0000000162939813 F F F
0.5982443689999997 0.5820530060000028 0.0000000000000000 F F F
0.5982443690000000 0.4179481269999956 0.0000000162939813 F F F
0.5982443690000000 0.8320533629998724 0.0000000000000000 F F F
0.5982443689998579 0.6679484249998566 0.0000000162939813 F F F
0.1674864555804879 0.0138350865617386 0.3513493824583636 T T T
0.3462774370500575 0.9426247449111138 0.3479318962392381 T T T
0.2944388387585278 0.0895693136078605 0.4150017838501333 T T T
0.4658708876476632 0.0135722352435984 0.4144540944382988 T T T
0.6290049032675055 0.1381488143652509 0.4081632620818212 T T T
0.6015491400818026 0.1192463040713804 0.3443591833001611 T T T
0.3916435148396478 0.2454409727849944 0.4104106771378413 T T T
0.5645393733344197 0.2733209773243213 0.3686473384565398 T T T

```

8.5. Final State B Configurations

B1, E(PBE-D3) = -702.56368 eV, E(HSE06-D3) = -813.04358 eV

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1.0000000000000000
15.3243999479999999 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

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```

Si O C H
96 1 4 40

```

Selective dynamics

Direct

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0.000000016986164 0.000000016986164 0.0354635925893945 F F F
0.5000006559493571 0.000000016986164 0.0354635925893945 F F F
0.0000000126289095 0.2500003288239867 0.0354635925893945 F F F
0.5000006668796504 0.2500003288239867 0.0354635925893945 F F F
0.2500003288239867 0.000000016986164 0.0354635925893945 F F F
0.7500009830747276 0.000000016986164 0.0354635925893945 F F F
0.0000000235592097 0.5000006559493571 0.0354635925893945 F F F
0.5000006778099506 0.5000006559493571 0.0354635925893945 F F F
0.2500003397542798 0.2500003288239867 0.0354635925893945 F F F
0.7500009940050278 0.2500003288239867 0.0354635925893945 F F F
0.0000000344895028 0.7500009830747274 0.0354635925893945 F F F
0.5000006887402436 0.7500009830747274 0.0354635925893945 F F F
0.2500003506845800 0.5000006559493571 0.0354635925893945 F F F
0.7500010049353210 0.5000006559493571 0.0354635925893945 F F F
0.2500003616148732 0.7500009830747274 0.0354635925893945 F F F
0.7500010158656139 0.7500009830747274 0.0354635925893945 F F F
0.1250001350555152 0.0000000041205368 0.0860282208949457 F F F
0.6250007893062559 0.0000000041205368 0.0860282208949457 F F F
0.1250001459858083 0.2500003312459071 0.0860282208949457 F F F
0.6250008002365490 0.2500003312459071 0.0860282208949457 F F F
0.3750004621808855 0.0000000041205368 0.0860282208949457 F F F

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0.8750011164316192 0.0000000041205368 0.0860282208949457 F F F
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0.6250008111668492 0.5000006583712775 0.0860282208949457 F F F
0.3750004731111787 0.2500003312459071 0.0860282208949457 F F F
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0.6250008220971425 0.7500009854966481 0.0860282208949457 F F F
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0.3750004949717720 0.7500009854966481 0.0860282208949457 F F F
0.8750011492225056 0.7500009854966481 0.0860282208949457 F F F
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0.1243058276591790 0.3754422956730665 0.1395978432117294 T T T
0.3730387175640557 0.1252953093177357 0.1342663957336629 T T T
0.1247716682755687 0.6255961581775509 0.1342107606360742 T T T
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0.9999831855146573 0.6247865832308030 0.1835359722419355 T T T
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0.2396352099150025 0.0028897504030570 0.2408915162442586 T T T
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0.5000006837654070 0.6711565893294209 0.0035690153482122 F F F
0.0000000364089985 0.8288453737646864 0.0035690153482122 F F F
0.5000006906597392 0.8288453737646864 0.0035690153482122 F F F
0.0000000404449665 0.9211569164547913 0.0035690153482122 F F F
0.5000006946957072 0.9211569164547913 0.0035690153482122 F F F
0.0000000254787054 0.5788450466393159 0.0035690153482122 F F F
0.5000006797294461 0.5788450466393159 0.0035690153482122 F F F
0.2500003526040757 0.5788450466393159 0.0035690153482122 F F F
0.7500010068548164 0.5788450466393159 0.0035690153482122 F F F
0.2500003566400366 0.6711565893294209 0.0035690153482122 F F F
0.7500010108907773 0.6711565893294209 0.0035690153482122 F F F
0.2500003635343688 0.8288453737646864 0.0035690153482122 F F F
0.7500010177851097 0.8288453737646864 0.0035690153482122 F F F
0.2500003675703368 0.9211569164547913 0.0035690153482122 F F F
0.7500010218210775 0.9211569164547913 0.0035690153482122 F F F
0.4250617401780352 0.2050611426751526 0.3725507354416356 T T T
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0.3086744627736875 0.3067476384457448 0.4101579301662363 T T T
0.2615225005238506 0.3166036041528876 0.3504531692334541 T T T
0.2533257840817458 0.1419949117855984 0.3538386120465880 T T T
0.2638156410520632 0.1568053909775287 0.4186772427991040 T T T
0.1092614832335543 0.1482971487643381 0.3947068784474502 T T T
0.1309814263171823 0.2561130211576087 0.4169870478947175 T T T

B2, E = -702.49971 eV

1.0000000000000000
15.3243999479999999 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H

96 1 4 40

Selective dynamics

Direct

0.0000000016986164 0.0000000016986164 0.0354635925893945 F F F
0.5000006559493571 0.0000000016986164 0.0354635925893945 F F F
0.0000000126289095 0.2500003288239867 0.0354635925893945 F F F
0.5000006668796504 0.2500003288239867 0.0354635925893945 F F F
0.2500003288239867 0.0000000016986164 0.0354635925893945 F F F
0.7500009830747276 0.0000000016986164 0.0354635925893945 F F F
0.0000000235592097 0.5000006559493571 0.0354635925893945 F F F
0.5000006778099506 0.5000006559493571 0.0354635925893945 F F F
0.2500003397542798 0.2500003288239867 0.0354635925893945 F F F
0.7500009940050278 0.2500003288239867 0.0354635925893945 F F F
0.0000000344895028 0.7500009830747274 0.0354635925893945 F F F
0.5000006887402436 0.7500009830747274 0.0354635925893945 F F F
0.2500003506845800 0.5000006559493571 0.0354635925893945 F F F
0.7500010049353210 0.5000006559493571 0.0354635925893945 F F F
0.2500003616148732 0.7500009830747274 0.0354635925893945 F F F
0.7500010158656139 0.7500009830747274 0.0354635925893945 F F F
0.1250001350555152 0.0000000041205368 0.0860282208949457 F F F
0.6250007893062559 0.0000000041205368 0.0860282208949457 F F F
0.1250001459858083 0.2500003312459071 0.0860282208949457 F F F
0.6250008002365490 0.2500003312459071 0.0860282208949457 F F F
0.3750004621808855 0.0000000041205368 0.0860282208949457 F F F
0.8750011164316192 0.0000000041205368 0.0860282208949457 F F F
0.1250001569161086 0.5000006583712775 0.0860282208949457 F F F
0.6250008111668492 0.5000006583712775 0.0860282208949457 F F F
0.3750004731111787 0.2500003312459071 0.0860282208949457 F F F
0.8750011273619194 0.2500003312459071 0.0860282208949457 F F F
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0.3750004949717720 0.7500009854966481 0.0860282208949457 F F F
0.8750011492225056 0.7500009854966481 0.0860282208949457 F F F
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0.3738184642531647 0.1251853802204665 0.1340420484538772 T T T
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0.4993318778561424 0.3769575037033503 0.1912716906312202 T T T
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0.0000802885576865 0.6249238196503095 0.1835315129580500 T T T
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0.2473666046531930 0.2447159364469153 0.2365847830232006 T T T
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0.3697037288458169 0.2036365837355627 0.2837608636220030 T T T
0.1248794702492287 0.7094694932988456 0.2955541632377759 T T T
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0.3748190965253232 0.6892031184096847 0.2669130108089670 T T T
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0.7501999490051096 0.1253540576294053 0.1834337618634888 T T T
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0.7511740092086768 0.3751861396708618 0.1919389357552845 T T T
0.5014082330735042 0.8740740810279014 0.1910546979150483 T T T
0.7501714300854946 0.6251573520471796 0.1833703065373559 T T T
0.7493569794469112 0.8751708519236298 0.1920614624582806 T T T
0.5082690207384731 0.0044297895909692 0.2385166838325843 T T T
0.9983812320485848 0.2428490040111044 0.2414120130944127 T T T
0.7429980594200596 0.0061589886833820 0.2396138771582853 T T T
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0.7594782411235429 0.2449953254153685 0.2400850300905388 T T T
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0.7583893121158124 0.5057666815214605 0.2398276689659130 T T T
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0.3532407377469052	0.2339197513999498	0.3518447016889307	T	T	T
0.3260044983421605	0.3305073460367396	0.3585225691695056	T	T	T
0.2370912136389231	0.3463449035920763	0.3833764500654859	T	T	T
0.1567056637411041	0.3309594394882593	0.3510043366113814	T	T	T
0.000000076540800	0.1711559350786800	0.0035690153482122	F	F	F
0.5000006619048207	0.1711559350786800	0.0035690153482122	F	F	F
0.0000000145484051	0.3288447195139526	0.0035690153482122	F	F	F
0.5000006687991458	0.3288447195139526	0.0035690153482122	F	F	F
0.0000000185843732	0.4211562622040503	0.0035690153482122	F	F	F
0.5000006728351138	0.4211562622040503	0.0035690153482122	F	F	F
0.0000000036181120	0.0788443923885822	0.0035690153482122	F	F	F
0.5000006578688527	0.0788443923885822	0.0035690153482122	F	F	F
0.2500003307434824	0.0788443923885822	0.0035690153482122	F	F	F
0.7500009849942231	0.0788443923885822	0.0035690153482122	F	F	F
0.2500003347794504	0.1711559350786800	0.0035690153482122	F	F	F
0.7500009890301913	0.1711559350786800	0.0035690153482122	F	F	F
0.2500003416737755	0.3288447195139526	0.0035690153482122	F	F	F
0.7500009959245233	0.3288447195139526	0.0035690153482122	F	F	F
0.2500003457097435	0.4211562622040503	0.0035690153482122	F	F	F
0.750000999604842	0.4211562622040503	0.0035690153482122	F	F	F
0.0000000295146663	0.6711565893294209	0.0035690153482122	F	F	F
0.5000006837654070	0.6711565893294209	0.0035690153482122	F	F	F
0.0000000364089985	0.8288453737646864	0.0035690153482122	F	F	F
0.5000006906597392	0.8288453737646864	0.0035690153482122	F	F	F
0.0000000404449665	0.9211569164547913	0.0035690153482122	F	F	F
0.5000006946957072	0.9211569164547913	0.0035690153482122	F	F	F
0.0000000254787054	0.5788450466393159	0.0035690153482122	F	F	F
0.5000006797294461	0.5788450466393159	0.0035690153482122	F	F	F
0.2500003526040757	0.5788450466393159	0.0035690153482122	F	F	F
0.7500010068548164	0.5788450466393159	0.0035690153482122	F	F	F
0.2500003566400366	0.6711565893294209	0.0035690153482122	F	F	F
0.7500010108907773	0.6711565893294209	0.0035690153482122	F	F	F
0.2500003635343688	0.8288453737646864	0.0035690153482122	F	F	F
0.7500010177851097	0.8288453737646864	0.0035690153482122	F	F	F
0.2500003675703368	0.9211569164547913	0.0035690153482122	F	F	F
0.7500010218210775	0.9211569164547913	0.0035690153482122	F	F	F
0.3015267081734610	0.1899137074306468	0.3653714478265286	T	T	T
0.4124890787340178	0.2183691506819700	0.3732853559394710	T	T	T
0.3763927359836040	0.3642993805158788	0.3805025892901689	T	T	T
0.3256473469197731	0.3650847434451047	0.3222253565129680	T	T	T
0.2312348859237049	0.3070338349736259	0.4177032338746147	T	T	T
0.2344614312169004	0.4154237074460777	0.3950104789417505	T	T	T
0.0984344691732971	0.3586584925314672	0.3693363496802370	T	T	T
0.1647490782633481	0.3656745233485019	0.3148780620363130	T	T	T

B3, E = -702.50647 eV

1.0000000000000000		
15.3243999479999999	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000
-0.0000007340000000	-0.0000007340000000	26.7875003810000010

Si O C H
96 1 4 40

Selective dynamics

Direct

0.0000000016986164	0.0000000016986164	0.0354635925893945	F	F	F
0.5000006559493571	0.0000000016986164	0.0354635925893945	F	F	F

0.0000000126289095 0.2500003288239867 0.0354635925893945 F F F
0.5000006668796504 0.2500003288239867 0.0354635925893945 F F F
0.2500003288239867 0.0000000016986164 0.0354635925893945 F F F
0.7500009830747276 0.0000000016986164 0.0354635925893945 F F F
0.0000000235592097 0.5000006559493571 0.0354635925893945 F F F
0.5000006778099506 0.5000006559493571 0.0354635925893945 F F F
0.2500003397542798 0.2500003288239867 0.0354635925893945 F F F
0.7500009940050278 0.2500003288239867 0.0354635925893945 F F F
0.0000000344895028 0.7500009830747274 0.0354635925893945 F F F
0.5000006887402436 0.7500009830747274 0.0354635925893945 F F F
0.2500003506845800 0.5000006559493571 0.0354635925893945 F F F
0.7500010049353210 0.5000006559493571 0.0354635925893945 F F F
0.2500003616148732 0.7500009830747274 0.0354635925893945 F F F
0.7500010158656139 0.7500009830747274 0.0354635925893945 F F F
0.1250001350555152 0.0000000041205368 0.0860282208949457 F F F
0.6250007893062559 0.0000000041205368 0.0860282208949457 F F F
0.1250001459858083 0.2500003312459071 0.0860282208949457 F F F
0.6250008002365490 0.2500003312459071 0.0860282208949457 F F F
0.3750004621808855 0.0000000041205368 0.0860282208949457 F F F
0.8750011164316192 0.0000000041205368 0.0860282208949457 F F F
0.1250001569161086 0.5000006583712775 0.0860282208949457 F F F
0.6250008111668492 0.5000006583712775 0.0860282208949457 F F F
0.3750004731111787 0.2500003312459071 0.0860282208949457 F F F
0.8750011273619194 0.2500003312459071 0.0860282208949457 F F F
0.1250001678464017 0.7500009854966481 0.0860282208949457 F F F
0.6250008220971425 0.7500009854966481 0.0860282208949457 F F F
0.3750004840414789 0.5000006583712775 0.0860282208949457 F F F
0.8750011382922127 0.5000006583712775 0.0860282208949457 F F F
0.3750004949717720 0.7500009854966481 0.0860282208949457 F F F
0.8750011492225056 0.7500009854966481 0.0860282208949457 F F F
0.1244463824551347 0.1239607676552424 0.1346904917076074 T T T
0.1238585738622602 0.3755130733692824 0.1395086620952134 T T T
0.3740987575786283 0.1251928642348621 0.1339495894678404 T T T
0.1248611556657974 0.6255944794123133 0.1341684996754175 T T T
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0.3748307243094438 0.8748017126339717 0.1395565485746121 T T T
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0.2505183157876640 0.1235418201606648 0.1831786150360503 T T T
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0.2499824632452636 0.3755770736225004 0.1908023668649464 T T T
0.0006547335166790 0.8754057804843609 0.1920505719287198 T T T
0.2500677520259990 0.6248010501373614 0.1830703989493496 T T T
0.2485271073264568 0.8734597980692163 0.1911421060397084 T T T
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0.2391081753391747 0.0023378729748669 0.2394817965464324 T T T
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0.2467821018287836 0.2435120501025578 0.2361350197249471 T T T
0.0083266204148219 0.7445480944674067 0.2397778908735334 T T T
0.2579045506495514 0.5056447710265298 0.2392262966790286 T T T
0.2413246883946223 0.7438748792794861 0.2395308100679586 T T T
0.1245901065217641 0.0400885433261441 0.2948348637971738 T T T
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0.1250266797305824 0.7092852710566647 0.2954513838768567 T T T
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0.8766871194839849 0.1257597126030476 0.1347916542917602 T T T
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0.8752496560893583 0.6243540421743150 0.1342501924659443 T T T
0.8751334085917580 0.8749161272964039 0.1397355760332214 T T T
0.4978784247618533 0.1261636580297285 0.1838237981658985 T T T
0.9993854083373792 0.3730200004017251 0.1930692856259593 T T T
0.7502707685653057 0.1254034835872857 0.1833971882534125 T T T
0.5002249910140669 0.6255007843801201 0.1831169115317534 T T T
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0.5013016270943405 0.8742285911714605 0.1912023643443246 T T T
0.7502522257797816 0.6251447417968291 0.1834045348165578 T T T
0.7493660451504084 0.8751834749939604 0.1920561111069705 T T T
0.5080912719661167 0.0047272766389834 0.2387377153669293 T T T
0.9987116594386520 0.2431797519279010 0.2422136120515569 T T T
0.7431479684955835 0.0062351133924486 0.2395612491865922 T T T
0.9921210015325518 0.5049707717571772 0.2397129322693010 T T T
0.7594076018383137 0.2449353191663829 0.2400613120616071 T T T
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0.7500009890301913 0.1711559350786800 0.0035690153482122 F F F
0.2500003416737755 0.3288447195139526 0.0035690153482122 F F F
0.7500009959245233 0.3288447195139526 0.0035690153482122 F F F
0.2500003457097435 0.4211562622040503 0.0035690153482122 F F F

0.7500009999604842	0.4211562622040503	0.0035690153482122	F	F	F
0.000000295146663	0.6711565893294209	0.0035690153482122	F	F	F
0.5000006837654070	0.6711565893294209	0.0035690153482122	F	F	F
0.000000364089985	0.8288453737646864	0.0035690153482122	F	F	F
0.5000006906597392	0.8288453737646864	0.0035690153482122	F	F	F
0.000000404449665	0.9211569164547913	0.0035690153482122	F	F	F
0.5000006946957072	0.9211569164547913	0.0035690153482122	F	F	F
0.000000254787054	0.5788450466393159	0.0035690153482122	F	F	F
0.5000006797294461	0.5788450466393159	0.0035690153482122	F	F	F
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0.7500010068548164	0.5788450466393159	0.0035690153482122	F	F	F
0.2500003566400366	0.6711565893294209	0.0035690153482122	F	F	F
0.7500010108907773	0.6711565893294209	0.0035690153482122	F	F	F
0.2500003635343688	0.8288453737646864	0.0035690153482122	F	F	F
0.7500010177851097	0.8288453737646864	0.0035690153482122	F	F	F
0.2500003675703368	0.9211569164547913	0.0035690153482122	F	F	F
0.7500010218210775	0.9211569164547913	0.0035690153482122	F	F	F
0.3011801902116993	0.1791580106928083	0.3644865479382658	T	T	T
0.4124628633939013	0.2061234109244458	0.3731791864343109	T	T	T
0.3192037562445850	0.3186403394888923	0.4111382398327035	T	T	T
0.3808943495926769	0.3638727024448259	0.3620717020296038	T	T	T
0.2416387068204398	0.4281413431719709	0.3587237909543272	T	T	T
0.2500468236979070	0.3612794064974862	0.3060992315168650	T	T	T
0.1477678428449557	0.3188282156442154	0.4018753046341453	T	T	T
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B4, E = -702.53883 eV

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15.3243999479999999	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000
-0.0000007340000000	-0.0000007340000000	26.7875003810000010

Si O C H
96 1 4 40

Selective dynamics

Direct

0.0000000016986164	0.0000000016986164	0.0354635925893945	F	F	F
0.5000006559493571	0.0000000016986164	0.0354635925893945	F	F	F
0.0000000126289095	0.2500003288239867	0.0354635925893945	F	F	F
0.5000006668796504	0.2500003288239867	0.0354635925893945	F	F	F
0.2500003288239867	0.0000000016986164	0.0354635925893945	F	F	F
0.7500009830747276	0.0000000016986164	0.0354635925893945	F	F	F
0.0000000235592097	0.5000006559493571	0.0354635925893945	F	F	F
0.5000006778099506	0.5000006559493571	0.0354635925893945	F	F	F
0.2500003397542798	0.2500003288239867	0.0354635925893945	F	F	F
0.7500009940050278	0.2500003288239867	0.0354635925893945	F	F	F
0.0000000344895028	0.7500009830747274	0.0354635925893945	F	F	F
0.5000006887402436	0.7500009830747274	0.0354635925893945	F	F	F
0.2500003506845800	0.5000006559493571	0.0354635925893945	F	F	F
0.7500010049353210	0.5000006559493571	0.0354635925893945	F	F	F
0.2500003616148732	0.7500009830747274	0.0354635925893945	F	F	F
0.7500010158656139	0.7500009830747274	0.0354635925893945	F	F	F
0.1250001350555152	0.0000000041205368	0.0860282208949457	F	F	F
0.6250007893062559	0.0000000041205368	0.0860282208949457	F	F	F
0.1250001459858083	0.2500003312459071	0.0860282208949457	F	F	F
0.6250008002365490	0.2500003312459071	0.0860282208949457	F	F	F
0.3750004621808855	0.0000000041205368	0.0860282208949457	F	F	F

0.8750011164316192 0.0000000041205368 0.0860282208949457 F F F
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0.5000006906597392 0.8288453737646864 0.0035690153482122 F F F
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B5, E = -702.39372 eV

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15.3243999479999999 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H

96 1 4 40

Selective dynamics

Direct

0.0000000016986164 0.0000000016986164 0.0354635925893945 F F F
0.5000006559493571 0.0000000016986164 0.0354635925893945 F F F
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0.5000006668796506 0.2500003288239867 0.0354635925893945 F F F
0.2500003288239867 0.0000000016986164 0.0354635925893945 F F F
0.7500009830747278 0.0000000016986164 0.0354635925893945 F F F
0.0000000235592097 0.5000006559493571 0.0354635925893945 F F F
0.5000006778099508 0.5000006559493571 0.0354635925893945 F F F
0.2500003397542798 0.2500003288239867 0.0354635925893945 F F F
0.7500009940050281 0.2500003288239867 0.0354635925893945 F F F
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B6, E = -702.55658 eV

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Si O C H
 96 1 4 40

Selective dynamics

Direct

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B7, E = -702.47289 eV

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Si O C H
96 1 4 40

Selective dynamics

Direct

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Si O C H

96 1 4 40

Selective dynamics

Direct

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TS B1 B2, E = -702.23986 eV

1.0000000000000000

15.3243999479999999 0.0000000000000000 0.0000000000000000

-0.0000006700000000 15.3243999479999999 0.0000000000000000

-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H

96 1 4 40

Selective dynamics

Direct

0.0000000016986164 0.0000000016986164 0.0354635925893950 F F F

0.5000006559493571 0.0000000016986164 0.0354635925893950 F F F

0.0000000126289095 0.2500003288239867 0.0354635925893950 F F F
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0.2500003288239867 0.0000000016986164 0.0354635925893950 F F F
0.7500009830747284 0.0000000016986164 0.0354635925893950 F F F
0.0000000235592097 0.5000006559493571 0.0354635925893950 F F F
0.5000006778099512 0.5000006559493571 0.0354635925893950 F F F
0.2500003397542798 0.2500003288239867 0.0354635925893950 F F F
0.7500009940050288 0.2500003288239867 0.0354635925893950 F F F
0.0000000344895028 0.7500009830747274 0.0354635925893950 F F F
0.5000006887402436 0.7500009830747274 0.0354635925893950 F F F
0.2500003506845800 0.5000006559493571 0.0354635925893950 F F F
0.7500010049353213 0.5000006559493571 0.0354635925893950 F F F
0.2500003616148732 0.7500009830747274 0.0354635925893950 F F F
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0.6250007893062559 0.0000000041205368 0.0860282208949541 F F F
0.1250001459858083 0.2500003312459071 0.0860282208949541 F F F
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TS B2 B3, E = -702.04637 eV

1.0000000000000000
15.3243999479999999 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H
96 1 4 40

Selective dynamics

Direct

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0.5000006559493571 0.0000000016986164 0.0354635925893957 F F F
0.0000000126289095 0.2500003288239867 0.0354635925893957 F F F
0.5000006668796507 0.2500003288239867 0.0354635925893957 F F F
0.2500003288239867 0.0000000016986164 0.0354635925893957 F F F
0.7500009830747284 0.0000000016986164 0.0354635925893957 F F F
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0.5000006778099512 0.5000006559493571 0.0354635925893957 F F F
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0.0000000364089985 0.8288453737646868 0.0035690153482123 F F F
0.5000006906597392 0.8288453737646868 0.0035690153482123 F F F
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0.5000006946957072 0.9211569164547923 0.0035690153482123 F F F
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0.2500003635343688 0.8288453737646868 0.0035690153482123 F F F
0.7500010177851101 0.8288453737646868 0.0035690153482123 F F F
0.2500003675703368 0.9211569164547923 0.0035690153482123 F F F
0.7500010218210775 0.9211569164547923 0.0035690153482123 F F F
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0.3851377566767906 0.3192145409695915 0.3961082065646050 T T T
0.2365923479434674 0.3871201318571856 0.4059927500936261 T T T
0.2934858877255814 0.4072628573471263 0.3505130582501381 T T T
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TS B3 B4, E = -702.27699 eV

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15.3243999479999999 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H

96 1 4 40

Selective dynamics

Direct

0.0000000016986164 0.0000000016986164 0.0354635925893946 F F F
0.5000006559493571 0.0000000016986164 0.0354635925893946 F F F
0.0000000126289095 0.2500003288239867 0.0354635925893946 F F F
0.5000006668796507 0.2500003288239867 0.0354635925893946 F F F
0.2500003288239867 0.0000000016986164 0.0354635925893946 F F F
0.7500009830747284 0.0000000016986164 0.0354635925893946 F F F
0.0000000235592097 0.5000006559493571 0.0354635925893946 F F F
0.5000006778099512 0.5000006559493571 0.0354635925893946 F F F
0.2500003397542798 0.2500003288239867 0.0354635925893946 F F F
0.7500009940050288 0.2500003288239867 0.0354635925893946 F F F
0.0000000344895028 0.7500009830747274 0.0354635925893946 F F F
0.5000006887402436 0.7500009830747274 0.0354635925893946 F F F
0.2500003506845800 0.5000006559493571 0.0354635925893946 F F F
0.7500010049353213 0.5000006559493571 0.0354635925893946 F F F
0.2500003616148732 0.7500009830747274 0.0354635925893946 F F F
0.7500010158656139 0.7500009830747274 0.0354635925893946 F F F
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0.6250007893062559 0.0000000041205368 0.0860282208949461 F F F
0.1250001459858083 0.2500003312459071 0.0860282208949461 F F F
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 0.2500003675703368 0.9211569164547923 0.0035690153482122 F F F
 0.7500010218210775 0.9211569164547923 0.0035690153482122 F F F
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TS B4 B5, E = -702.38846 eV

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 -0.0000006700000000 15.3243999479999999 0.0000000000000000
 -0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H
 96 1 4 40

Selective dynamics

Direct

0.0000000016986164 0.0000000016986164 0.0354635925893950 F F F
 0.5000006559493571 0.0000000016986164 0.0354635925893950 F F F

0.0000000126289095 0.2500003288239867 0.0354635925893950 F F F
0.5000006668796507 0.2500003288239867 0.0354635925893950 F F F
0.2500003288239867 0.0000000016986164 0.0354635925893950 F F F
0.7500009830747284 0.0000000016986164 0.0354635925893950 F F F
0.0000000235592097 0.5000006559493571 0.0354635925893950 F F F
0.5000006778099512 0.5000006559493571 0.0354635925893950 F F F
0.2500003397542798 0.2500003288239867 0.0354635925893950 F F F
0.7500009940050288 0.2500003288239867 0.0354635925893950 F F F
0.0000000344895028 0.7500009830747274 0.0354635925893950 F F F
0.5000006887402436 0.7500009830747274 0.0354635925893950 F F F
0.2500003506845800 0.5000006559493571 0.0354635925893950 F F F
0.7500010049353213 0.5000006559493571 0.0354635925893950 F F F
0.2500003616148732 0.7500009830747274 0.0354635925893950 F F F
0.7500010158656139 0.7500009830747274 0.0354635925893950 F F F
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0.6250007893062559 0.0000000041205368 0.0860282208949469 F F F
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0.1250001569161086 0.5000006583712775 0.0860282208949469 F F F
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0.8750011273619194 0.2500003312459071 0.0860282208949469 F F F
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0.6250008220971425 0.7500009854966488 0.0860282208949469 F F F
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0.3750004949717720 0.7500009854966488 0.0860282208949469 F F F
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TS B5 B6, E = -702.16267 eV

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-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H

96 1 4 40

Selective dynamics

Direct

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0.2500003288239867 0.0000000016986164 0.0354635925893948 F F F
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0.2500003616148732 0.7500009830747274 0.0354635925893948 F F F
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TS B6 B7, E = -702.20201 eV

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Si O C H

96 1 4 40

Selective dynamics

Direct

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0.2500003288239867 0.0000000016986164 0.0354635925893945 F F F
0.7500009830747281 0.0000000016986164 0.0354635925893945 F F F
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0.2500003397542798 0.2500003288239867 0.0354635925893945 F F F
0.7500009940050283 0.2500003288239867 0.0354635925893945 F F F
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0.2500003506845800 0.5000006559493571 0.0354635925893945 F F F
0.7500010049353213 0.5000006559493571 0.0354635925893945 F F F
0.2500003616148732 0.7500009830747274 0.0354635925893945 F F F
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0.8755488074582861 0.3750114441401990 0.1388125620016880 T T T
0.6254019926768632 0.8748042690532970 0.1386086360700392 T T T
0.8751149728372298 0.6243809520744247 0.1342474272759318 T T T
0.8750824679014183 0.8749995858347634 0.1398317160252338 T T T
0.4987852248845627 0.1246227423212057 0.1824669246376673 T T T
0.9990563544498126 0.3738356874204547 0.1924619206204631 T T T
0.7503954006002652 0.1250966391152648 0.1834584459440951 T T T
0.4999233675746561 0.6251925003678329 0.1832179425501817 T T T
0.7512131721180207 0.3752278406453568 0.1918640917584831 T T T
0.5010336990826402 0.8737888623198118 0.1912487333032027 T T T
0.7500549787304206 0.6251745117129962 0.1833578253598960 T T T
0.7490990035485763 0.8751894365272900 0.1920801026621983 T T T
0.5074508385413691 0.0047843272251749 0.2381455545949310 T T T
0.9957148161571366 0.2427598936137333 0.2396901994360852 T T T
0.7422503065178027 0.0059996785459630 0.2397987647588780 T T T
0.9918248460571565 0.5050620331277615 0.2397603017127863 T T T
0.7594674090140625 0.2450158576274885 0.2399687800430573 T T T
0.5079876864082609 0.7440899840783205 0.2398309612041149 T T T
0.7584187788270290 0.5057666615890737 0.2397831762373397 T T T
0.7419500168709107 0.7444401591845061 0.2397814409308384 T T T
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0.8753275582036627 0.0634979966879918 0.2676304551504377 T T T
0.6253106108535670 0.5624680479437287 0.2675602257632869 T T T
0.8768426702406608 0.2101833947300155 0.2942725935665075 T T T
0.6250309290765601 0.7094042948562117 0.2953017290508388 T T T
0.8752016923987044 0.5406899254379490 0.2953378149897996 T T T
0.8751107771820702 0.6877163703654431 0.2676989193590196 T T T
0.1197081426023987 0.2574077368370162 0.3389316875842611 T T T

0.3867483587489896	0.2284770561720224	0.3532369363014126	T	T	T
0.3292712753032118	0.1749309993067531	0.3889884398184786	T	T	T
0.2327346035323388	0.2032401954224992	0.3972811962903093	T	T	T
0.1955725189969522	0.2805301554259304	0.3672906529971867	T	T	T
0.000000076540800	0.1711559350786800	0.0035690153482122	F	F	F
0.5000006619048207	0.1711559350786800	0.0035690153482122	F	F	F
0.0000000145484051	0.3288447195139526	0.0035690153482122	F	F	F
0.5000006687991458	0.3288447195139526	0.0035690153482122	F	F	F
0.0000000185843732	0.4211562622040503	0.0035690153482122	F	F	F
0.5000006728351138	0.4211562622040503	0.0035690153482122	F	F	F
0.0000000036181120	0.0788443923885894	0.0035690153482122	F	F	F
0.5000006578688527	0.0788443923885894	0.0035690153482122	F	F	F
0.2500003307434824	0.0788443923885894	0.0035690153482122	F	F	F
0.7500009849942231	0.0788443923885894	0.0035690153482122	F	F	F
0.2500003347794504	0.1711559350786800	0.0035690153482122	F	F	F
0.7500009890301915	0.1711559350786800	0.0035690153482122	F	F	F
0.2500003416737755	0.3288447195139526	0.0035690153482122	F	F	F
0.7500009959245233	0.3288447195139526	0.0035690153482122	F	F	F
0.2500003457097435	0.4211562622040503	0.0035690153482122	F	F	F
0.750000999604842	0.4211562622040503	0.0035690153482122	F	F	F
0.0000000295146663	0.6711565893294213	0.0035690153482122	F	F	F
0.5000006837654070	0.6711565893294213	0.0035690153482122	F	F	F
0.0000000364089985	0.8288453737646868	0.0035690153482122	F	F	F
0.5000006906597392	0.8288453737646868	0.0035690153482122	F	F	F
0.0000000404449665	0.9211569164547917	0.0035690153482122	F	F	F
0.5000006946957072	0.9211569164547917	0.0035690153482122	F	F	F
0.0000000254787054	0.5788450466393159	0.0035690153482122	F	F	F
0.5000006797294461	0.5788450466393159	0.0035690153482122	F	F	F
0.2500003526040757	0.5788450466393159	0.0035690153482122	F	F	F
0.7500010068548164	0.5788450466393159	0.0035690153482122	F	F	F
0.2500003566400366	0.6711565893294213	0.0035690153482122	F	F	F
0.7500010108907773	0.6711565893294213	0.0035690153482122	F	F	F
0.2500003635343688	0.8288453737646868	0.0035690153482122	F	F	F
0.7500010177851101	0.8288453737646868	0.0035690153482122	F	F	F
0.2500003675703368	0.9211569164547917	0.0035690153482122	F	F	F
0.7500010218210775	0.9211569164547917	0.0035690153482122	F	F	F
0.4557619823679115	0.2125109308240991	0.3607399467743460	T	T	T
0.3806342430175287	0.2993711117102531	0.3594800459914668	T	T	T
0.3301503631030233	0.1063185669973426	0.3764271415283789	T	T	T
0.3621166024135473	0.1745108770757529	0.4255567651510299	T	T	T
0.1897232566384069	0.1473052467104459	0.3896155165753346	T	T	T
0.2240018895494358	0.2173892413571087	0.4372119303347659	T	T	T
0.1744692322517139	0.3332710396658937	0.3924039763764322	T	T	T
0.2449396000135478	0.3088661281609730	0.3418979379679198	T	T	T

TS B7 B8, E = -702.31820 eV

1.0000000000000000		
15.3243999479999999	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000
-0.0000007340000000	-0.0000007340000000	26.7875003810000010

Si O C H

96 1 4 40

Selective dynamics

Direct

0.0000000016986164	0.0000000016986164	0.0354635925893945	F	F	F
0.5000006559493571	0.0000000016986164	0.0354635925893945	F	F	F
0.0000000126289095	0.2500003288239867	0.0354635925893945	F	F	F

0.5000006668796507 0.2500003288239867 0.0354635925893945 F F F
0.2500003288239867 0.0000000016986164 0.0354635925893945 F F F
0.7500009830747281 0.0000000016986164 0.0354635925893945 F F F
0.0000000235592097 0.5000006559493571 0.0354635925893945 F F F
0.5000006778099511 0.5000006559493571 0.0354635925893945 F F F
0.2500003397542798 0.2500003288239867 0.0354635925893945 F F F
0.7500009940050283 0.2500003288239867 0.0354635925893945 F F F
0.0000000344895028 0.7500009830747274 0.0354635925893945 F F F
0.5000006887402436 0.7500009830747274 0.0354635925893945 F F F
0.2500003506845800 0.5000006559493571 0.0354635925893945 F F F
0.7500010049353213 0.5000006559493571 0.0354635925893945 F F F
0.2500003616148732 0.7500009830747274 0.0354635925893945 F F F
0.7500010158656139 0.7500009830747274 0.0354635925893945 F F F
0.1250001350555152 0.0000000041205368 0.0860282208949458 F F F
0.6250007893062559 0.0000000041205368 0.0860282208949458 F F F
0.1250001459858083 0.2500003312459071 0.0860282208949458 F F F
0.6250008002365490 0.2500003312459071 0.0860282208949458 F F F
0.3750004621808854 0.0000000041205368 0.0860282208949458 F F F
0.8750011164316192 0.0000000041205368 0.0860282208949458 F F F
0.1250001569161086 0.5000006583712775 0.0860282208949458 F F F
0.6250008111668492 0.5000006583712775 0.0860282208949458 F F F
0.3750004731111787 0.2500003312459071 0.0860282208949458 F F F
0.8750011273619194 0.2500003312459071 0.0860282208949458 F F F
0.1250001678464017 0.7500009854966485 0.0860282208949458 F F F
0.6250008220971425 0.7500009854966485 0.0860282208949458 F F F
0.3750004840414789 0.5000006583712775 0.0860282208949458 F F F
0.8750011382922129 0.5000006583712775 0.0860282208949458 F F F
0.3750004949717720 0.7500009854966485 0.0860282208949458 F F F
0.8750011492225056 0.7500009854966485 0.0860282208949458 F F F
0.1258050146222107 0.1240742567059174 0.1350674750744116 T T T
0.1240969654265985 0.3754590571894131 0.1395668664999303 T T T
0.3736841045982637 0.1251295861380211 0.1340927629857936 T T T
0.1248085995763700 0.6255786012187512 0.1341995518615157 T T T
0.3745838589152153 0.3751294541304569 0.1384649131807232 T T T
0.1244600633651918 0.8748325871774729 0.1386443727285631 T T T
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0.3746388712185658 0.8748156485428684 0.1396517048058960 T T T
0.0012066834166381 0.1271530519088414 0.1844338433246376 T T T
0.4998418162002136 0.3774218697230528 0.1904801787260337 T T T
0.2514382151660133 0.1246655090988158 0.1847579510255639 T T T
0.9999949023331762 0.6246929620939226 0.1834898997825395 T T T
0.2501441746607501 0.3756513296964967 0.1911442748313862 T T T
0.0001292179979767 0.8744258978235502 0.1916277864905190 T T T
0.2498921727669962 0.6246132177087400 0.1832512138453225 T T T
0.2486482288556353 0.8735499290762366 0.1916693352318923 T T T
0.0047722881148883 0.0050170714864759 0.2389288467268281 T T T
0.4969613400798917 0.2468392188877097 0.2371021533102730 T T T
0.2396300716190002 0.0024185574388503 0.2406384670142848 T T T
0.4920616942598502 0.5062059430946089 0.2396040898760397 T T T
0.2481220839429815 0.2451241570113378 0.2378788706042554 T T T
0.0079988716306062 0.7442069777144491 0.2397414277010828 T T T
0.2575024078784106 0.5053746369045059 0.2395430092880332 T T T
0.2413194649705139 0.7435454409998595 0.2398470650096547 T T T
0.1215734242231868 0.0429816089251724 0.2918702753488951 T T T
0.1253672252337186 0.2025703153840552 0.2853065066331422 T T T
0.3724126391123522 0.0527965878797930 0.2691365867715165 T T T
0.1245756409769774 0.5622494214733412 0.2677509693831741 T T T

0.3730825776927020	0.2074126657065525	0.2836530890917596	T	T	T
0.1246113940143159	0.7094508310226566	0.2955885202159430	T	T	T
0.3746605022992368	0.5398707068590575	0.2950867175510384	T	T	T
0.3746342816913770	0.6872254180667973	0.2676162947468940	T	T	T
0.6253468364314042	0.1247084134279021	0.1345032288687123	T	T	T
0.6260537280218443	0.3753995733727043	0.1393108093215083	T	T	T
0.8769025829348421	0.1257049343113237	0.1346375889835857	T	T	T
0.6251138020670456	0.6255975601343116	0.1342360612833189	T	T	T
0.8758249380205806	0.3748453736198503	0.1389902962635230	T	T	T
0.6251029319205036	0.8749012371823398	0.1387154568117999	T	T	T
0.8751058283681064	0.6243799084511213	0.1342443760715358	T	T	T
0.8746030507021862	0.8748010108491893	0.1395920061364687	T	T	T
0.4987789152565558	0.1246977379938489	0.1826068752694131	T	T	T
0.9993667379978682	0.3733367178038481	0.1928810924952176	T	T	T
0.7506930594449736	0.1253766777218248	0.1834780949125059	T	T	T
0.4999735360879262	0.6253043054448921	0.1832027528145444	T	T	T
0.7513535429432565	0.3751142210438398	0.1919477927873579	T	T	T
0.5006976594802588	0.8742697618434242	0.1915266416433279	T	T	T
0.7500601840903857	0.6251614636044881	0.1833738938464379	T	T	T
0.7489372359562741	0.8751632495723707	0.1920867050626118	T	T	T
0.5064055047986933	0.0054762485832234	0.2385424608371587	T	T	T
0.9977197578636346	0.2429916467699056	0.2413205836491375	T	T	T
0.7417792264353128	0.0060699935840498	0.2397443844333109	T	T	T
0.9919362403225694	0.5050325703678309	0.2397323314897202	T	T	T
0.7599811766262385	0.2450526304326134	0.2402512336562347	T	T	T
0.5078670320198189	0.7441952914130753	0.2398258037572684	T	T	T
0.7584537695435006	0.5057340362773710	0.2398004597871950	T	T	T
0.7418333279801876	0.7444299199333491	0.2398261100679693	T	T	T
0.6233018889257883	0.0407790659316215	0.2941053729081221	T	T	T
0.6272878877434095	0.1872262389118332	0.2671714798595154	T	T	T
0.8743621327604212	0.0636040604225406	0.2678302821521502	T	T	T
0.6253418680872094	0.5624738763923091	0.2675599447701226	T	T	T
0.8772025798957951	0.2101784750229699	0.2949160486105058	T	T	T
0.6248916906057645	0.7094087856352644	0.2953153606495478	T	T	T
0.8752810675557653	0.5406132577400778	0.2953204253375917	T	T	T
0.8749707969037495	0.6875869795147551	0.2676902854979230	T	T	T
0.1283905566628645	0.2507059581398764	0.3409655524850458	T	T	T
0.3754622428132995	0.2485013211752515	0.3510063815540002	T	T	T
0.3385324694722093	0.1870229348422966	0.3909077491274443	T	T	T
0.2440135216296632	0.1576763637119809	0.3831535835408960	T	T	T
0.1742902381942226	0.2300507878754691	0.3861742283606112	T	T	T
0.0000000076540800	0.1711559350786800	0.0035690153482122	F	F	F
0.5000006619048207	0.1711559350786800	0.0035690153482122	F	F	F
0.0000000145484051	0.3288447195139526	0.0035690153482122	F	F	F
0.5000006687991458	0.3288447195139526	0.0035690153482122	F	F	F
0.0000000185843732	0.4211562622040503	0.0035690153482122	F	F	F
0.5000006728351138	0.4211562622040503	0.0035690153482122	F	F	F
0.0000000036181120	0.0788443923885823	0.0035690153482122	F	F	F
0.5000006578688527	0.0788443923885823	0.0035690153482122	F	F	F
0.2500003307434824	0.0788443923885823	0.0035690153482122	F	F	F
0.7500009849942231	0.0788443923885823	0.0035690153482122	F	F	F
0.2500003347794504	0.1711559350786800	0.0035690153482122	F	F	F
0.7500009890301915	0.1711559350786800	0.0035690153482122	F	F	F
0.2500003416737755	0.3288447195139526	0.0035690153482122	F	F	F
0.7500009959245233	0.3288447195139526	0.0035690153482122	F	F	F
0.2500003457097435	0.4211562622040503	0.0035690153482122	F	F	F
0.750000999604842	0.4211562622040503	0.0035690153482122	F	F	F

0.000000295146663 0.6711565893294213 0.0035690153482122 F F F
0.5000006837654070 0.6711565893294213 0.0035690153482122 F F F
0.000000364089985 0.8288453737646868 0.0035690153482122 F F F
0.5000006906597392 0.8288453737646868 0.0035690153482122 F F F
0.000000404449665 0.9211569164547917 0.0035690153482122 F F F
0.5000006946957072 0.9211569164547917 0.0035690153482122 F F F
0.000000254787054 0.5788450466393159 0.0035690153482122 F F F
0.5000006797294461 0.5788450466393159 0.0035690153482122 F F F
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0.7500010177851101 0.8288453737646868 0.0035690153482122 F F F
0.2500003675703368 0.9211569164547917 0.0035690153482122 F F F
0.7500010218210775 0.9211569164547917 0.0035690153482122 F F F
0.4438602244753715 0.2643564007585553 0.3598324499766892 T T T
0.3400965883269857 0.3112975652209413 0.3505718566857871 T T T
0.3800046249453236 0.1282678283718003 0.3928833254961327 T T T
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0.2385709898366896 0.1239478973493306 0.3467421110557494 T T T
0.2286170238020455 0.1068963146894426 0.4108447650531110 T T T
0.1243237616602439 0.2122062123887995 0.4139252437553960 T T T
0.2045058054980814 0.2915340574569860 0.3989517934212076 T T T

TS B8 B1, E = -702.26601 eV

1.0000000000000000
15.3243999479999999 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H

96 1 4 40

Selective dynamics

Direct

0.000000016986164 0.000000016986164 0.0354635925893945 F F F
0.5000006559493571 0.000000016986164 0.0354635925893945 F F F
0.000000126289095 0.2500003288239867 0.0354635925893945 F F F
0.5000006668796505 0.2500003288239867 0.0354635925893945 F F F
0.2500003288239867 0.000000016986164 0.0354635925893945 F F F
0.7500009830747277 0.000000016986164 0.0354635925893945 F F F
0.000000235592097 0.5000006559493571 0.0354635925893945 F F F
0.5000006778099507 0.5000006559493571 0.0354635925893945 F F F
0.2500003397542798 0.2500003288239867 0.0354635925893945 F F F
0.7500009940050280 0.2500003288239867 0.0354635925893945 F F F
0.000000344895028 0.7500009830747274 0.0354635925893945 F F F
0.5000006887402436 0.7500009830747274 0.0354635925893945 F F F
0.2500003506845800 0.5000006559493571 0.0354635925893945 F F F
0.7500010049353211 0.5000006559493571 0.0354635925893945 F F F
0.2500003616148732 0.7500009830747274 0.0354635925893945 F F F
0.7500010158656139 0.7500009830747274 0.0354635925893945 F F F
0.1250001350555152 0.0000000041205368 0.0860282208949457 F F F
0.6250007893062559 0.0000000041205368 0.0860282208949457 F F F
0.1250001459858083 0.2500003312459071 0.0860282208949457 F F F
0.6250008002365490 0.2500003312459071 0.0860282208949457 F F F
0.3750004621808854 0.0000000041205368 0.0860282208949457 F F F
0.8750011164316192 0.0000000041205368 0.0860282208949457 F F F

0.1250001569161086 0.5000006583712775 0.0860282208949457 F F F
0.6250008111668492 0.5000006583712775 0.0860282208949457 F F F
0.3750004731111787 0.2500003312459071 0.0860282208949457 F F F
0.8750011273619194 0.2500003312459071 0.0860282208949457 F F F
0.1250001678464017 0.7500009854966482 0.0860282208949457 F F F
0.6250008220971425 0.7500009854966482 0.0860282208949457 F F F
0.3750004840414789 0.5000006583712775 0.0860282208949457 F F F
0.8750011382922128 0.5000006583712775 0.0860282208949457 F F F
0.3750004949717720 0.7500009854966482 0.0860282208949457 F F F
0.8750011492225056 0.7500009854966482 0.0860282208949457 F F F
0.1258574735126374 0.1240888536870814 0.1351099707666112 T T T
0.1239105627793878 0.3754526170057682 0.1395495809656020 T T T
0.3739406133561133 0.1251157952283213 0.1340170500517586 T T T
0.1248101922726870 0.6255799019589188 0.1342079519155807 T T T
0.3745189785653687 0.3751480345230835 0.1384568745960203 T T T
0.1244811442994319 0.8748235670888541 0.1386342824540285 T T T
0.3749065043169877 0.6244224639371759 0.1342038706901479 T T T
0.3747745148798881 0.8747964379722813 0.1396305660318078 T T T
0.0011892118125913 0.1273339001363092 0.1844913051842287 T T T
0.4995023624775511 0.3770455747666412 0.1906609796865198 T T T
0.2517622179826966 0.1247012976880773 0.1846449442217309 T T T
0.9999946101904899 0.6247957144711600 0.1835028758743724 T T T
0.2499960262356402 0.3758983605287481 0.1910501802432741 T T T
0.0002841125422076 0.8746651091329095 0.1917285688822390 T T T
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0.4919174618181867 0.5060578239522859 0.2396300674904988 T T T
0.2474897967562963 0.2453355544147270 0.2376466487652259 T T T
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0.7508063218400900 0.1253874990248222 0.1834143458302250 T T T
0.4999623352690232 0.6251905512262336 0.1832151029518145 T T T
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0.5007542744316720 0.8742043145508189 0.1916096422812240 T T T
0.7500572807541944 0.6251540918470414 0.1833791776045884 T T T

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0.7582990962444376 0.5057124838372018 0.2397720862787033 T T T
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0.6259450326851161 0.1873141905411779 0.2670771700118313 T T T
0.8749378177917372 0.0636898164996453 0.2678470575760250 T T T
0.6251940395874467 0.5623934529739764 0.2675722267191241 T T T
0.8760722167055541 0.2102781635065498 0.2949235232775021 T T T
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0.8751181686933786 0.5406549547364951 0.2953095502464961 T T T
0.8750095598288372 0.6876359332285065 0.2676934383568593 T T T
0.1362550791010262 0.2467037925618459 0.3413172120879055 T T T
0.3816698863145977 0.2544938712429131 0.3497991506438010 T T T
0.3222794401522761 0.2273246636998238 0.3940448599598865 T T T
0.2488744336368885 0.1597635424716103 0.3860552459494648 T T T
0.1560200312425718 0.1957853895064714 0.3848053885403272 T T T
0.0000000076540800 0.1711559350786800 0.0035690153482122 F F F
0.5000006619048207 0.1711559350786800 0.0035690153482122 F F F
0.0000000145484051 0.3288447195139526 0.0035690153482122 F F F
0.5000006687991458 0.3288447195139526 0.0035690153482122 F F F
0.0000000185843732 0.4211562622040503 0.0035690153482122 F F F
0.5000006728351138 0.4211562622040503 0.0035690153482122 F F F
0.0000000036181120 0.0788443923885823 0.0035690153482122 F F F
0.5000006578688527 0.0788443923885823 0.0035690153482122 F F F
0.2500003307434824 0.0788443923885823 0.0035690153482122 F F F
0.7500009849942231 0.0788443923885823 0.0035690153482122 F F F
0.2500003347794504 0.1711559350786800 0.0035690153482122 F F F
0.7500009890301914 0.1711559350786800 0.0035690153482122 F F F
0.2500003416737755 0.3288447195139526 0.0035690153482122 F F F
0.7500009959245233 0.3288447195139526 0.0035690153482122 F F F
0.2500003457097435 0.4211562622040503 0.0035690153482122 F F F
0.750000999604842 0.4211562622040503 0.0035690153482122 F F F
0.0000000295146663 0.6711565893294210 0.0035690153482122 F F F
0.5000006837654070 0.6711565893294210 0.0035690153482122 F F F
0.0000000364089985 0.8288453737646865 0.0035690153482122 F F F
0.5000006906597392 0.8288453737646865 0.0035690153482122 F F F
0.0000000404449665 0.9211569164547914 0.0035690153482122 F F F
0.5000006946957072 0.9211569164547914 0.0035690153482122 F F F
0.0000000254787054 0.5788450466393159 0.0035690153482122 F F F
0.5000006797294461 0.5788450466393159 0.0035690153482122 F F F
0.2500003526040757 0.5788450466393159 0.0035690153482122 F F F
0.7500010068548164 0.5788450466393159 0.0035690153482122 F F F
0.2500003566400366 0.6711565893294210 0.0035690153482122 F F F
0.7500010108907773 0.6711565893294210 0.0035690153482122 F F F
0.2500003635343688 0.8288453737646865 0.0035690153482122 F F F
0.7500010177851099 0.8288453737646865 0.0035690153482122 F F F
0.2500003675703368 0.9211569164547914 0.0035690153482122 F F F
0.7500010218210775 0.9211569164547914 0.0035690153482122 F F F
0.4507316748785802 0.2444112938778538 0.3597722908596705 T T T
0.3756965784775968 0.3252504671501399 0.3425048165138578 T T T
0.3655129245243515 0.2020346771935438 0.4234472208387537 T T T

0.2927657535431054 0.2868969103410448 0.4096979805275966 T T T
0.2604428061808697 0.1206675549795956 0.3518968645456480 T T T
0.2502933822463796 0.1118811386860142 0.4167922901892600 T T T
0.1094390733655687 0.1409001008427697 0.3875365834655322 T T T
0.1450923767668720 0.2391128444485108 0.4170813590505095 T T T

8.6. Final State C Configurations

Cb(4x2), E = -387.98123 eV

1.0000000000000000
7.6621999740000000 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H
48 1 4 24

Selective dynamics

Direct

0.0982437263469365 0.0000000011734684 0.0289689852776363 F F F
0.0982437493469348 0.2500002971734646 0.0289689852776363 F F F
0.5982443673469362 0.0000000011734684 0.0289689852776363 F F F
0.0982437713469366 0.5000005951734678 0.0289689852776363 F F F
0.5982443673469362 0.2500002971734646 0.0289689852776363 F F F
0.0982437933469384 0.7500008931734712 0.0289689852776363 F F F
0.5982444273469341 0.5000005951734678 0.0289689852776363 F F F
0.5982444273469341 0.7500008931734712 0.0289689852776363 F F F
0.3480383385581050 0.9981421732642418 0.0800122532992163 F F F
0.3480377191238375 0.2523206682297854 0.0807251537912919 F F F
0.8480882003325618 0.9990134760524754 0.0809062178506253 F F F
0.3480599805555897 0.4977572267302506 0.0807011518149352 F F F
0.8481536924995370 0.2521531409645306 0.0801095804747902 F F F
0.3479654336356290 0.7518208992697737 0.0800015227840163 F F F
0.8482636818747693 0.4982203957226120 0.0800102540313006 F F F
0.8484488576981875 0.7510569402139853 0.0809839353321493 F F F
0.3479546708138848 0.1242490783610799 0.1276474675566445 T T T
0.3477435076006796 0.3749890003043999 0.1349121972347027 T T T
0.8483064410559746 0.1259876368459884 0.1288310516425061 T T T
0.3482826403887215 0.6256822946792950 0.1275266692085158 T T T
0.8486806331551655 0.3753208140083074 0.1326896889370080 T T T
0.3479105106077418 0.8748976064563119 0.1332474963463132 T T T
0.8500785285167923 0.6241593836909146 0.1289542826985563 T T T
0.8477945807474750 0.8751159677095952 0.1343165596077031 T T T
0.1007466652961288 0.1273181813445902 0.1777983240108024 T T T
0.0940584611264047 0.3746982527110991 0.1860983493366515 T T T
0.5955267168988095 0.1273406594613712 0.1775392223094598 T T T
0.1024512360180238 0.6215087623596199 0.1782385631969904 T T T
0.6022772137525438 0.3749671281606003 0.1854776702070209 T T T
0.0996898031125059 0.8755707177929215 0.1860355772056777 T T T
0.5964044862740989 0.6227115709766510 0.1770887077763921 T T T
0.5957938821243840 0.8757817090219364 0.1861080696479848 T T T
0.1064051432741218 0.0059153054585786 0.2337704493204932 T T T
0.0864989318947905 0.2447117460680795 0.2333288683871794 T T T
0.5871491096130903 0.0062332981140729 0.2337656439125804 T T T
0.0906881299970298 0.5040491013317268 0.2341542842252702 T T T
0.6093283674341486 0.2451848258320868 0.2326647211549009 T T T
0.1035363105545953 0.7446850505336616 0.2333637692545872 T T T

0.6066148565354231	0.5052292157643200	0.2322141318646031	T	T	T
0.5909336471520723	0.7445296084783476	0.2330550885611742	T	T	T
0.3465489140994896	0.0591088955187745	0.2777232330644427	T	T	T
0.3497187895612280	0.2189508561759354	0.2761579375080387	T	T	T
0.8468730831184309	0.0675517161844701	0.2622547995293046	T	T	T
0.3510849962278128	0.5305966831369299	0.2783946815450659	T	T	T
0.8461363286360470	0.2140012875145307	0.2870866904345861	T	T	T
0.3472718696671888	0.6882387469989787	0.2732965659287031	T	T	T
0.8461022180008962	0.5347639829205089	0.2862252321234339	T	T	T
0.8472089154721620	0.6811178367503452	0.2626370711544632	T	T	T
0.3672141796113718	0.2691988166517421	0.3312263734675545	T	T	T
0.3801015930392921	0.4834182553322805	0.3439503435657805	T	T	T
0.2159748336542615	0.4551735179243667	0.3725259237660527	T	T	T
0.1283450676273407	0.3713980841118392	0.3539788887267265	T	T	T
0.2231696100492154	0.2856810298722172	0.3645468722880004	T	T	T
0.0982437210000029	0.9179475529999908	0.0000000000000000	F	F	F
0.0982437879999978	0.0820524620000000	0.0000000162939813	F	F	F
0.0982437429999976	0.1679478439999969	0.0000000000000000	F	F	F
0.0982438099999996	0.3320527369999980	0.0000000162939813	F	F	F
0.5982443090000018	0.0820524470000024	0.0000000000000000	F	F	F
0.5982443089999947	0.9179475379999857	0.0000000162939813	F	F	F
0.0982437660000031	0.4179481569999908	0.0000000000000000	F	F	F
0.0982438329999979	0.5820530649999895	0.0000000162939813	F	F	F
0.5982443089999876	0.3320527079999992	0.0000000000000000	F	F	F
0.5982443090000018	0.1679478289999992	0.0000000162939813	F	F	F
0.0982437950000019	0.6679484840000003	0.0000000000000000	F	F	F
0.0982438469999991	0.8320534229999836	0.0000000162939813	F	F	F
0.5982443689999997	0.5820530060000026	0.0000000000000000	F	F	F
0.5982443689999999	0.4179481269999955	0.0000000162939813	F	F	F
0.5982443689999999	0.8320533629999929	0.0000000000000000	F	F	F
0.5982443689999857	0.6679484249999845	0.0000000162939813	F	F	F
0.4696815011060304	0.4276694460048916	0.3392911866326178	T	T	T
0.4531170567614408	0.5329499306393441	0.3652633792173612	T	T	T
0.2502438928368683	0.4461201398234064	0.4122685348851343	T	T	T
0.1182905988111317	0.5080727670385226	0.3716295276223246	T	T	T
-0.0017192841049100	0.3662615813865314	0.3714268294614345	T	T	T
0.1023233517677071	0.3756064328965830	0.3134412380235126	T	T	T
0.2782185837441800	0.2860294708852765	0.4026003879716357	T	T	T
0.1286841926826869	0.2313360147268126	0.3622733023402077	T	T	T

Cb(2x2), E(PBE-D3) = -388.06775 eV,, E(HSE06-D3) = -449.28334 eV

1.0000000000000000		
7.6621999740000000	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000
-0.0000007340000000	-0.0000007340000000	26.7875003810000010

Si O C H
48 1 4 24

Selective dynamics

Direct

0.0982437263469365	0.0000000011734684	0.0289689852776363	F	F	F
0.0982437493469277	0.2500002971734574	0.0289689852776363	F	F	F
0.5982443673469362	0.0000000011734684	0.0289689852776363	F	F	F
0.0982437713469366	0.5000005951734678	0.0289689852776363	F	F	F
0.5982443673469362	0.2500002971734574	0.0289689852776363	F	F	F
0.0982437933469313	0.7500008931734712	0.0289689852776363	F	F	F
0.5982444273469341	0.5000005951734678	0.0289689852776363	F	F	F

0.5982444273469341 0.7500008931734712 0.0289689852776363 F F F
0.3480383385581050 0.9981421732642418 0.0800122532992163 F F F
0.3480377191238304 0.2523206682297712 0.0807251537912919 F F F
0.8480882003325405 0.9990134760524754 0.0809062178506253 F F F
0.3480599805555897 0.4977572267302436 0.0807011518149352 F F F
0.8481536924995225 0.2521531409645164 0.0801095804747902 F F F
0.3479654336356290 0.7518208992697737 0.0800015227840163 F F F
0.8482636818747551 0.4982203957225977 0.0800102540313006 F F F
0.8484488576981735 0.7510569402139566 0.0809839353321493 F F F
0.3477915949665828 0.1242397223302135 0.1277347551404968 T T T
0.3479302378328693 0.3746690363579998 0.1342930029069865 T T T
0.8479112017888719 0.1260186059903397 0.1286734699144340 T T T
0.3488982366260341 0.6249051777610447 0.1273049529761315 T T T
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0.0995394486337084 0.1266935571372809 0.1774650777812970 T T T
0.0948430591735627 0.3715610695759193 0.1852783507234241 T T T
0.5960472121311630 0.1267135034354662 0.1773536160666968 T T T
0.1034901098011148 0.6258018928853823 0.1778585402106533 T T T
0.6015598933000610 0.3718481520309316 0.1849080221529976 T T T
0.0988395643880760 0.8771051279062400 0.1866948968664685 T T T
0.5956991351538174 0.6264210062715887 0.1772724694068699 T T T
0.5967167424897298 0.8772360383618482 0.1867458431318401 T T T
0.1104753050052940 0.0077944821146952 0.2345752191324063 T T T
0.0864538385028978 0.2428655072317402 0.2334714356531950 T T T
0.5828996192614403 0.0079528602851817 0.2346285339574699 T T T
0.1043330743983170 0.5024828637680679 0.2314630308579862 T T T
0.6083145840965344 0.2433449837298482 0.2330176559675653 T T T
0.0856044127001501 0.7457286045372975 0.2337747537885198 T T T
0.5949303931373447 0.5031309094367725 0.2304649729820617 T T T
0.6108554315624239 0.7456282160478507 0.2335770079985008 T T T
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0.3489753469462101 0.2161473298881076 0.2766097369252404 T T T
0.8467286601425290 0.0667159843819256 0.2618454357384261 T T T
0.3509915460645328 0.5398175040078085 0.2786484403377921 T T T
0.8458072271540621 0.2133787434175771 0.2873671011134385 T T T
0.3481371556688393 0.6941750736313885 0.2637764851226882 T T T
0.8491726362249381 0.5657835021684657 0.2609420965845493 T T T
0.8481429158824478 0.7113769222766495 0.2881402463059940 T T T
0.3651069334013249 0.2741013819938845 0.3296162626121935 T T T
0.3688347334553071 0.4920930155277728 0.3443967758577167 T T T
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0.1219638773829048 0.3760046217823870 0.3498233626454524 T T T
0.2212198613177246 0.2921344613736439 0.3626037553563681 T T T
0.0982437210000029 0.9179475529999692 0.0000000000000000 F F F
0.0982437879999978 0.0820524620000000 0.0000000162939813 F F F
0.0982437429999976 0.1679478439999969 0.0000000000000000 F F F
0.0982438099999925 0.3320527369999980 0.0000000162939813 F F F
0.5982443090000018 0.0820524470000024 0.0000000000000000 F F F
0.5982443089999973 0.9179475379999573 0.0000000162939813 F F F
0.0982437660000031 0.4179481569999838 0.0000000000000000 F F F
0.0982438329999979 0.5820530649999682 0.0000000162939813 F F F
0.5982443089999663 0.3320527079999992 0.0000000000000000 F F F
0.5982443090000018 0.1679478289999992 0.0000000162939813 F F F
0.0982437950000019 0.6679484840000003 0.0000000000000000 F F F

0.0982438469999920 0.8320534229999625 0.0000000162939813 F F F
 0.5982443689999997 0.5820530060000026 0.0000000000000000 F F F
 0.5982443689999999 0.4179481269999955 0.0000000162939813 F F F
 0.5982443689999999 0.8320533629999716 0.0000000000000000 F F F
 0.5982443689999644 0.6679484249999632 0.0000000162939813 F F F
 0.4604867881171602 0.4369349062034446 0.3410700405877289 T T T
 0.4341845952488054 0.5420194503206934 0.3673729456453625 T T T
 0.2210245534798370 0.4553547275925533 0.4097172636962729 T T T
 0.0983883433651224 0.5135462171128853 0.3652829696564682 T T T
 0.9890987029529212 0.3685738818595727 0.3651494798425113 T T T
 0.1041125967763569 0.3786380468101976 0.3088918290626780 T T T
 0.2763589016376424 0.2963387728354399 0.4005915197224641 T T T
 0.1285908282422651 0.2368968488966717 0.3620497375881818 T T T

Cc(4x2), E = -387.92392 eV

1.0000000000000000
 7.6621999740000000 0.0000000000000000 0.0000000000000000
 -0.0000006700000000 15.3243999479999999 0.0000000000000000
 -0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H
 48 1 4 24

Selective dynamics

Direct

0.0982437263469294 0.0000000016016131 0.0289689852776363 F F F
 0.0982437493469277 0.2500002971734503 0.0289689852776363 F F F
 0.5982443673469362 0.0000000016016131 0.0289689852776363 F F F
 0.0982437713469366 0.5000005951734678 0.0289689852776363 F F F
 0.5982443673469362 0.2500002971734503 0.0289689852776363 F F F
 0.0982437933469313 0.7500008931734712 0.0289689852776363 F F F
 0.5982444273469341 0.5000005951734678 0.0289689852776363 F F F
 0.5982444273469341 0.7500008931734712 0.0289689852776363 F F F
 0.3480383385581050 0.9981421732642418 0.0800122532992163 F F F
 0.3480377191238233 0.2523206682297712 0.0807251537912919 F F F
 0.8480882003325334 0.9990134760524754 0.0809062178506253 F F F
 0.3480599805555897 0.4977572267302364 0.0807011518149352 F F F
 0.8481536924995157 0.2521531409645164 0.0801095804747902 F F F
 0.3479654336356290 0.7518208992697737 0.0800015227840163 F F F
 0.8482636818747340 0.4982203957225907 0.0800102540313006 F F F
 0.8484488576981593 0.7510569402139426 0.0809839353321493 F F F
 0.3483306903488705 0.1242721718618035 0.1277068970289444 T T T
 0.3476074363558782 0.3749619407535751 0.1349115467969426 T T T
 0.8493497464580863 0.1260824414209377 0.1289679406967563 T T T
 0.3477371024185910 0.6257683786651344 0.1274587176126320 T T T
 0.8485944873118942 0.3751656008914234 0.1328471694108346 T T T
 0.3478397766406863 0.8749068460742438 0.1332644928987694 T T T
 0.8494480763199624 0.6242621942115797 0.1287953984198144 T T T
 0.8478220311810745 0.8748603721525615 0.1341565252604001 T T T
 0.1018742569625784 0.1278761852922326 0.1782344632497368 T T T
 0.0943229599054989 0.3746970736455495 0.1862599286860656 T T T
 0.5961478143581683 0.1274184494706586 0.1775712339541075 T T T
 0.1014333845442670 0.6218353041992423 0.1779344691896813 T T T
 0.6017275424043929 0.3752197024913418 0.1856040552378979 T T T
 0.0992076226946361 0.8747266620151496 0.1859499821241329 T T T
 0.5959826453685988 0.6229827046628411 0.1768609949146007 T T T
 0.5962588409003090 0.8748504094247126 0.1859431900969245 T T T
 0.1047087163867240 0.0051287282122390 0.2334545215459096 T T T

0.0882835534081556 0.2452382117632859 0.2342492718227044 T T T
0.5899144351689156 0.0053563264925904 0.2333111689373089 T T T
0.0893534478840872 0.5045471161612189 0.2336516965545617 T T T
0.6087004277706584 0.2452717032616240 0.2328174337460425 T T T
0.1041644126751013 0.7440898849748401 0.2335014583445891 T T T
0.6052702703133748 0.5058996700054498 0.2320478525817642 T T T
0.5897431705739359 0.7440093734014148 0.2331766136602029 T T T
0.3472991007403273 0.0574405043097958 0.2759266356990267 T T T
0.3512266593645175 0.2162094014018335 0.2769298691392470 T T T
0.8473102321280445 0.0681198816945042 0.2627245671221371 T T T
0.3489969308973492 0.5317201463216702 0.2779158351303957 T T T
0.8459238658194151 0.2149426375181092 0.2872952304090432 T T T
0.3470920631119204 0.6894191782927386 0.2750062959290311 T T T
0.8451876374993214 0.5347793364426435 0.2859409141702202 T T T
0.8467760584750759 0.6811294842456246 0.2624800480043890 T T T
0.3737943997244775 0.2606227082636025 0.3332992866765145 T T T
0.3670235156540015 0.4728082150176811 0.3406005722239999 T T T
0.2008069395353250 0.4273520761815114 0.3592283415719383 T T T
0.2373193798375263 0.3527061733662832 0.3963792449671688 T T T
0.2432947842323490 0.2630893772771500 0.3718774784755373 T T T
0.0982437210000029 0.9179475529999623 0.0000000000000000 F F F
0.0982437879999907 0.0820524620000000 0.0000000162939813 F F F
0.0982437429999905 0.1679478439999969 0.0000000000000000 F F F
0.0982438099999925 0.3320527369999980 0.0000000162939813 F F F
0.5982443090000018 0.0820524470000024 0.0000000000000000 F F F
0.5982443089999665 0.9179475379999431 0.0000000162939813 F F F
0.0982437660000031 0.4179481569999766 0.0000000000000000 F F F
0.0982438329999979 0.5820530649999611 0.0000000162939813 F F F
0.5982443089999523 0.3320527079999992 0.0000000000000000 F F F
0.5982443090000018 0.1679478289999992 0.0000000162939813 F F F
0.0982437950000019 0.6679484840000003 0.0000000000000000 F F F
0.0982438469999920 0.8320534229999481 0.0000000162939813 F F F
0.5982443689999997 0.5820530060000026 0.0000000000000000 F F F
0.5982443689999999 0.4179481269999955 0.0000000162939813 F F F
0.5982443689999999 0.8320533629999647 0.0000000000000000 F F F
0.5982443689999501 0.6679484249999490 0.0000000162939813 F F F
0.4693546372838851 0.4235307874083376 0.3338705960774767 T T T
0.4198778500623848 0.5173600868095997 0.3691092746746744 T T T
0.1129530496606841 0.4760139163306241 0.3760223405561016 T T T
0.1269783137151708 0.4002725775344882 0.3273406965938208 T T T
0.3606138358180473 0.3649372684977429 0.4164264017615561 T T T
0.1336566921307807 0.3498652446109992 0.4249091800375704 T T T
0.2748941839382468 0.2121100445801421 0.3995663070987618 T T T
0.1136485287252202 0.2477358861414790 0.3559173437907591 T T T

Cc(2x2), E = -388.02703 eV

1.0000000000000000
7.6621999740000000 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H
48 1 4 24

Selective dynamics

Direct

0.0982437263469294 0.0000000016016131 0.0289689852776363 F F F
0.0982437493469277 0.2500002971734503 0.0289689852776363 F F F

0.5982443673469362 0.0000000016016131 0.0289689852776363 F F F
0.0982437713469366 0.5000005951734678 0.0289689852776363 F F F
0.5982443673469362 0.2500002971734503 0.0289689852776363 F F F
0.0982437933469313 0.7500008931734712 0.0289689852776363 F F F
0.5982444273469341 0.5000005951734678 0.0289689852776363 F F F
0.5982444273469341 0.7500008931734712 0.0289689852776363 F F F
0.3480383385581050 0.9981421732642418 0.0800122532992163 F F F
0.3480377191238233 0.2523206682297712 0.0807251537912919 F F F
0.8480882003325405 0.9990134760524754 0.0809062178506253 F F F
0.3480599805555897 0.4977572267302364 0.0807011518149352 F F F
0.8481536924995157 0.2521531409645164 0.0801095804747902 F F F
0.3479654336356290 0.7518208992697737 0.0800015227840163 F F F
0.8482636818747409 0.4982203957225977 0.0800102540313006 F F F
0.8484488576981661 0.7510569402139495 0.0809839353321493 F F F
0.3478688030381897 0.1242504096868329 0.1278064238636471 T T T
0.3476545455704914 0.3746398089605363 0.1342845931781646 T T T
0.8486282251568085 0.1261410871235730 0.128770088963447 T T T
0.3485935533377082 0.6249814557854921 0.1272256819746507 T T T
0.8483454956759688 0.3752108019377696 0.1326921286732600 T T T
0.3479182680673667 0.8746795814534313 0.1339189841480001 T T T
0.8493513593729443 0.6247898813350835 0.1290524266689911 T T T
0.8479191015159409 0.8758494997904048 0.1342956696716376 T T T
0.1001354628511706 0.1272587262132075 0.1778119147175977 T T T
0.0950224813975862 0.3712635994819303 0.1854684029586887 T T T
0.5964385214698730 0.1268217756438326 0.1773342813312039 T T T
0.1030014172663302 0.6261546619906184 0.1776213580112152 T T T
0.6008269625382957 0.3718633917508936 0.1850377637252599 T T T
0.0984278888176045 0.8769451083560195 0.1865669580382762 T T T
0.5953626502781121 0.6267149714839300 0.1771485153849237 T T T
0.5972745850175654 0.8769399375455460 0.1865659275427139 T T T
0.1098427121887723 0.0075080497099614 0.2343647732457702 T T T
0.0883559189246614 0.2431294874809638 0.2344271565774595 T T T
0.5847858736596880 0.0075444932886179 0.2342667414930077 T T T
0.1027869014603969 0.5028073201677112 0.2308893295050628 T T T
0.6070972214439153 0.2432447827971082 0.2332376666832405 T T T
0.0852966497747525 0.7457216118756301 0.2337390114846944 T T T
0.5932351717842124 0.5035682510792084 0.2302875329287526 T T T
0.6105543155513486 0.7456246491978995 0.2336165336315623 T T T
0.3473264127963679 0.0527508920640609 0.2834687690101582 T T T
0.3502667617018626 0.2125497908612339 0.2775300555191437 T T T
0.8472050347327040 0.0672089391196875 0.2621641670067951 T T T
0.3485203031851645 0.5402062101153441 0.2783144101135708 T T T
0.8453194018222305 0.2142501037142173 0.2874813343772823 T T T
0.3478035251377490 0.6945313089098687 0.2641097064258619 T T T
0.8479091467207415 0.5658580206954782 0.2606378536571010 T T T
0.8478794606812426 0.7113155246995637 0.2880780844595948 T T T
0.3694711661217165 0.2653969728550272 0.3320410447653301 T T T
0.3591576249424813 0.4811063572554503 0.3411040377755662 T T T
0.1927382593046414 0.4323532191375517 0.3567158679550939 T T T
0.2284594339299263 0.3580067485354405 0.3942598266435187 T T T
0.2381130554766575 0.2678971035476952 0.3702977582557559 T T T
0.0982437210000029 0.9179475529999623 0.0000000000000000 F F F
0.0982437879999907 0.0820524620000000 0.0000000162939813 F F F
0.0982437429999905 0.1679478439999969 0.0000000000000000 F F F
0.0982438099999925 0.3320527369999980 0.0000000162939813 F F F
0.5982443090000018 0.0820524470000024 0.0000000000000000 F F F
0.5982443089999665 0.9179475379999504 0.0000000162939813 F F F

0.098243766000031 0.4179481569999766 0.0000000000000000 F F F
 0.0982438329999979 0.5820530649999611 0.0000000162939813 F F F
 0.5982443089999592 0.3320527079999992 0.0000000000000000 F F F
 0.5982443090000018 0.1679478289999992 0.0000000162939813 F F F
 0.0982437950000019 0.6679484840000003 0.0000000000000000 F F F
 0.0982438469999920 0.8320534229999481 0.0000000162939813 F F F
 0.5982443689999997 0.5820530060000026 0.0000000000000000 F F F
 0.5982443689999999 0.4179481269999955 0.0000000162939813 F F F
 0.5982443689999999 0.8320533629999716 0.0000000000000000 F F F
 0.5982443689999573 0.6679484249999562 0.0000000162939813 F F F
 0.4653337020752563 0.4334350464166490 0.3357228742175762 T T T
 0.4025639649429296 0.5262339490286015 0.3705975433960603 T T T
 0.0984090598714711 0.4792403406526961 0.3723190854419941 T T T
 0.1283989983814261 0.4040970319117452 0.3235107013470700 T T T
 0.3501757182231693 0.3712615203234633 0.4148761433739144 T T T
 0.1233618834629345 0.3549876482518115 0.4223344914119023 T T T
 0.2698289354270471 0.2180189732333167 0.3986326239261384 T T T
 0.1092053227986597 0.2512160754897153 0.3542651601023369 T T T

TS Cb Cc, E = -387.55180 eV

1.0000000000000000
 7.6621999740000000 0.0000000000000000 0.0000000000000000
 -0.0000006700000000 15.3243999479999999 0.0000000000000000
 -0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H
 48 1 4 24

Selective dynamics

Direct

0.0982437263469365 0.0000000013875407 0.0289689852776365 F F F
 0.0982437493469206 0.2500002971734362 0.0289689852776365 F F F
 0.5982443673469362 0.0000000013875407 0.0289689852776365 F F F
 0.0982437713469366 0.5000005951734678 0.0289689852776365 F F F
 0.5982443673469362 0.2500002971734362 0.0289689852776365 F F F
 0.0982437933469313 0.7500008931734712 0.0289689852776365 F F F
 0.5982444273469341 0.5000005951734678 0.0289689852776365 F F F
 0.5982444273469341 0.7500008931734712 0.0289689852776365 F F F
 0.3480383385581050 0.9981421732642418 0.0800122532992241 F F F
 0.3480377191237949 0.2523206682297499 0.0807251537912997 F F F
 0.8480882003324979 0.9990134760524754 0.0809062178506331 F F F
 0.3480599805555897 0.4977572267302151 0.0807011518149430 F F F
 0.8481536924994799 0.2521531409644950 0.0801095804747980 F F F
 0.3479654336356290 0.7518208992697737 0.0800015227840241 F F F
 0.8482636818746982 0.4982203957225766 0.0800102540313084 F F F
 0.8484488576981164 0.7510569402139069 0.0809839353321571 F F F
 0.3486825323594564 0.1242039357937484 0.1277270730000964 T T T
 0.3473148263692010 0.3748994622173675 0.1348197251030221 T T T
 0.8514342461534791 0.1259279400734918 0.1287280249151634 T T T
 0.3472741676616111 0.6257841978680880 0.1272797596637095 T T T
 0.8486046758386403 0.3752076621632296 0.1327273247088859 T T T
 0.3478624759272260 0.8749868205351332 0.1332886571262116 T T T
 0.8483650825824085 0.6242181785100748 0.1290739853334069 T T T
 0.8478271632459159 0.8750897770832694 0.1344894435959041 T T T
 0.1025945530897017 0.1280764642968842 0.1784665472204975 T T T
 0.0940808940596602 0.3737755202499463 0.1861972263825648 T T T
 0.5982382620523169 0.1265527040113065 0.1767080681436012 T T T
 0.1015937883588953 0.6222761599617052 0.1779328254753046 T T T

0.6015675784390282	0.3742758532855657	0.1852803446815468	T	T	T
0.100037164777785	0.87640588450214822	0.1862903883536786	T	T	T
0.5940155464849696	0.6229301622923198	0.1772553955261440	T	T	T
0.5954328834222428	0.8764242743345624	0.1862696734620088	T	T	T
0.1084691781599133	0.0065815704006405	0.2343328005828711	T	T	T
0.0880544989871943	0.2449734061936691	0.2347734551248934	T	T	T
0.5875799476207109	0.0070776936036623	0.2337833973621178	T	T	T
0.0897351136929804	0.5041000239612728	0.2331040865341845	T	T	T
0.6093669267353949	0.2438445112313868	0.2316537445734393	T	T	T
0.1040483407758829	0.7450504921851658	0.2334285672307007	T	T	T
0.6017983565184163	0.5047273329697527	0.2319952482347737	T	T	T
0.5890733386635254	0.7450532291856964	0.2332157553175036	T	T	T
0.3481776404182517	0.0567027475494569	0.2799696831561809	T	T	T
0.3529449499914855	0.2162100244626882	0.2766652685706978	T	T	T
0.8480105665703409	0.0680320703589913	0.2623930464262400	T	T	T
0.3471709205589644	0.5292383087041805	0.2787990413912093	T	T	T
0.8445637304100464	0.2148037751522053	0.2872868247150824	T	T	T
0.3465954651703202	0.6871007240202434	0.2732853637185601	T	T	T
0.8436196630092858	0.5361431755163172	0.2839637302909934	T	T	T
0.8462533932171038	0.6820907301037982	0.2620329908848648	T	T	T
0.3972696816340676	0.2686279770803202	0.3293028775807063	T	T	T
0.3583691280812878	0.4688221233996675	0.3414048170547517	T	T	T
0.1814560532219869	0.4357449851555117	0.3616359545714796	T	T	T
0.1649129806364376	0.3393163022356229	0.3793217429189600	T	T	T
0.3242676555311876	0.2801174597779216	0.3778933964626177	T	T	T
0.0982437210000029	0.9179475529999266	0.0000000000000000	F	F	F
0.0982437879999836	0.0820524620000000	0.0000000162939813	F	F	F
0.0982437429999905	0.1679478439999969	0.0000000000000000	F	F	F
0.0982438099999853	0.3320527369999980	0.0000000162939813	F	F	F
0.5982443090000018	0.0820524470000024	0.0000000000000000	F	F	F
0.5982443089999313	0.9179475379999076	0.0000000162939813	F	F	F
0.0982437660000031	0.4179481569999628	0.0000000000000000	F	F	F
0.0982438329999979	0.5820530649999256	0.0000000162939813	F	F	F
0.5982443089999165	0.3320527079999994	0.0000000000000000	F	F	F
0.5982443090000018	0.1679478289999992	0.0000000162939813	F	F	F
0.0982437950000019	0.6679484840000008	0.0000000000000000	F	F	F
0.0982438469999848	0.8320534229999127	0.0000000162939813	F	F	F
0.5982443689999997	0.5820530060000032	0.0000000000000000	F	F	F
0.5982443690000008	0.4179481269999958	0.0000000162939813	F	F	F
0.5982443690000001	0.8320533629999365	0.0000000000000000	F	F	F
0.5982443689999161	0.6679484249999135	0.0000000162939813	F	F	F
0.4456173384463323	0.4139972576184631	0.3321482940853779	T	T	T
0.4292071274173048	0.5088162037535495	0.3688493792055633	T	T	T
0.1404667766524568	0.4791812760351591	0.3921661631976877	T	T	T
0.0800388062619674	0.4451846500187794	0.3329669086981711	T	T	T
0.1191004013800439	0.3381665752245776	0.4183703580471649	T	T	T
0.0605625095031669	0.3071746178388175	0.3575995765978698	T	T	T
0.4309981034490708	0.3069314671282117	0.4008936300514063	T	T	T
0.2889521324856016	0.2158454874473018	0.3936023194542699	T	T	T

8.7. Transition States of Reaction A

TS Ib Ac, E(PBE-D3) = -385.47349 eV, E(HSE06-D3) = -446.40813 eV

1.0000000000000000		
7.6621999740000000	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000
-0.0000007340000000	-0.0000007340000000	26.7875003810000010

Si H C O
48 24 4 1

Selective dynamics

Direct

0.0982437263469365	0.0000000013607817	0.0289689852776371	F	F	F
0.0982437493469206	0.2500002971734362	0.0289689852776371	F	F	F
0.5982443673469362	0.0000000013607817	0.0289689852776371	F	F	F
0.0982437713469366	0.5000005951734678	0.0289689852776371	F	F	F
0.5982443673469362	0.2500002971734362	0.0289689852776371	F	F	F
0.0982437933469313	0.7500008931734712	0.0289689852776371	F	F	F
0.5982444273469341	0.5000005951734678	0.0289689852776371	F	F	F
0.5982444273469341	0.7500008931734712	0.0289689852776371	F	F	F
0.3481230376947772	0.9989071622797876	0.0798151623121752	F	F	F
0.3481346066161493	0.2526030942439519	0.0806783164695472	F	F	F
0.8481566327504082	0.9986779124980032	0.0808364981489218	F	F	F
0.3481126591339319	0.4979994052466957	0.0807215086139789	F	F	F
0.8481875685981143	0.2521401069244223	0.0801652446756149	F	F	F
0.3480948846987602	0.7525621000566581	0.0800264606093845	F	F	F
0.8482343583851488	0.4976939015568007	0.0800855033682053	F	F	F
0.8483816353192921	0.7516257018052465	0.0808204111694577	F	F	F
0.3479668101274999	0.1247929238406606	0.1276509706572879	T	T	T
0.3483146400957894	0.3755094969592991	0.1351128475672616	T	T	T
0.8482737486466799	0.1256635945954514	0.1280506709788591	T	T	T
0.3481753727091001	0.6261532721337787	0.1274322951915565	T	T	T
0.8482727709929431	0.3752668537367873	0.1334586765653341	T	T	T
0.3483336839462834	0.8759161652312368	0.1334643152674587	T	T	T
0.8483412826125590	0.6238025508328690	0.1276179513195790	T	T	T
0.8485161982062082	0.8751833305633362	0.1347625654383923	T	T	T
0.0988048761422256	0.1268230734186378	0.1770589008283247	T	T	T
0.0954273308483936	0.3748786011790666	0.1866046689209155	T	T	T
0.5973783646130076	0.1275339238648976	0.1768921822044069	T	T	T
0.0984228672137139	0.6251727865963062	0.1769360635738093	T	T	T
0.6012203125632742	0.3749189724544569	0.1865882773996322	T	T	T
0.100333988465537	0.8754866009006449	0.1867000441466101	T	T	T
0.5980791700890975	0.6254237691448672	0.1768402182412034	T	T	T
0.5966436794971540	0.8756108743424976	0.1865392191480044	T	T	T
0.1114792291282643	0.0067191917136866	0.2339666417065459	T	T	T
0.0871764589818265	0.2436470821096804	0.2331912575717704	T	T	T
0.5856795969838886	0.0074967225745656	0.2331097853430478	T	T	T
0.0815436211402682	0.5060131906796584	0.2337820182008313	T	T	T
0.6100191226961877	0.2439310875768854	0.2333771050915557	T	T	T
0.1145436120770015	0.7441250340205657	0.2338025183346353	T	T	T
0.6143160316739515	0.5062356440096134	0.2335705388222558	T	T	T
0.5820232302362514	0.7443206655400566	0.2337516483771996	T	T	T
0.3494582860509010	0.0510200826516357	0.2838953174881597	T	T	T
0.3479858117789095	0.2050064826332431	0.2735075690202389	T	T	T
0.8486614599176899	0.0662253411261753	0.2618011271061356	T	T	T
0.3479647994558476	0.5625535005024633	0.2615212434257799	T	T	T
0.8495143387789925	0.2129146569230750	0.2878261102852835	T	T	T
0.3483636961979908	0.7093999444431055	0.2893530646837661	T	T	T
0.8476932929009748	0.5407161299852568	0.2893771849151981	T	T	T
0.8481736273115335	0.6877325250495238	0.2616991116012196	T	T	T
0.0982437210000029	0.9179475529999129	0.0000000000000000	F	F	F
0.0982437879999907	0.0820524620000000	0.0000000162939813	F	F	F
0.0982437429999905	0.1679478439999969	0.0000000000000000	F	F	F
0.0982438099999853	0.3320527369999980	0.0000000162939813	F	F	F
0.5982443090000018	0.0820524470000024	0.0000000000000000	F	F	F

0.5982443089999236	0.9179475379998863	0.0000000162939813	F	F	F
0.0982437660000031	0.4179481569999628	0.0000000000000000	F	F	F
0.0982438329999979	0.5820530649999114	0.0000000162939813	F	F	F
0.5982443089999027	0.3320527079999994	0.0000000000000000	F	F	F
0.5982443090000018	0.1679478289999992	0.0000000162939813	F	F	F
0.0982437950000019	0.6679484840000008	0.0000000000000000	F	F	F
0.0982438469999920	0.8320534229998984	0.0000000162939813	F	F	F
0.5982443689999997	0.5820530060000032	0.0000000000000000	F	F	F
0.5982443690000008	0.4179481269999958	0.0000000162939813	F	F	F
0.5982443690000001	0.8320533629999218	0.0000000000000000	F	F	F
0.5982443689999082	0.6679484249999064	0.0000000162939813	F	F	F
0.3320954362964136	0.1374209149475653	0.4070042267022714	T	T	T
0.5274926855532451	0.0909240111331268	0.3762259373933858	T	T	T
0.6048567560214524	0.2117213247881883	0.4476258285635198	T	T	T
0.6895148574172382	0.2271777085696560	0.3865902105334982	T	T	T
0.3485199997568740	0.3070742528179669	0.4283459921272300	T	T	T
0.5463193758200066	0.3652369865065581	0.4175760106272558	T	T	T
0.3158624605062470	0.3733294834282575	0.3458828965986183	T	T	T
0.5301967844458622	0.3387030005208511	0.3274200410744522	T	T	T
0.4630877765931522	0.1478398363343952	0.3922520206109470	T	T	T
0.5667413344237550	0.2237139666072038	0.4081254310510390	T	T	T
0.4665360515634973	0.3098589788872245	0.4048972547117813	T	T	T
0.4151168472630882	0.3217042183937168	0.3503857374469890	T	T	T
0.3435861990740910	0.2402534363447502	0.3344908166982302	T	T	T

TS Ic At, E = -385.42820 eV

1.0000000000000000		
7.6621999740000000	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000
-0.0000007340000000	-0.0000007340000000	26.7875003810000010

Si O C H
48 1 4 24

Selective dynamics

Direct

0.0982437263469365	0.0000000011734684	0.0289689852776362	F	F	F
0.0982437493468993	0.2500002971733863	0.0289689852776362	F	F	F
0.5982443673469362	0.0000000011734684	0.0289689852776362	F	F	F
0.0982437713469366	0.5000005951734678	0.0289689852776362	F	F	F
0.5982443673469362	0.2500002971733863	0.0289689852776362	F	F	F
0.0982437933469100	0.7500008931734712	0.0289689852776362	F	F	F
0.5982444273469341	0.5000005951734678	0.0289689852776362	F	F	F
0.5982444273469341	0.7500008931734712	0.0289689852776362	F	F	F
0.3481091979665720	0.9987821640746901	0.0798473667218076	F	F	F
0.3481187753265615	0.2525569462024109	0.0806859696266926	F	F	F
0.8481454509827415	0.9987327431440605	0.0808478902570613	F	F	F
0.3481040515230518	0.4979598335936046	0.0807181823396235	F	F	F
0.8481820332878129	0.2521422366695063	0.0801561492179843	F	F	F
0.3480737325642806	0.7524409888169927	0.0800223858013211	F	F	F
0.8482391498050106	0.4977799300152697	0.0800732077249080	F	F	F
0.8483926193681626	0.7515327669047025	0.0808471308038961	F	F	F
0.3482470397234394	0.1247178483115619	0.1276510026642299	T	T	T
0.3484589240011786	0.3755076981072349	0.1350942210790720	T	T	T
0.8479716404229620	0.1257250671988501	0.1281165171615157	T	T	T
0.3480150197432366	0.6260875833120281	0.1274366266056290	T	T	T
0.8484644963333707	0.3753077954368678	0.1334485081745740	T	T	T
0.3483961889984784	0.8758156574995439	0.1334646909476334	T	T	T

0.8482037415311225	0.6237853540830685	0.1276802163653699	T	T	T
0.8486135237252626	0.8751441389728640	0.1346984637880198	T	T	T
0.0989562796663535	0.1269387251001604	0.1769206327887147	T	T	T
0.0957149723524751	0.3749412684823952	0.1865846057752805	T	T	T
0.5972480677765049	0.1277463078881667	0.1771387573252312	T	T	T
0.0983493638815176	0.6251930636481617	0.1769546152625168	T	T	T
0.6013832893351605	0.3750602169835560	0.1865794214333434	T	T	T
0.1003163853107552	0.8754260830099128	0.1866438698024169	T	T	T
0.5978361745134251	0.6254514337150852	0.1768719531681171	T	T	T
0.5968728408987616	0.8755390568248416	0.1864917821441239	T	T	T
0.1108003000106592	0.0068249332212176	0.2336870846823302	T	T	T
0.0880911614285438	0.2436879787477579	0.2331254801497522	T	T	T
0.5859912628237751	0.0071607926230755	0.2332511407257982	T	T	T
0.0821068107229408	0.5060721126124221	0.2337663005103252	T	T	T
0.6103052680220031	0.2443567492579817	0.2335914094484366	T	T	T
0.1147949623022839	0.7441739834757684	0.2338073735939830	T	T	T
0.6149107484957810	0.5062794600147527	0.2336554642525996	T	T	T
0.5822514304625983	0.7443476488886844	0.2337598011935640	T	T	T
0.3488641955266161	0.0506568946287658	0.2835163010533535	T	T	T
0.3485443977360987	0.2046439644373379	0.2735849813441931	T	T	T
0.8484811268950310	0.0664151895992617	0.2618273441594425	T	T	T
0.3484743284615703	0.5626151751100466	0.2615576541638305	T	T	T
0.8503657569415708	0.2131802927890760	0.2877357859010417	T	T	T
0.3486081501168314	0.7095067634065515	0.2893816550243073	T	T	T
0.8483612058859435	0.5408046023190494	0.2894073104388610	T	T	T
0.8484798267384690	0.6877612397362611	0.2616870475561228	T	T	T
0.3428357498240970	0.2351932253949514	0.3351028083794247	T	T	T
0.4837108905184309	0.1410596366565002	0.3877485896253319	T	T	T
0.4899209550561352	0.2177065419100614	0.4209861939623849	T	T	T
0.5367273342660894	0.3017514733478137	0.3932191648347469	T	T	T
0.3928316962715641	0.3181642375050160	0.3548149347393306	T	T	T
0.0982437210000029	0.9179475529997987	0.0000000000000000	F	F	F
0.0982437879999694	0.0820524620000000	0.0000000162939813	F	F	F
0.0982437429999763	0.1679478439999968	0.0000000000000000	F	F	F
0.0982438099999570	0.3320527369999979	0.0000000162939813	F	F	F
0.5982443090000018	0.0820524470000024	0.0000000000000000	F	F	F
0.5982443089998029	0.9179475379997228	0.0000000162939813	F	F	F
0.0982437660000031	0.4179481569999126	0.0000000000000000	F	F	F
0.0982438329999979	0.5820530649997977	0.0000000162939813	F	F	F
0.5982443089997602	0.3320527079999991	0.0000000000000000	F	F	F
0.5982443090000018	0.1679478289999992	0.0000000162939813	F	F	F
0.0982437950000019	0.6679484840000001	0.0000000000000000	F	F	F
0.0982438469999707	0.8320534229997492	0.0000000162939813	F	F	F
0.5982443689999997	0.5820530060000024	0.0000000000000000	F	F	F
0.5982443689999997	0.4179481269999954	0.0000000162939813	F	F	F
0.5982443689999997	0.8320533629998010	0.0000000000000000	F	F	F
0.5982443689997723	0.6679484249997785	0.0000000162939813	F	F	F
0.3991886911721636	0.0857974538096826	0.3960985087914892	T	T	T
0.5950882335958525	0.1282418841979620	0.3633220683349236	T	T	T
0.3677193533798828	0.2247202595394384	0.4422777810630478	T	T	T
0.5942489464463350	0.2040022400194701	0.4488036102268893	T	T	T
0.5493922961151156	0.3576369174833616	0.4187304792913409	T	T	T
0.6623452436129043	0.2929323814572626	0.3737660286658624	T	T	T
0.2765222510579903	0.3477563551285741	0.3721929397137416	T	T	T
0.4395287394322551	0.3617840143792037	0.3248269946581814	T	T	T

8.8. Transition States of Reaction B

TS Ib B2, E(PBE-D3) = -699.83974 eV, E(HSE06-D3) = -809.94973 eV

1.0000000000000000

15.3244190216000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 15.3244190216000007 0.0000000000000000

0.0000000000000000 0.0000000000000000 26.7875003810000010

Si O C H

96 1 4 40

Selective dynamics

Direct

0.0000000000000000 0.0000000000000000 0.0354635925893945 F F F

0.5000000319229088 0.0000000000000000 0.0354635925893945 F F F

0.0000000000000000 0.2500000159614544 0.0354635925893945 F F F

0.5000000319229088 0.2500000159614544 0.0354635925893945 F F F

0.2500000159614544 0.0000000000000000 0.0354635925893945 F F F

0.7500000478843631 0.0000000000000000 0.0354635925893945 F F F

0.0000000000000000 0.5000000319229088 0.0354635925893945 F F F

0.5000000319229088 0.5000000319229088 0.0354635925893945 F F F

0.2500000159614544 0.2500000159614544 0.0354635925893945 F F F

0.7500000478843631 0.2500000159614544 0.0354635925893945 F F F

0.0000000000000000 0.7500000478843631 0.0354635925893945 F F F

0.5000000319229088 0.7500000478843631 0.0354635925893945 F F F

0.2500000159614544 0.5000000319229088 0.0354635925893945 F F F

0.7500000478843631 0.5000000319229088 0.0354635925893945 F F F

0.2500000159614544 0.7500000478843631 0.0354635925893945 F F F

0.7500000478843631 0.7500000478843631 0.0354635925893945 F F F

0.1249999753530631 0.0000000000000000 0.0860282208949457 F F F

0.6250000072759718 0.0000000000000000 0.0860282208949457 F F F

0.1249999753530631 0.2500000159614544 0.0860282208949457 F F F

0.6250000072759718 0.2500000159614544 0.0860282208949457 F F F

0.3749999913145174 0.0000000000000000 0.0860282208949457 F F F

0.8750000232374191 0.0000000000000000 0.0860282208949457 F F F

0.1249999753530631 0.5000000319229088 0.0860282208949457 F F F

0.6250000072759718 0.5000000319229088 0.0860282208949457 F F F

0.3749999913145174 0.2500000159614544 0.0860282208949457 F F F

0.8750000232374191 0.2500000159614544 0.0860282208949457 F F F

0.1249999753530631 0.7500000478843631 0.0860282208949457 F F F

0.6250000072759718 0.7500000478843631 0.0860282208949457 F F F

0.3749999913145174 0.5000000319229088 0.0860282208949457 F F F

0.8750000232374191 0.5000000319229088 0.0860282208949457 F F F

0.3749999913145174 0.7500000478843631 0.0860282208949457 F F F

0.8750000232374191 0.7500000478843631 0.0860282208949457 F F F

0.1251309029155436 0.1242514530845753 0.1344134072495180 T T T

0.1248782574657312 0.3752837561401847 0.1397174218145238 T T T

0.3734952876589617 0.1253885256962732 0.1344535379753751 T T T

0.1249051317842671 0.6256131091656130 0.1342306982168964 T T T

0.3746416852461891 0.3749433068706054 0.1387724651135045 T T T

0.1247595853904713 0.8749684058249443 0.1388070565643744 T T T

0.3749746949673778 0.6244175944305894 0.1341923600613697 T T T

0.3746692292755256 0.8750202636347879 0.1398561252567987 T T T

0.0001455956743257 0.1251497731947353 0.1833058706262776 T T T

0.4996433655795371 0.3764265010330661 0.1911955645522170 T T T

0.2496056017109183 0.1256197862087163 0.1842334948152100 T T T

0.9999180570323958 0.6252026993097388 0.1833932068164117 T T T

0.2505682624991721 0.3743871131013279 0.1920312380528912 T T T

0.0009487170477058 0.8760463167471286 0.1922819246787952 T T T

0.2500047022002079	0.6252397326774712	0.1833136043056101	T	T	T
0.2487138722191489	0.8756320150435002	0.1921047642663609	T	T	T
0.0094311225569896	0.0066157929097130	0.2403121319908621	T	T	T
0.4970793586574018	0.2456719911981793	0.2381705393703655	T	T	T
0.2393359307784451	0.0056964727829296	0.2405084369915613	T	T	T
0.4920323137267104	0.5059446917315853	0.2398352158182888	T	T	T
0.2509414837469706	0.2436493738934118	0.2396486920755194	T	T	T
0.0080740827275321	0.7447813544497208	0.2397716723659897	T	T	T
0.2579949011312692	0.5054727501279359	0.2394772502472051	T	T	T
0.2417713679965132	0.7446316526776826	0.2397767197828955	T	T	T
0.1242655499241678	0.0410373177738350	0.2972033603386350	T	T	T
0.1211462154385359	0.1981442243574776	0.2820491195972252	T	T	T
0.3742229167005817	0.0577494639398068	0.2668958527033283	T	T	T
0.1248374183398724	0.5624445603153276	0.2673670356296611	T	T	T
0.3770708149000654	0.2078108658514495	0.2892885049011795	T	T	T
0.1249422103119997	0.7092364121549792	0.2952512113747545	T	T	T
0.3747261041429155	0.5405489745859100	0.2952758492581609	T	T	T
0.3748463599226213	0.6879532909400439	0.2677508066657523	T	T	T
0.6247867530464362	0.1244756202305410	0.1342864694657919	T	T	T
0.6256305793211538	0.3752855681148404	0.1395311673157309	T	T	T
0.8754381533730609	0.1253787960057053	0.1343446136097128	T	T	T
0.6250461291113538	0.6255943643027067	0.1343202047275156	T	T	T
0.8753459296528945	0.3750429822445369	0.1387384142967392	T	T	T
0.6253128859967489	0.8749256852201270	0.1387594313293761	T	T	T
0.8749923583982735	0.6243912476915909	0.1342052598736529	T	T	T
0.8752900403286361	0.8750453571262398	0.1398787566821937	T	T	T
0.4990420566824696	0.1245546155366526	0.1829780004680259	T	T	T
0.9992242348119831	0.3740592142950021	0.1920439122409547	T	T	T
0.7498909715980488	0.1250646990767521	0.1833545715233029	T	T	T
0.4998716956415947	0.6250904155322274	0.1833621391582270	T	T	T
0.7512413900926234	0.3750355566901362	0.1919117433624677	T	T	T
0.5010655500437267	0.8746763245338087	0.1916767713738423	T	T	T
0.7501113338087251	0.6250607361154294	0.1834520467496361	T	T	T
0.7493316744841039	0.8753686143312223	0.1920923695924301	T	T	T
0.5085892132441501	0.0051830677584022	0.2393642935611169	T	T	T
0.9950232878117973	0.2422669801736532	0.2386050020727879	T	T	T
0.7427242036536867	0.0061409745766525	0.2399241590310268	T	T	T
0.9918376667911488	0.5052603507004036	0.2394857293686314	T	T	T
0.7599084506108866	0.2447855961667358	0.2399276180310821	T	T	T
0.5081313112671495	0.7443616725178615	0.2398251789296282	T	T	T
0.7585103008139171	0.5055618655931227	0.2398531776816810	T	T	T
0.7421843663044640	0.7445091204277219	0.2398273390924928	T	T	T
0.6251386132019121	0.0403118000708176	0.2952636206720882	T	T	T
0.6277966576018628	0.1871939234212334	0.2675352546142022	T	T	T
0.8762273946884207	0.0633216790264655	0.2675623644244141	T	T	T
0.6253889683186458	0.5623715324751899	0.2676584392296206	T	T	T
0.8774396727804046	0.2103324472751922	0.2941912017902411	T	T	T
0.6251639000116285	0.7093086363632111	0.2952513437648108	T	T	T
0.8754734828673065	0.5403349643929332	0.2954125302474822	T	T	T
0.8752571776178044	0.6876897707456351	0.2678498485422196	T	T	T
0.1141892962820705	0.2460726782441398	0.3419878271786416	T	T	T
0.2460414646813760	0.2380669016247197	0.3656652218108860	T	T	T
0.2553773315438761	0.3339929762346401	0.3636647833892681	T	T	T
0.1681577314622160	0.3757291569892729	0.3798127096553827	T	T	T
0.0991043005641501	0.3390000556995147	0.3449732009816344	T	T	T
0.0000000000000000	0.1711557218778097	0.0035690153482122	F	F	F
0.5000000319229088	0.1711557218778097	0.0035690153482122	F	F	F

0.0000000000000000	0.3288443100450991	0.0035690153482122	F	F	F
0.5000000319229088	0.3288443100450991	0.0035690153482122	F	F	F
0.0000000000000000	0.4211557378392641	0.0035690153482122	F	F	F
0.5000000319229088	0.4211557378392641	0.0035690153482122	F	F	F
0.0000000000000000	0.0788442940836447	0.0035690153482122	F	F	F
0.5000000319229088	0.0788442940836447	0.0035690153482122	F	F	F
0.2500000159614544	0.0788442940836447	0.0035690153482122	F	F	F
0.7500000478843631	0.0788442940836447	0.0035690153482122	F	F	F
0.2500000159614544	0.1711557218778097	0.0035690153482122	F	F	F
0.7500000478843631	0.1711557218778097	0.0035690153482122	F	F	F
0.2500000159614544	0.3288443100450991	0.0035690153482122	F	F	F
0.7500000478843631	0.3288443100450991	0.0035690153482122	F	F	F
0.2500000159614544	0.4211557378392641	0.0035690153482122	F	F	F
0.7500000478843631	0.4211557378392641	0.0035690153482122	F	F	F
0.0000000000000000	0.6711557538007185	0.0035690153482122	F	F	F
0.5000000319229088	0.6711557538007185	0.0035690153482122	F	F	F
0.0000000000000000	0.8288443419680007	0.0035690153482122	F	F	F
0.5000000319229088	0.8288443419680007	0.0035690153482122	F	F	F
0.0000000000000000	0.9211557697621728	0.0035690153482122	F	F	F
0.5000000319229088	0.9211557697621728	0.0035690153482122	F	F	F
0.0000000000000000	0.5788443260065463	0.0035690153482122	F	F	F
0.5000000319229088	0.5788443260065463	0.0035690153482122	F	F	F
0.2500000159614544	0.5788443260065463	0.0035690153482122	F	F	F
0.7500000478843631	0.5788443260065463	0.0035690153482122	F	F	F
0.2500000159614544	0.6711557538007185	0.0035690153482122	F	F	F
0.7500000478843631	0.6711557538007185	0.0035690153482122	F	F	F
0.2500000159614544	0.8288443419680007	0.0035690153482122	F	F	F
0.7500000478843631	0.8288443419680007	0.0035690153482122	F	F	F
0.2500000159614544	0.9211557697621728	0.0035690153482122	F	F	F
0.7500000478843631	0.9211557697621728	0.0035690153482122	F	F	F
0.2516461490205302	0.1940832968712272	0.3342416403907222	T	T	T
0.2412428312452306	0.2061632957193211	0.4021276928517850	T	T	T
0.307655558005225	0.3558527720046953	0.3889690970075890	T	T	T
0.2730323461347197	0.3560096699961051	0.3257885436577794	T	T	T
0.1530042370740077	0.3583662831022778	0.4187515049264334	T	T	T
0.1718947954715517	0.4473702382270162	0.3773631910744442	T	T	T
0.0321052540058204	0.3496709234283486	0.3585662457926446	T	T	T
0.1051578446926413	0.3687746319734515	0.3075107456869191	T	T	T

TS Ic B3, E = -699.74583 eV

1.0000000000000000		
15.3243999479999999	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000
-0.0000007340000000	-0.0000007340000000	26.7875003810000010

Si O C H

96 1 4 40

Selective dynamics

Direct

0.0000000016986164	0.0000000016986164	0.0354635925893945	F	F	F
0.5000006559493571	0.0000000016986164	0.0354635925893945	F	F	F
0.0000000126289095	0.2500003288239867	0.0354635925893945	F	F	F
0.5000006668796505	0.2500003288239867	0.0354635925893945	F	F	F
0.2500003288239867	0.0000000016986164	0.0354635925893945	F	F	F
0.7500009830747277	0.0000000016986164	0.0354635925893945	F	F	F
0.0000000235592097	0.5000006559493571	0.0354635925893945	F	F	F
0.5000006778099507	0.5000006559493571	0.0354635925893945	F	F	F

0.2500003397542798 0.2500003288239867 0.0354635925893945 F F F
0.7500009940050280 0.2500003288239867 0.0354635925893945 F F F
0.0000000344895028 0.7500009830747274 0.0354635925893945 F F F
0.5000006887402436 0.7500009830747274 0.0354635925893945 F F F
0.2500003506845800 0.5000006559493571 0.0354635925893945 F F F
0.7500010049353211 0.5000006559493571 0.0354635925893945 F F F
0.2500003616148732 0.7500009830747274 0.0354635925893945 F F F
0.7500010158656139 0.7500009830747274 0.0354635925893945 F F F
0.1250001350555152 0.0000000041205368 0.0860282208949457 F F F
0.6250007893062559 0.0000000041205368 0.0860282208949457 F F F
0.1250001459858083 0.2500003312459071 0.0860282208949457 F F F
0.6250008002365490 0.2500003312459071 0.0860282208949457 F F F
0.3750004621808854 0.0000000041205368 0.0860282208949457 F F F
0.8750011164316192 0.0000000041205368 0.0860282208949457 F F F
0.1250001569161086 0.5000006583712775 0.0860282208949457 F F F
0.6250008111668492 0.5000006583712775 0.0860282208949457 F F F
0.3750004731111787 0.2500003312459071 0.0860282208949457 F F F
0.8750011273619194 0.2500003312459071 0.0860282208949457 F F F
0.1250001678464017 0.7500009854966482 0.0860282208949457 F F F
0.6250008220971425 0.7500009854966482 0.0860282208949457 F F F
0.3750004840414789 0.5000006583712775 0.0860282208949457 F F F
0.8750011382922128 0.5000006583712775 0.0860282208949457 F F F
0.3750004949717720 0.7500009854966482 0.0860282208949457 F F F
0.8750011492225056 0.7500009854966482 0.0860282208949457 F F F
0.1249728309666391 0.1242764872309923 0.1344012478108858 T T T
0.1248097339929482 0.3752389501001276 0.1397263267149433 T T T
0.3734089804669167 0.1254218480212368 0.1344571901176782 T T T
0.1249330147244453 0.6256452366882892 0.1341746038785543 T T T
0.3744792843618299 0.3748589159248038 0.1388068060958011 T T T
0.1247629369200321 0.8749613830264660 0.1387766087448705 T T T
0.3752584597402832 0.6244910155130763 0.1340923503591961 T T T
0.3747601648855577 0.8750091167641522 0.1398150594937339 T T T
0.0001446672143775 0.1253521045029156 0.1834222806087409 T T T
0.4995841666111838 0.3765604529208880 0.1911332316183669 T T T
0.2494323676084324 0.1256393965337637 0.1842090828848357 T T T
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0.2503715022550539 0.3743472686520389 0.1921332626166729 T T T
0.0009128912868661 0.8760054170760470 0.1922118989464189 T T T
0.2502422473369715 0.6255391617417809 0.1830010586366279 T T T
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0.0093943216624612 0.0065006660045929 0.2402231268845146 T T T
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0.4918228116890705 0.5059527607511819 0.2398474376302021 T T T
0.2502462933888915 0.2434263656713452 0.2398476935415313 T T T
0.0081456131710104 0.7448499896953010 0.2397615394302588 T T T
0.2578873512911145 0.5060489252189762 0.2389745321976278 T T T
0.2419000282802032 0.7446001200431254 0.2396582668162186 T T T
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0.1207700463042335 0.1975576995051662 0.2828046562216553 T T T
0.3740815316051940 0.0575468011065910 0.2667999470223096 T T T
0.1247773767431956 0.5626298722159400 0.2672040069959095 T T T
0.3771140724471079 0.2074368431058193 0.2886971863814462 T T T
0.1250624081197522 0.7093848154647937 0.2951845970155738 T T T
0.3742290587225054 0.5401036531875704 0.2951783904064664 T T T
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0.6248046383088270 0.1244816048290363 0.1342632550621902 T T T

0.6256332253383636 0.3752854963493706 0.1395085380387492 T T T
0.8754840676734769 0.1254151512970866 0.1343663595954269 T T T
0.6251488422108826 0.6255945660908692 0.1343176763244358 T T T
0.8753765343990099 0.3750304516963699 0.1387513395567697 T T T
0.6253427454806667 0.8749223662043850 0.1387568287667668 T T T
0.8751199243545277 0.6243736763400628 0.1342094504925563 T T T
0.8752759351757832 0.8750292813355809 0.1398446209964722 T T T
0.4990134400742551 0.1245034213376876 0.1829299635947240 T T T
0.9992241138856353 0.3740208958636034 0.1921185893926021 T T T
0.7498774531782122 0.1250737429782317 0.1833160318286776 T T T
0.4999941478215263 0.6251082647219166 0.1833690225256824 T T T
0.7512251558965142 0.3750394869541824 0.1918887389324966 T T T
0.5010871214431338 0.8746618901476578 0.1916901609441097 T T T
0.7502172254859756 0.6250728123840578 0.1834264270984457 T T T
0.7493565511073835 0.8753632928997278 0.1920734450776639 T T T
0.5086440385709107 0.0052158226161377 0.2393586457046706 T T T
0.9952130272552228 0.2423930131643981 0.2388675615478193 T T T
0.7427975720568761 0.0061648561303168 0.2398614160145862 T T T
0.9917906859204586 0.5052012942818720 0.2395793066520949 T T T
0.7599515389895924 0.2447892651532759 0.2398901276490005 T T T
0.5080698088285732 0.7443361655485436 0.2398455654258929 T T T
0.7583676768649702 0.5055874880165784 0.2397972461255259 T T T
0.7422412906543052 0.7445029531366739 0.2397791260628786 T T T
0.6252264129445576 0.0403014261985890 0.2952031705205224 T T T
0.6279007805301445 0.1871498684953779 0.2675009619406299 T T T
0.8762962174377216 0.0633703353347106 0.2675231322314622 T T T
0.6252133512276669 0.5623662623762966 0.2676069113899573 T T T
0.8773174291706166 0.2103083489862799 0.2942469599188968 T T T
0.6251981328213632 0.7092799165738312 0.2951757023795750 T T T
0.8753018421947883 0.5404381430101258 0.2953618386463972 T T T
0.8753323647304201 0.6877372814453846 0.2678038873526872 T T T
0.1106212034123304 0.2399945230531684 0.3435264404200971 T T T
0.2446047385390153 0.2274506445590379 0.3713505683713990 T T T
0.2448671611106140 0.3182668245798205 0.3898068959633433 T T T
0.1877910503732499 0.3752057938252067 0.3557184230288212 T T T
0.0985891098250335 0.3318836061930969 0.3519628878080358 T T T
0.000000076540800 0.1711559350786800 0.0035690153482122 F F F
0.5000006619048207 0.1711559350786800 0.0035690153482122 F F F
0.000000145484051 0.3288447195139526 0.0035690153482122 F F F
0.5000006687991458 0.3288447195139526 0.0035690153482122 F F F
0.000000185843732 0.4211562622040503 0.0035690153482122 F F F
0.5000006728351138 0.4211562622040503 0.0035690153482122 F F F
0.000000036181120 0.0788443923885823 0.0035690153482122 F F F
0.5000006578688527 0.0788443923885823 0.0035690153482122 F F F
0.2500003307434824 0.0788443923885823 0.0035690153482122 F F F
0.7500009849942231 0.0788443923885823 0.0035690153482122 F F F
0.2500003347794504 0.1711559350786800 0.0035690153482122 F F F
0.7500009890301914 0.1711559350786800 0.0035690153482122 F F F
0.2500003416737755 0.3288447195139526 0.0035690153482122 F F F
0.7500009959245233 0.3288447195139526 0.0035690153482122 F F F
0.2500003457097435 0.4211562622040503 0.0035690153482122 F F F
0.7500009999604842 0.4211562622040503 0.0035690153482122 F F F
0.000000295146663 0.6711565893294210 0.0035690153482122 F F F
0.5000006837654070 0.6711565893294210 0.0035690153482122 F F F
0.0000000364089985 0.8288453737646865 0.0035690153482122 F F F
0.5000006906597392 0.8288453737646865 0.0035690153482122 F F F
0.0000000404449665 0.9211569164547914 0.0035690153482122 F F F

0.5000006946957072	0.9211569164547914	0.0035690153482122	F	F	F
0.0000000254787054	0.5788450466393159	0.0035690153482122	F	F	F
0.5000006797294461	0.5788450466393159	0.0035690153482122	F	F	F
0.2500003526040757	0.5788450466393159	0.0035690153482122	F	F	F
0.7500010068548164	0.5788450466393159	0.0035690153482122	F	F	F
0.2500003566400366	0.6711565893294210	0.0035690153482122	F	F	F
0.7500010108907773	0.6711565893294210	0.0035690153482122	F	F	F
0.2500003635343688	0.8288453737646865	0.0035690153482122	F	F	F
0.7500010177851099	0.8288453737646865	0.0035690153482122	F	F	F
0.2500003675703368	0.9211569164547914	0.0035690153482122	F	F	F
0.7500010218210775	0.9211569164547914	0.0035690153482122	F	F	F
0.2536224843162309	0.2131845544898042	0.3322737717231394	T	T	T
0.2435823843424129	0.1716275015860488	0.3966838446096128	T	T	T
0.2220691655693468	0.3204028239010674	0.4287928340896288	T	T	T
0.3119642057541619	0.3444432095680284	0.3899180052511506	T	T	T
0.1827184228764434	0.4423418529470071	0.3700359776848169	T	T	T
0.2179559467695298	0.3792519524532108	0.3184137197705147	T	T	T
0.0615178172559454	0.3383450591633301	0.3869923163848647	T	T	T
0.0592951099689602	0.3604125439737816	0.3214669989295985	T	T	T

8.9. Transition States of Reaction C

TS Ib(4x2) Cb(4x2), E = -385.80561 eV

```

1.0000000000000000
 7.6621999740000000  0.0000000000000000  0.0000000000000000
-0.0000006700000000  15.3243999479999999  0.0000000000000000
-0.0000007340000000 -0.0000007340000000  26.7875003810000010

```

Si O C H

48 1 4 24

Selective dynamics

Direct

0.0982437263469365	0.0000000011734684	0.0289689852776363	F	F	F
0.0982437493469206	0.2500002971734503	0.0289689852776363	F	F	F
0.5982443673469362	0.0000000011734684	0.0289689852776363	F	F	F
0.0982437713469366	0.5000005951734678	0.0289689852776363	F	F	F
0.5982443673469362	0.2500002971734503	0.0289689852776363	F	F	F
0.0982437933469313	0.7500008931734712	0.0289689852776363	F	F	F
0.5982444273469341	0.5000005951734678	0.0289689852776363	F	F	F
0.5982444273469341	0.7500008931734712	0.0289689852776363	F	F	F
0.3481418597251962	0.9990771598388480	0.0797713643150431	F	F	F
0.3481561371700012	0.2526658555804390	0.0806679081758262	F	F	F
0.8481718399543968	0.9986033428192300	0.0808210048818765	F	F	F
0.3481243654847078	0.4980532226948499	0.0807260323471014	F	F	F
0.8481950966200174	0.2521372104710693	0.0801776144980267	F	F	F
0.3481236516016965	0.7527268113426544	0.0800320023483821	F	F	F
0.8482278420540940	0.4975769028533037	0.0801022254430706	F	F	F
0.8483666970129423	0.7517520932699711	0.0807840724666278	F	F	F
0.3477334405480190	0.1248731268707299	0.1272868678442351	T	T	T
0.3477745551828276	0.3754413510913254	0.1346429589488155	T	T	T
0.8476627659698890	0.1257143515598792	0.1283677233121797	T	T	T
0.3495398714916245	0.6261165924806534	0.1276867068823940	T	T	T
0.8475767376580404	0.3748386791929305	0.1333457126236043	T	T	T
0.3482395898664621	0.8760132434379705	0.1335282888632946	T	T	T
0.8493669613660089	0.6240369582331421	0.1273499342263944	T	T	T
0.8482172868884189	0.8754212592679397	0.1353602146365756	T	T	T
0.0992735019166319	0.1253122552079294	0.1768138937986649	T	T	T
0.0956088922123095	0.3736266082291374	0.1860106579545574	T	T	T

0.5959711518684090	0.1252691589339711	0.1768280790441711	T	T	T
0.0988009176870952	0.6269276621923164	0.1766057359338761	T	T	T
0.5996027526987816	0.3740858391295443	0.1861231146088093	T	T	T
0.1014345433455574	0.8770111499264689	0.1871598770967281	T	T	T
0.6006178365700890	0.6265431251610410	0.1767560607082913	T	T	T
0.5949567066066043	0.8769354297580841	0.1871970962063699	T	T	T
0.1174911313614967	0.0082153684805440	0.2347332433319040	T	T	T
0.0897155283219218	0.2421264818257596	0.2327460350254091	T	T	T
0.5772585426107751	0.0081280661102319	0.2348369909000496	T	T	T
0.0830217412793349	0.5061748413951086	0.2314286510526503	T	T	T
0.6032253096655622	0.2425959898238350	0.2323985823007655	T	T	T
0.1158959765293864	0.7449584010929788	0.2339731262909275	T	T	T
0.6153264602547562	0.5061304879559105	0.2317210978603604	T	T	T
0.5820457702754299	0.7448925238705205	0.2341380797561811	T	T	T
0.3470486910751415	0.0452982355170142	0.2912023412883813	T	T	T
0.3478534790209540	0.2028414211386663	0.2752544518302503	T	T	T
0.8472740262788897	0.0623256746585216	0.2603580947086901	T	T	T
0.3492899946257467	0.5564796387826419	0.2637480916389480	T	T	T
0.8452675719587645	0.2088044039148425	0.2838155566790931	T	T	T
0.3487296859085988	0.7055467037098416	0.2888157992418504	T	T	T
0.8503166577283945	0.5408870184710525	0.2860233333451130	T	T	T
0.8490985620124682	0.6899349613744995	0.2614355709423782	T	T	T
0.3630021108996938	0.2625605719468020	0.3312493200834647	T	T	T
0.3455955972470044	0.3955450096937969	0.3168807024119955	T	T	T
0.2317931748053955	0.4141850183376726	0.3602746863288455	T	T	T
0.1223063121560199	0.3324366710212922	0.3722358164278837	T	T	T
0.2426679778415715	0.2536504407952429	0.3724005973089538	T	T	T
0.0982437210000029	0.9179475529999479	0.0000000000000000	F	F	F
0.0982437879999978	0.0820524620000000	0.0000000162939813	F	F	F
0.0982437429999976	0.1679478439999969	0.0000000000000000	F	F	F
0.0982438099999853	0.3320527369999980	0.0000000162939813	F	F	F
0.5982443090000018	0.0820524470000024	0.0000000000000000	F	F	F
0.5982443089999450	0.9179475379999292	0.0000000162939813	F	F	F
0.0982437660000031	0.4179481569999766	0.0000000000000000	F	F	F
0.0982438329999979	0.5820530649999399	0.0000000162939813	F	F	F
0.5982443089999379	0.3320527079999993	0.0000000000000000	F	F	F
0.5982443090000018	0.1679478289999992	0.0000000162939813	F	F	F
0.0982437950000019	0.6679484840000004	0.0000000000000000	F	F	F
0.0982438469999920	0.8320534229999339	0.0000000162939813	F	F	F
0.5982443689999997	0.5820530060000028	0.0000000000000000	F	F	F
0.5982443690000000	0.4179481269999956	0.0000000162939813	F	F	F
0.5982443690000000	0.8320533629999503	0.0000000000000000	F	F	F
0.5982443689999428	0.6679484249999419	0.0000000162939813	F	F	F
0.2884363165485583	0.3798439342926667	0.2807382503456118	T	T	T
0.4866362951031426	0.4042233396188517	0.3183328562804141	T	T	T
0.3096280617248759	0.4352714256257877	0.3925751404884216	T	T	T
0.1382618814927683	0.4671314448278315	0.3510796588687511	T	T	T
0.0542562881247118	0.3399123656697973	0.4081477691613901	T	T	T
0.0213968348274135	0.3233969958393816	0.3432901291844982	T	T	T
0.3217513000809014	0.2501660330179212	0.4066901931392614	T	T	T
0.1683704921949143	0.1923633271501891	0.3682344906422105	T	T	T

TS Ib(2x2) Cb(2x2), E = -385.99952 eV

1.0000000000000000		
7.6621999740000000	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000

-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si O C H

48 1 4 24

Selective dynamics

Direct

0.0982437263469365	0.0000000011734684	0.0289689852776366	F	F	F
0.0982437493469135	0.2500002971734290	0.0289689852776366	F	F	F
0.5982443673469362	0.0000000011734684	0.0289689852776366	F	F	F
0.0982437713469366	0.5000005951734678	0.0289689852776366	F	F	F
0.5982443673469362	0.2500002971734290	0.0289689852776366	F	F	F
0.0982437933469313	0.7500008931734712	0.0289689852776366	F	F	F
0.5982444273469341	0.5000005951734678	0.0289689852776366	F	F	F
0.5982444273469341	0.7500008931734712	0.0289689852776366	F	F	F
0.3481446276708269	0.9991021594798544	0.0797649234331114	F	F	F
0.3481593034279200	0.2526750851887343	0.0806663775443905	F	F	F
0.8481740763078065	0.9985923766900563	0.0808187264602590	F	F	F
0.3481260870068681	0.4980611370254172	0.0807266976019686	F	F	F
0.8481962036819520	0.2521367845220510	0.0801794335895717	F	F	F
0.3481278820286001	0.7527510335905845	0.0800328173099782	F	F	F
0.8482268837701037	0.4975596971615705	0.0801046845717092	F	F	F
0.8483645002031182	0.7517706802500910	0.0807787285397420	F	F	F
0.3482194049930541	0.1249237197853871	0.1274823517770647	T	T	T
0.3478851468852728	0.3748634477211883	0.1344042281161582	T	T	T
0.8484252241364666	0.1257745592288912	0.1282242847275081	T	T	T
0.3482373661488248	0.6252431885337242	0.1271219936648236	T	T	T
0.8482571494649149	0.3751014562375149	0.1339104198686172	T	T	T
0.3482266144702881	0.8755448050392652	0.1340026323054833	T	T	T
0.8482246889168946	0.6251808138280897	0.1277720137833327	T	T	T
0.8483260817418987	0.8759882091514813	0.1345750581911082	T	T	T
0.0994481349121714	0.1259967874595493	0.1769464060868819	T	T	T
0.0975146720817362	0.3727642623681819	0.1865019625623532	T	T	T
0.5972246297154317	0.1258405902619674	0.1768057024564194	T	T	T
0.0995563296439293	0.6261938363914379	0.1767930488159891	T	T	T
0.5986153432155409	0.3728992624881943	0.1862363345463397	T	T	T
0.0989657869894814	0.8776310136154488	0.1869336674964890	T	T	T
0.5969373313271434	0.6260546736191158	0.1767961420383653	T	T	T
0.5976240478332100	0.8775881722392753	0.1868723833738926	T	T	T
0.1156979505212300	0.0086079870482505	0.2346220375554297	T	T	T
0.0900200582988848	0.2416748818195219	0.2337929494274701	T	T	T
0.5808724955118102	0.0085372102856658	0.2345505957908449	T	T	T
0.1112430425672430	0.5054240906358120	0.2321791950406393	T	T	T
0.6050061274961065	0.2419341438989009	0.2332796638062791	T	T	T
0.0838678743446014	0.7454428447322472	0.2336729345783455	T	T	T
0.5867706585384431	0.5050845705609928	0.2320363749880988	T	T	T
0.6132908072455820	0.7454608380000950	0.2335988610241203	T	T	T
0.3484113019029611	0.0414149811411721	0.2905772761307149	T	T	T
0.3489100471408426	0.1977827117084056	0.2749545717413340	T	T	T
0.8481251461417078	0.0651690131733143	0.2613432013480913	T	T	T
0.3498105966319260	0.5393252304693897	0.2857076062898774	T	T	T
0.8462651193448314	0.2119709206819072	0.2865327869642208	T	T	T
0.3487518745802984	0.6900091230370329	0.2625004995803215	T	T	T
0.8488765139219998	0.5637860324351870	0.2612586884477267	T	T	T
0.8484792974535998	0.7103904702658085	0.2887294138707605	T	T	T
0.3626159248652955	0.2508924016349300	0.3339421864398285	T	T	T
0.3466491918850495	0.3768384188626722	0.3306966041304802	T	T	T
0.2587252505958805	0.3865009326135856	0.3802660070639700	T	T	T
0.1450552687085614	0.3051548499387498	0.3889608283174723	T	T	T

0.2580392325239459	0.2266377963665774	0.3769130058510021	T	T	T
0.0982437210000029	0.9179475529998919	0.0000000000000000	F	F	F
0.0982437879999907	0.0820524620000000	0.0000000162939813	F	F	F
0.0982437429999905	0.1679478439999969	0.0000000000000000	F	F	F
0.0982438099999783	0.3320527369999980	0.0000000162939813	F	F	F
0.5982443090000018	0.0820524470000024	0.0000000000000000	F	F	F
0.5982443089998971	0.9179475379998507	0.0000000162939813	F	F	F
0.0982437660000031	0.4179481569999552	0.0000000000000000	F	F	F
0.0982438329999979	0.5820530649998901	0.0000000162939813	F	F	F
0.5982443089998817	0.3320527079999994	0.0000000000000000	F	F	F
0.5982443090000018	0.1679478289999992	0.0000000162939813	F	F	F
0.0982437950000019	0.6679484840000008	0.0000000000000000	F	F	F
0.0982438469999848	0.8320534229998628	0.0000000162939813	F	F	F
0.5982443689999997	0.5820530060000032	0.0000000000000000	F	F	F
0.5982443690000008	0.4179481269999958	0.0000000162939813	F	F	F
0.5982443690000001	0.8320533629998944	0.0000000000000000	F	F	F
0.5982443689998872	0.6679484249998922	0.0000000162939813	F	F	F
0.2679013632566152	0.3749662649626249	0.2967608811268488	T	T	T
0.4867495520738385	0.3849776917687735	0.3260680381465436	T	T	T
0.3567763115611441	0.3940706533092216	0.4099552242550484	T	T	T
0.1760252324415575	0.4450242460992963	0.3805242987837930	T	T	T
0.0955434273738462	0.3026619157490422	0.4274756790510360	T	T	T
0.0315306846016568	0.3059853096114481	0.3636033672126159	T	T	T
0.3494221769464615	0.2107757217423366	0.4073302720266602	T	T	T
0.1805250513042181	0.1682420491854421	0.3678091648561632	T	T	T

TS Ic(4x2) Cc(4x2), E = -385.79189 eV

1.0000000000000000		
7.6621999740000000	0.0000000000000000	0.0000000000000000
-0.0000006700000000	15.3243999479999999	0.0000000000000000
-0.0000007340000000	-0.0000007340000000	26.7875003810000010

Si H C O

48 24 4 1

Selective dynamics

Direct

0.0982437263469293	0.0000000013072636	0.0289689852776387	F	F	F
0.0982437493469135	0.2500002971734290	0.0289689852776387	F	F	F
0.5982443673469362	0.0000000013072636	0.0289689852776387	F	F	F
0.0982437713469366	0.5000005951734678	0.0289689852776387	F	F	F
0.5982443673469362	0.2500002971734290	0.0289689852776387	F	F	F
0.0982437933469313	0.7500008931734712	0.0289689852776387	F	F	F
0.5982444273469341	0.5000005951734678	0.0289689852776387	F	F	F
0.5982444273469341	0.7500008931734712	0.0289689852776387	F	F	F
0.3481418597252164	0.9990771598388067	0.0797713643150508	F	F	F
0.3481561371700014	0.2526658555804175	0.0806679081758339	F	F	F
0.8481718399543112	0.9986033428192300	0.0808210048818842	F	F	F
0.3481243654847006	0.4980532226948505	0.0807260323471091	F	F	F
0.8481950966199410	0.2521372104710693	0.0801776144980344	F	F	F
0.3481236516017174	0.7527268113426615	0.0800320023483685	F	F	F
0.8482278420540941	0.4975769028532753	0.0801022254430783	F	F	F
0.8483666970129234	0.7517520932699213	0.0807840724666355	F	F	F
0.3484854848820174	0.1248513006578068	0.1273589995508804	T	T	T
0.3475175512344828	0.3754521432427633	0.1346896389516579	T	T	T
0.8488641434257911	0.1256997962539608	0.1282200761315765	T	T	T
0.3487093791782889	0.6260799974608390	0.1276542181496004	T	T	T
0.8477643875015888	0.3748638253873370	0.1333753813350044	T	T	T

0.3481119823140469 0.8761720893736037 0.1335186481929585 T T T
0.8488221512127173 0.6239801362431975 0.1275043737744341 T T T
0.8481712792469309 0.8753618267955652 0.1352795897197944 T T T
0.1000398124084378 0.1256403011103790 0.1768781451635287 T T T
0.0954922239150591 0.3735426570346546 0.1862853283397536 T T T
0.5974965578005584 0.1254745109091962 0.1766026712873926 T T T
0.0984456217365106 0.6269353310279177 0.1768811884113358 T T T
0.5995709003995722 0.3740830162906368 0.1860276225755442 T T T
0.1011271930792924 0.8771383571796746 0.1871251403410622 T T T
0.5995047573462206 0.6266274841278875 0.1767125335177899 T T T
0.5950611138852485 0.8770484569030417 0.1870520286596723 T T T
0.1167869883073227 0.0083389336397398 0.2347150946546936 T T T
0.0907287191548605 0.2419939204191375 0.2331050506274001 T T T
0.5797054460913584 0.0083172164073312 0.2345712141821683 T T T
0.0789106201173002 0.5058940446288908 0.2319603627843092 T T T
0.6068679149278089 0.2425044833442465 0.2321873172997763 T T T
0.1155710003840058 0.7452826105430591 0.2340729365330537 T T T
0.6102861195345025 0.5062536334433353 0.2316387736498821 T T T
0.5800028976415894 0.7451621095706903 0.2339415848959369 T T T
0.3485967769547369 0.0449316983459750 0.2903375705122218 T T T
0.3513832521639930 0.2018983484589539 0.2745073116840889 T T T
0.8481351575007423 0.0640491173032243 0.2608976411608335 T T T
0.3450688834147180 0.5565737693687323 0.2640417852890845 T T T
0.8467508939246979 0.2110813148543206 0.2852634561604796 T T T
0.3475863524243909 0.7059891523578702 0.2892073058205542 T T T
0.8449736050547924 0.5425844083843482 0.2855299971758752 T T T
0.8475102387030856 0.6909781624576178 0.2609444599259593 T T T
0.0982437210000029 0.9179475529998919 0.0000000000000000 F F F
0.0982437879999836 0.0820524620000000 0.0000000162939813 F F F
0.0982437429999905 0.1679478439999969 0.0000000000000000 F F F
0.0982438099999783 0.3320527369999980 0.0000000162939813 F F F
0.5982443090000018 0.0820524470000024 0.0000000000000000 F F F
0.5982443089998971 0.9179475379998584 0.0000000162939813 F F F
0.0982437660000031 0.4179481569999484 0.0000000000000000 F F F
0.0982438329999979 0.5820530649998901 0.0000000162939813 F F F
0.5982443089998817 0.3320527079999994 0.0000000000000000 F F F
0.5982443090000018 0.1679478289999992 0.0000000162939813 F F F
0.0982437950000019 0.6679484840000008 0.0000000000000000 F F F
0.0982438469999848 0.8320534229998700 0.0000000162939813 F F F
0.5982443689999997 0.5820530060000032 0.0000000000000000 F F F
0.5982443690000008 0.4179481269999958 0.0000000162939813 F F F
0.5982443690000001 0.8320533629999005 0.0000000000000000 F F F
0.5982443689998872 0.6679484249998853 0.0000000162939813 F F F
0.3239072182518755 0.3777959742474747 0.2761407080432083 T T T
0.4599310096686082 0.4109022196366319 0.3303274554472581 T T T
0.1533724766785704 0.4647457889284322 0.3617241283236885 T T T
0.0574916239393680 0.3789350397908353 0.3268207554163894 T T T
0.3110921859175565 0.3584708988065221 0.4157540792107998 T T T
0.0838883220179646 0.3335719161472189 0.4161351980426272 T T T
0.3015346587240357 0.2019272883414939 0.3979334677753840 T T T
0.1217152267791181 0.2164018884680022 0.3554874921291746 T T T
0.3317964832161536 0.3928480247853138 0.3157566610338652 T T T
0.1749547713860155 0.3977085707102663 0.3479124053018074 T T T
0.2014028997356920 0.3356810933832228 0.3925885831054483 T T T
0.2415828072381765 0.2464835598384673 0.3706099666253718 T T T
0.3662196361019403 0.2606570119012563 0.3309314893346763 T T T

TS Ic(2x2) Cc(2x2), E(PBE-D3/PAW) = -386.02722 eV, E(HSE06-D3/PAW) = -447.11262 eV, E(PBE-D3/TZ2P) = -373.5400 eV

1.0000000000000000

7.6621999740000000 0.0000000000000000 0.0000000000000000
-0.0000006700000000 15.3243999479999999 0.0000000000000000
-0.0000007340000000 -0.0000007340000000 26.7875003810000010

Si H C O

48 24 4 1

Selective dynamics

Direct

0.0982437263469365 0.0000000013072636 0.0289689852776365 F F F
0.0982437493469206 0.2500002971734290 0.0289689852776365 F F F
0.5982443673469362 0.0000000013072636 0.0289689852776365 F F F
0.0982437713469366 0.5000005951734678 0.0289689852776365 F F F
0.5982443673469362 0.2500002971734290 0.0289689852776365 F F F
0.0982437933469384 0.7500008931734712 0.0289689852776365 F F F
0.5982444273469341 0.5000005951734678 0.0289689852776365 F F F
0.5982444273469341 0.7500008931734712 0.0289689852776365 F F F
0.3481418597251913 0.9990771598388200 0.0797713643150438 F F F
0.3481561371700014 0.2526658555804175 0.0806679081758268 F F F
0.8481718399543261 0.9986033428192375 0.0808210048818772 F F F
0.3481243654847078 0.4980532226948505 0.0807260323471020 F F F
0.8481950966199463 0.2521372104710693 0.0801776144980273 F F F
0.3481236516016917 0.7527268113426694 0.0800320023483614 F F F
0.8482278420541078 0.4975769028532895 0.0801022254430712 F F F
0.8483666970128763 0.7517520932699289 0.0807840724666285 F F F
0.3482949604752222 0.1248927287223099 0.1274667986914153 T T T
0.3478421064934121 0.3748822067597946 0.1343897639746308 T T T
0.8485788461985851 0.1257555552611038 0.1281895763333375 T T T
0.3480875807572971 0.6252232819444214 0.1271257478441344 T T T
0.8482186011528030 0.3751224157183813 0.1339148001270526 T T T
0.3481677563786230 0.8755484374487409 0.1340379622574052 T T T
0.8478101044110071 0.6251921197287114 0.1277751637651588 T T T
0.8482855338023788 0.8759903487539145 0.1345621074641550 T T T
0.0995211264886722 0.1259388487286894 0.1769196129314265 T T T
0.0975287921983223 0.3727150046089709 0.1865046957820913 T T T
0.5974453054882997 0.1258096204120827 0.1767310044889549 T T T
0.0991948478781286 0.6261802770727921 0.1767108611764420 T T T
0.5984973391400180 0.3730625809782686 0.1862482578199246 T T T
0.0987844384713590 0.8777618310625362 0.1869477077080621 T T T
0.5966134457924748 0.6259169812608458 0.1769088057378255 T T T
0.5976975701134370 0.8776409351045381 0.1868860613277870 T T T
0.1157285197186851 0.0087037202965974 0.2347170352509092 T T T
0.0902593093125285 0.2415740091995743 0.2337607060623530 T T T
0.5812244469582760 0.0086384591159435 0.2345514487406306 T T T
0.1104270316828905 0.5054774089318953 0.2320762009327168 T T T
0.6058128130062950 0.2419749822184043 0.2331087999769815 T T T
0.0834519292539257 0.7454756758556588 0.2335806766117729 T T T
0.5858453043173144 0.5050288997162375 0.2323281478835412 T T T
0.6130818801329484 0.7454787139767709 0.2336504919195207 T T T
0.3488669012147040 0.0412458665606999 0.2906633095921024 T T T
0.3499855863770532 0.1973475574983481 0.2745250198120519 T T T
0.8482946820286330 0.065552520922767 0.2614723121144573 T T T
0.3481917471513931 0.5394105064498513 0.2858189796583534 T T T
0.8463460992295107 0.2126843561435676 0.2867449591797893 T T T
0.3482496176159705 0.6900812846123787 0.2624956802833284 T T T
0.8481906572004427 0.5637574741218090 0.2613667872748485 T T T

0.8483419880722072	0.7104310301875859	0.2887512257395324	T	T	T
0.0982437210000029	0.9179475529998982	0.0000000000000000	F	F	F
0.0982437879999978	0.0820524620000000	0.0000000162939813	F	F	F
0.0982437429999976	0.1679478439999969	0.0000000000000000	F	F	F
0.0982438099999783	0.3320527369999980	0.0000000162939813	F	F	F
0.5982443090000018	0.0820524470000024	0.0000000000000000	F	F	F
0.5982443089999023	0.9179475379998721	0.0000000162939813	F	F	F
0.0982437660000031	0.4179481569999552	0.0000000000000000	F	F	F
0.0982438329999979	0.5820530649998972	0.0000000162939813	F	F	F
0.5982443089998881	0.3320527079999994	0.0000000000000000	F	F	F
0.5982443090000018	0.1679478289999992	0.0000000162939813	F	F	F
0.0982437950000019	0.6679484840000008	0.0000000000000000	F	F	F
0.0982438469999920	0.8320534229998842	0.0000000162939813	F	F	F
0.5982443689999997	0.5820530060000032	0.0000000000000000	F	F	F
0.5982443690000008	0.4179481269999958	0.0000000162939813	F	F	F
0.5982443690000001	0.8320533629999076	0.0000000000000000	F	F	F
0.5982443689999003	0.6679484249998993	0.0000000162939813	F	F	F
0.3107897100369931	0.3735290235989649	0.2895422632591877	T	T	T
0.4730968352714733	0.3884383428091977	0.3402299706141372	T	T	T
0.1999540926952056	0.4452155828154371	0.3867078177066630	T	T	T
0.0671954753282709	0.3772006693927176	0.3484068832794896	T	T	T
0.3341378129137962	0.3187776960666019	0.4279438990468767	T	T	T
0.1043462638489763	0.3013040238110956	0.4294769303242586	T	T	T
0.3024803236143063	0.1709183992291276	0.3939171729845139	T	T	T
0.1169129087969787	0.2038023573957221	0.3572729723887778	T	T	T
0.3382412242103549	0.3760806625785220	0.3294397142856293	T	T	T
0.1946987048018738	0.3823516938706580	0.3671337268527040	T	T	T
0.2180415325253447	0.3070420084848897	0.4046477416215530	T	T	T
0.2421993736687277	0.2254046364826140	0.3734823143748353	T	T	T
0.3608271666349216	0.2507625015116235	0.3337382465376390	T	T	T

8.10. Diethylether on Si(001)

Diethylether Molecule, E = -79.96444 eV

```

1.0000000000000000
7.6622000000000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 15.3244000000000007 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.6488380432000014

```

H C O

10 4 1

Direct

0.8222022544735654	0.5777961969033253	0.30991549451084800
0.5891808913264749	0.5776832830661368	0.31007441941222200
0.8226539441017805	0.4219995600378881	0.30993452080965600
0.5896331689566753	0.4218704889247204	0.31005384829227500
0.7056760880483587	0.7162073503345302	0.34243541023168700
0.7066504301515831	0.2834505809524003	0.34244320741657800
0.5900534416881500	0.6551827858337638	0.38269474513663900
0.8226752790933977	0.6553516067725673	0.38250840496602000
0.8232140185953299	0.3444522599823865	0.38253750565303900
0.5906033403907170	0.3443608775002706	0.38266891500753700
0.7059254265399650	0.5770978020524972	0.33152808698816400
0.7063144972552310	0.4225692230451781	0.33152580457257400
0.7060960285688459	0.6555339625102676	0.36159902172791700
0.7067225247595355	0.3441338899561276	0.36159853892680000

0.7063527966373763 0.4998356379790978 0.35735127259942500

Diethylether Slab, E = -313.62042 eV

1.0000000000000000

7.6622095108000003 0.0000000000000000 0.0000000000000000
0.0000000000000000 15.3244190216000007 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.6488380432000014

Si H

48 16

Selective dynamics

Direct

0.0000000000000000 0.0000000000000000 0.0309956599290166 F F F
0.0000000000000000 0.2500000159614544 0.0309956599290166 F F F
0.5000000319229088 0.0000000000000000 0.0309956599290166 F F F
0.0000000000000000 0.5000000319229088 0.0309956599290166 F F F
0.5000000319229088 0.2500000159614544 0.0309956599290166 F F F
0.0000000000000000 0.7500000478843631 0.0309956599290166 F F F
0.5000000319229088 0.5000000319229088 0.0309956599290166 F F F
0.5000000319229088 0.7500000478843631 0.0309956599290166 F F F
0.2499999507061261 0.0000000000000000 0.0751898294690930 F F F
0.2499999507061261 0.2500000159614544 0.0751898294690930 F F F
0.7499999826290349 0.0000000000000000 0.0751898294690930 F F F
0.2499999507061261 0.5000000319229088 0.0751898294690930 F F F
0.7499999826290349 0.2500000159614544 0.0751898294690930 F F F
0.2499999507061261 0.7500000478843631 0.0751898294690930 F F F
0.7499999826290349 0.5000000319229088 0.0751898294690930 F F F
0.7499999826290349 0.7500000478843631 0.0751898294690930 F F F
0.2499999507061261 0.1244328412915507 0.1173549825298820 T T T
0.2499999507061261 0.3749999913145174 0.1221879551124780 T T T
0.7499999826290349 0.1255671746699036 0.1173550477852070 T T T
0.2499999507061261 0.6255670760821488 0.1173550151575470 T T T
0.7499999826290349 0.3749999913145174 0.1213351658845190 T T T
0.2499999507061261 0.8750000232374191 0.1213350680015290 T T T
0.7499999826290349 0.6244328079591313 0.1173550477852070 T T T
0.7499999826290349 0.8750000232374191 0.1221879551124780 T T T
0.0000000000000000 0.1250003016297043 0.1602985337469810 T T T
0.9982723637638244 0.3749999913145174 0.1678266491767670 T T T
0.4999999014122523 0.1250003016297043 0.1602985337469810 T T T
0.0000000000000000 0.6249996809993235 0.1602985337469810 T T T
0.5017276014942382 0.3749999913145174 0.1678266491767670 T T T
0.0017279611032990 0.8750000232374191 0.1678264860384520 T T T
0.4999999014122523 0.6249996809993235 0.1602985337469810 T T T
0.4982720708196098 0.8750000232374191 0.1678264860384520 T T T
0.0162464886694309 0.0056880459792410 0.2096157031661020 T T T
0.9837540972190126 0.2443120352375416 0.2096159641874070 T T T
0.4837535432534779 0.0056880459792410 0.2096157031661020 T T T
0.9837542277296691 0.5056879473914861 0.2096159641874070 T T T
0.5162457375283935 0.2443121004928699 0.2096159641874070 T T T
0.0162463581587744 0.7443120019051221 0.2096157031661020 T T T
0.5162458680390500 0.5056878821361579 0.2096159968150720 T T T
0.4837535432534779 0.7443120019051221 0.2096157357937670 T T T
0.2499999507061261 0.0405486824083923 0.2581541807799470 T T T
0.2499999507061261 0.1876281244951130 0.2340310812756260 T T T
0.7499999826290349 0.0623711084024023 0.2340307549989960 T T T
0.2499999507061261 0.5623719233892501 0.2340310812756260 T T T
0.7499999826290349 0.2094503547231312 0.2581540828969620 T T T

0.2499999507061261	0.7094513002206355	0.2581541807799470	T	T	T
0.7499999826290349	0.5405496279059037	0.2581541155246220	T	T	T
0.7499999826290349	0.6876288742266325	0.2340307549989960	T	T	T
0.0000000000000000	0.1711557218778097	0.0031193677215796	F	F	F
0.0000000000000000	0.3288443100450991	0.0031193677215796	F	F	F
0.0000000000000000	0.4211557378392641	0.0031193677215796	F	F	F
0.0000000000000000	0.0788442940836447	0.0031193677215796	F	F	F
0.5000000319229088	0.0788442940836447	0.0031193677215796	F	F	F
0.5000000319229088	0.1711557218778097	0.0031193677215796	F	F	F
0.5000000319229088	0.3288443100450991	0.0031193677215796	F	F	F
0.5000000319229088	0.4211557378392641	0.0031193677215796	F	F	F
0.0000000000000000	0.6711557538007185	0.0031193677215796	F	F	F
0.0000000000000000	0.8288443419680007	0.0031193677215796	F	F	F
0.0000000000000000	0.9211557697621728	0.0031193677215796	F	F	F
0.0000000000000000	0.5788443260065463	0.0031193677215796	F	F	F
0.5000000319229088	0.5788443260065463	0.0031193677215796	F	F	F
0.5000000319229088	0.6711557538007185	0.0031193677215796	F	F	F
0.5000000319229088	0.8288443419680007	0.0031193677215796	F	F	F
0.5000000319229088	0.9211557697621728	0.0031193677215796	F	F	F

Diethylether Intermediate, E = -394.78825 eV

1.0000000000000000					
7.6622095108000003	0.0000000000000000	0.0000000000000000			
0.0000000000000000	15.3244190216000007	0.0000000000000000			
0.0000000000000000	0.0000000000000000	30.6488380432000014			

Si H C O

48 26 4 1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0309956611947584	F	F	F
0.0000000000000000	0.2500000159614544	0.0309956611947584	F	F	F
0.5000000319229088	0.0000000000000000	0.0309956611947584	F	F	F
0.0000000000000000	0.5000000319229088	0.0309956611947584	F	F	F
0.5000000319229088	0.2500000159614544	0.0309956611947584	F	F	F
0.0000000000000000	0.7500000478843631	0.0309956611947584	F	F	F
0.5000000319229088	0.5000000319229088	0.0309956611947584	F	F	F
0.5000000319229088	0.7500000478843631	0.0309956611947584	F	F	F
0.2499999507061261	0.0000000000000000	0.0751898325395501	F	F	F
0.2499999507061261	0.2500000159614544	0.0751898325395501	F	F	F
0.7499999826290349	0.0000000000000000	0.0751898325395501	F	F	F
0.2499999507061261	0.5000000319229088	0.0751898325395501	F	F	F
0.7499999826290349	0.2500000159614544	0.0751898325395501	F	F	F
0.2499999507061261	0.7500000478843631	0.0751898325395501	F	F	F
0.7499999826290349	0.5000000319229088	0.0751898325395501	F	F	F
0.7499999826290349	0.7500000478843631	0.0751898325395501	F	F	F
0.2499319490763979	0.1245008266732819	0.1173117331527426	T	T	T
0.2500783495378188	0.3751236897127729	0.1221375782999375	T	T	T
0.7496168923086479	0.1251339794254619	0.1174444595848523	T	T	T
0.2499112381758728	0.6256349092440407	0.1173447250878331	T	T	T
0.7501741721328629	0.3749578374579289	0.1213048972015733	T	T	T
0.2499962648937438	0.8751074130119377	0.1213899288797649	T	T	T
0.7500063701620872	0.6244052791212943	0.1172303265694545	T	T	T
0.7499563869041141	0.8751527204266519	0.1222205088564457	T	T	T
-0.0001965412062727	0.1254001376260701	0.1599249311759151	T	T	T
0.9984266280921574	0.3741037872215847	0.1677623652022032	T	T	T
0.4997137343723312	0.1254880743818553	0.1601220755163801	T	T	T

-0.0003382529839455 0.6253685356763682 0.1602543468404779 T T T
0.5018468673305758 0.3741352250611305 0.1677601158685161 T T T
0.0016259782211267 0.8763434288188960 0.1678971759342811 T T T
0.5002623174297427 0.6254137017578846 0.1602193853804496 T T T
0.4983015339531476 0.8764154760925854 0.1679363043653514 T T T
0.0168207136449637 0.0072398788507873 0.2096872723361939 T T T
0.9878915202511904 0.2424370470722279 0.2087229637010248 T T T
0.4823469703508639 0.0071965684180677 0.2098811390528321 T T T
0.9840474068736631 0.5053403955048689 0.2092513505712294 T T T
0.5117962224136157 0.2426443978470065 0.2089776014862966 T T T
0.0158875051706272 0.7451241221365905 0.2094846729038079 T T T
0.5169074245847477 0.5054441297166674 0.2092503797790923 T T T
0.4845920458265199 0.7451042389289058 0.2094573570698643 T T T
0.2492547303342341 0.0404852690310052 0.2587865915165204 T T T
0.2496952810384203 0.1943895696177111 0.2413273345542440 T T T
0.7496807070441095 0.0636221126099839 0.2336863552466614 T T T
0.2503677885499698 0.5629300915841075 0.2334049873830464 T T T
0.7500270074443456 0.2109050098042473 0.2568247488337453 T T T
0.2503263015007573 0.7095321180157091 0.2577607525979994 T T T
0.7504766844374688 0.5403500520085576 0.2579804437108411 T T T
0.7502937420982358 0.6880377508755843 0.2340676446723852 T T T
0.0000000000000000 0.1711557218778097 0.0031193678489601 F F F
0.0000000000000000 0.3288443100450991 0.0031193678489601 F F F
0.0000000000000000 0.4211557378392641 0.0031193678489601 F F F
0.0000000000000000 0.0788442940836447 0.0031193678489601 F F F
0.5000000319229088 0.0788442940836447 0.0031193678489601 F F F
0.5000000319229088 0.1711557218778097 0.0031193678489601 F F F
0.5000000319229088 0.3288443100450991 0.0031193678489601 F F F
0.5000000319229088 0.4211557378392641 0.0031193678489601 F F F
0.0000000000000000 0.6711557538007185 0.0031193678489601 F F F
0.0000000000000000 0.8288443419680007 0.0031193678489601 F F F
0.0000000000000000 0.9211557697621728 0.0031193678489601 F F F
0.0000000000000000 0.5788443260065463 0.0031193678489601 F F F
0.5000000319229088 0.5788443260065463 0.0031193678489601 F F F
0.5000000319229088 0.6711557538007185 0.0031193678489601 F F F
0.5000000319229088 0.8288443419680007 0.0031193678489601 F F F
0.5000000319229088 0.9211557697621728 0.0031193678489601 F F F
0.1142717622660066 0.3688461011568722 0.3027485127412267 T T T
0.2755082947141330 0.3645601554375502 0.2608469696630317 T T T
0.0845246559419232 0.1627868452857246 0.3244496906869127 T T T
0.1100374625174192 0.2626756861232731 0.3537332812164000 T T T
0.3564447465941625 0.3749870552679166 0.3596291079614257 T T T
0.2663877947847075 0.1387255611042703 0.3916825544609457 T T T
0.5149222282921513 0.3626851198955062 0.3169483738821555 T T T
0.3858499107952666 0.4588924424811661 0.3202381885508557 T T T
0.3888905695369992 0.1182710037817198 0.3434212380207098 T T T
0.4213359106650653 0.2175306756830456 0.3730705652057801 T T T
0.2488008595272370 0.3484884813580436 0.2951920409978013 T T T
0.1800947501291575 0.2109804057859291 0.3361124392386118 T T T
0.3843411893284892 0.3876669447420897 0.3250280505366300 T T T
0.3237883287536306 0.1694499428128448 0.3625665336612267 T T T
0.2525672184464105 0.2523076327008668 0.2964318891239413 T T T

Diethylether TS(2x2), E = -394.15404 eV

1.0000000000000000

7.6622095108000003 0.0000000000000000 0.0000000000000000

```

0.0000000000000000 15.3244190216000007 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.6488380432000014
Si H C O
48 26 4 1
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0309956611947584 F F F
0.0000000000000000 0.2500000159614544 0.0309956611947584 F F F
0.5000000319229088 0.0000000000000000 0.0309956611947584 F F F
0.0000000000000000 0.5000000319229088 0.0309956611947584 F F F
0.5000000319229088 0.2500000159614544 0.0309956611947584 F F F
0.0000000000000000 0.7500000478843631 0.0309956611947584 F F F
0.5000000319229088 0.5000000319229088 0.0309956611947584 F F F
0.5000000319229088 0.7500000478843631 0.0309956611947584 F F F
0.2499999507061261 0.0000000000000000 0.0751898325395501 F F F
0.2499999507061261 0.2500000159614544 0.0751898325395501 F F F
0.749999826290349 0.0000000000000000 0.0751898325395501 F F F
0.2499999507061261 0.5000000319229088 0.0751898325395501 F F F
0.749999826290349 0.2500000159614544 0.0751898325395501 F F F
0.2499999507061261 0.7500000478843631 0.0751898325395501 F F F
0.749999826290349 0.5000000319229088 0.0751898325395501 F F F
0.749999826290349 0.7500000478843631 0.0751898325395501 F F F
0.2499613173423646 0.1244436287328135 0.1173453529461466 T T T
0.2497266244349799 0.3744969199242720 0.1215456851288318 T T T
0.7503145885007144 0.1251675367555695 0.1176945265077410 T T T
0.2500051109483797 0.6245718677885986 0.1172056631608647 T T T
0.7501607574327116 0.3752168355538866 0.1213765578519475 T T T
0.2498982302041316 0.8745684138377028 0.1218359759206437 T T T
0.7507795639671505 0.6257220945132553 0.1175497606883575 T T T
0.7498818366762582 0.8758233677581481 0.1218264865950937 T T T
0.0008145485162896 0.1259867934981335 0.1602802653198056 T T T
0.9994277662795089 0.3726521985486457 0.1673871523900133 T T T
0.4994864896329185 0.1257018152089620 0.1601370898698392 T T T
0.0014501072024253 0.6256735179784155 0.1605089442407330 T T T
0.5003892434425654 0.3730152862473854 0.1672056453425917 T T T
0.9999408732887988 0.8768909428417555 0.1679438756581564 T T T
0.4995097330113378 0.6266749365011092 0.1601140087067558 T T T
0.4997836363934619 0.8771091912551808 0.1679603940793024 T T T
0.0161379372433826 0.0074746227122896 0.2099759325669788 T T T
0.9925547411686433 0.2424490484157918 0.2093344226402985 T T T
0.4833941935489499 0.0075803657167775 0.2100657134332988 T T T
0.0102884201727908 0.5039874205335039 0.2082893936636595 T T T
0.5090814636701362 0.2424255424287825 0.2089537087959376 T T T
0.9843150728743647 0.7457091834768489 0.2096319364663006 T T T
0.4867600392644835 0.5051166611056250 0.2076778751537774 T T T
0.5149812492329642 0.7458624375291387 0.2095431144988541 T T T
0.2497104561142915 0.0421584290391546 0.2580920972981742 T T T
0.2514894964258723 0.1990977326558093 0.2451604767559364 T T T
0.7498991166203502 0.0648218300835953 0.2337350878920979 T T T
0.2489598965555500 0.5397361600279423 0.2544204433003654 T T T
0.7501171538930353 0.2120939172899226 0.2558228484930300 T T T
0.2495483843993116 0.6905790214471542 0.2344276823121213 T T T
0.7483932633645387 0.5629265260494405 0.2337572622263988 T T T
0.7493715680949242 0.7099720443440759 0.2578851425201223 T T T
0.0000000000000000 0.1711557218778097 0.0031193678489601 F F F
0.0000000000000000 0.3288443100450991 0.0031193678489601 F F F
0.0000000000000000 0.4211557378392641 0.0031193678489601 F F F

```

0.0000000000000000	0.0788442940836447	0.0031193678489601	F	F	F
0.5000000319229088	0.0788442940836447	0.0031193678489601	F	F	F
0.5000000319229088	0.1711557218778097	0.0031193678489601	F	F	F
0.5000000319229088	0.3288443100450991	0.0031193678489601	F	F	F
0.5000000319229088	0.4211557378392641	0.0031193678489601	F	F	F
0.0000000000000000	0.6711557538007185	0.0031193678489601	F	F	F
0.0000000000000000	0.8288443419680007	0.0031193678489601	F	F	F
0.0000000000000000	0.9211557697621728	0.0031193678489601	F	F	F
0.0000000000000000	0.5788443260065463	0.0031193678489601	F	F	F
0.5000000319229088	0.5788443260065463	0.0031193678489601	F	F	F
0.5000000319229088	0.6711557538007185	0.0031193678489601	F	F	F
0.5000000319229088	0.8288443419680007	0.0031193678489601	F	F	F
0.5000000319229088	0.9211557697621728	0.0031193678489601	F	F	F
0.1716328466581336	0.3905675685698365	0.3089567030929068	T	T	T
0.2945517264678246	0.3731160913549339	0.2577439695130295	T	T	T
0.0649925614149994	0.1734098788087850	0.3222257372712287	T	T	T
0.0958486540426173	0.2754996779173504	0.3484020928368494	T	T	T
0.4486756685696471	0.3955871196218075	0.3516330450925590	T	T	T
0.2123236434815349	0.1538226828981770	0.3951325330832583	T	T	T
0.5491969163962230	0.3297741718546205	0.3100202780706641	T	T	T
0.5371537446486497	0.4437588102558907	0.3033667457511309	T	T	T
0.3508795484413543	0.1195483706275235	0.3516255068115254	T	T	T
0.3877978854990864	0.2221417337221189	0.3777632704238267	T	T	T
0.2958598960427664	0.3761107247489899	0.2933111897437868	T	T	T
0.1650136971222955	0.2192516244995347	0.3341812588400777	T	T	T
0.4653800763562058	0.3870929112988003	0.3163369062325056	T	T	T
0.2868458279735105	0.1763789349521202	0.3665759030197875	T	T	T
0.2625173181115924	0.2514276435732677	0.2967117672764441	T	T	T

Diethylether C(2x2), E = -396.42490 eV

1.0000000000000000		
7.6622095108000003	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.3244190216000007	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.6488380432000014

Si H C O

48 26 4 1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0309956611947584	F	F	F
0.0000000000000000	0.2500000159614544	0.0309956611947584	F	F	F
0.5000000319229088	0.0000000000000000	0.0309956611947584	F	F	F
0.0000000000000000	0.5000000319229088	0.0309956611947584	F	F	F
0.5000000319229088	0.2500000159614544	0.0309956611947584	F	F	F
0.0000000000000000	0.7500000478843631	0.0309956611947584	F	F	F
0.5000000319229088	0.5000000319229088	0.0309956611947584	F	F	F
0.5000000319229088	0.7500000478843631	0.0309956611947584	F	F	F
0.2499999507061261	0.0000000000000000	0.0751898325395501	F	F	F
0.2499999507061261	0.2500000159614544	0.0751898325395501	F	F	F
0.7499999826290349	0.0000000000000000	0.0751898325395501	F	F	F
0.2499999507061261	0.5000000319229088	0.0751898325395501	F	F	F
0.7499999826290349	0.2500000159614544	0.0751898325395501	F	F	F
0.2499999507061261	0.7500000478843631	0.0751898325395501	F	F	F
0.7499999826290349	0.5000000319229088	0.0751898325395501	F	F	F
0.7499999826290349	0.7500000478843631	0.0751898325395501	F	F	F
0.2500358550679678	0.1243831383924138	0.1176488617655056	T	T	T
0.2497085281539191	0.3745849166823122	0.1215309620143358	T	T	T

0.7500890681010288 0.1252622917174458 0.1179747881838586 T T T
0.2498507057680851 0.6247043186903029 0.1172727359728713 T T T
0.7502423731367264 0.3751306912433596 0.1207512095474811 T T T
0.2500018027996389 0.8747448093426490 0.1215673172808192 T T T
0.7500774779310611 0.6253758911279175 0.1183693473601433 T T T
0.7499914954169244 0.8759042507565311 0.1212690952931600 T T T
0.0010491604058344 0.1272162144899751 0.1606978911727417 T T T
0.9978365188187696 0.3712227686509368 0.1668654890307346 T T T
0.4990852707156156 0.1272287195697318 0.1606731725254256 T T T
0.0029801541655225 0.6258431527617868 0.1608795820210539 T T T
0.5020811892834536 0.3717073646524928 0.1665702941848169 T T T
-0.0007393992303453 0.8769710912343769 0.1671840981384031 T T T
0.4968733012457531 0.6262017009074374 0.160743772884114 T T T
0.5007422414134428 0.8771913679010882 0.1671864185370684 T T T
0.0099803193539671 0.0066003337245326 0.2094724069770503 T T T
0.9902315089621099 0.2431664212162244 0.2099074903093681 T T T
0.4886739765721054 0.0067292021368402 0.2095594209403751 T T T
1.0046500876330915 0.5021602620223994 0.2076000197342096 T T T
0.5099408200321222 0.2437865273388177 0.2095039896391562 T T T
-0.0145609535429520 0.7468623164468569 0.2089352121619147 T T T
0.4949316400688980 0.5025050610955302 0.2072865021906282 T T T
0.5152146133552694 0.7471026085099822 0.2088968762188753 T T T
0.2491114688561634 0.0509057787298066 0.2517358891177675 T T T
0.2516142335193846 0.2102504206395765 0.2472677455471565 T T T
0.7494077394049274 0.0673420456466448 0.2345850009291606 T T T
0.2500180844514868 0.5446898299433699 0.2481378508119458 T T T
0.7489292612896337 0.2146864912626578 0.2570703090473366 T T T
0.2504935200613098 0.6980332970977284 0.2344926434545608 T T T
0.7496770986721005 0.5659345706008567 0.2330605481698406 T T T
0.7501780336941571 0.7119201909566736 0.2571266301012609 T T T
0.0000000000000000 0.1711557218778097 0.0031193678489601 F F F
0.0000000000000000 0.3288443100450991 0.0031193678489601 F F F
0.0000000000000000 0.4211557378392641 0.0031193678489601 F F F
0.0000000000000000 0.0788442940836447 0.0031193678489601 F F F
0.5000000319229088 0.0788442940836447 0.0031193678489601 F F F
0.5000000319229088 0.1711557218778097 0.0031193678489601 F F F
0.5000000319229088 0.3288443100450991 0.0031193678489601 F F F
0.5000000319229088 0.4211557378392641 0.0031193678489601 F F F
0.0000000000000000 0.6711557538007185 0.0031193678489601 F F F
0.0000000000000000 0.8288443419680007 0.0031193678489601 F F F
0.0000000000000000 0.9211557697621728 0.0031193678489601 F F F
0.0000000000000000 0.5788443260065463 0.0031193678489601 F F F
0.5000000319229088 0.5788443260065463 0.0031193678489601 F F F
0.5000000319229088 0.6711557538007185 0.0031193678489601 F F F
0.5000000319229088 0.8288443419680007 0.0031193678489601 F F F
0.5000000319229088 0.9211557697621728 0.0031193678489601 F F F
0.1354468170678370 0.5320275004147046 0.3228938953438351 T T T
0.2401829103489711 0.4345547550618996 0.3057596157798968 T T T
0.0467481408471859 0.1957780396693465 0.3230676463103478 T T T
0.1173861508643260 0.2928781034791066 0.3492549328932180 T T T
0.4138329704032631 0.5087496019800770 0.3659260032816666 T T T
0.1986417332637920 0.1624853325960046 0.3941333234103391 T T T
0.5359950700590356 0.5043677526515885 0.3168083631038343 T T T
0.4360980483713000 0.6036467303920859 0.3328808186291847 T T T
0.3160279738065278 0.1176612735332078 0.3491080434218481 T T T
0.3911808958611325 0.2154581863189579 0.3744765574542608 T T T
0.2538154564609204 0.5062371341324429 0.3070250583317045 T T T

0.1638005689263590 0.2324346475710488 0.3335263662996001 T T T
0.4184392435696446 0.5323681097887289 0.3320239830379414 T T T
0.2740947854845099 0.1788911195950819 0.3646806435386825 T T T
0.2649288208562944 0.2584929611024531 0.2961372349662152 T T T