

Electronic Supplemental Information

Initial stages of CO₂ adsorption on CaO: A combined experimental and computational study

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S1. Computational Details

S1.1. Cluster models

The CaO(001) surface was modeled with twelve neutral cluster models using the periodic electrostatic embedded cluster method (PEECM): T1, T2, T3, T4, and T5 represent terrace models; MS1 and MS2 represent monatomic step models; DS represents a diatomic step model; E represents an edge model; RC represents a reverse corner model; and C1 and C2 represent corner models. These cluster models are depicted in Figure S1. To appropriately model the morphologies of the monatomic step, diatomic step, and edge clusters within the PEECM formalism, a rectangular array of point charges was removed from the embedding, amounting to 966.4 pm in the $-x$ direction and 507.36 pm in both the $+y$ and $-y$ directions, one, two, and six layers deep, respectively. For the corner models, all six layers of point charges were removed from the periodic array, starting with the edge cluster model and removing additional point charges in the $+x$ direction 990.56 pm and 483.2 pm in the $-y$ direction. For the reverse corner model, a single layer of point charges was removed from the embedding 966.4 pm in the $-x$ direction and 483.2 pm in the $-y$ direction.

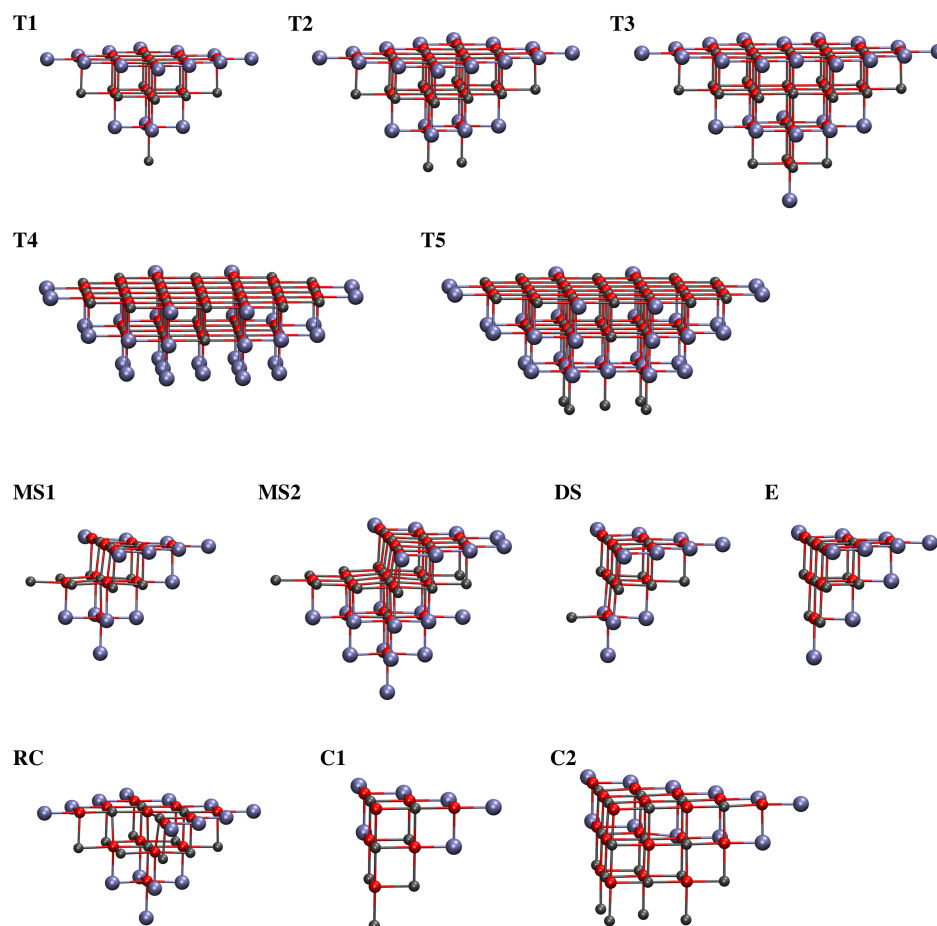


Figure S1. Cluster models (angled view) for different morphological sites of CaO(001) optimized with B3LYP: terrace models T1, T2, T3, T4, and T5; step-edge models MS1, MS2, DS, and E; corner models RC, C1, and C2. Color code: red, O; gray, Ca; purple, Ca effective core potential.

To test the effect of the number of point charge layers in the PEECM formalism on the calculated adsorption energies, we performed additional calculations with 10 atomic point charge layers. The change in CO₂ adsorption energy was very low upon inclusion of 10 atomic point charge layers instead of 6, as shown in Table S1. Therefore, we used 6 layers of point charges for the duration of the study.

Table S1. Calculated CO₂ adsorption energies, ΔE_{el} (kJ/mol), defined by the reaction $\text{CO}_2 + \text{CaO} \rightarrow \text{CO}_2 \bullet \text{CaO}$, with 10 layers of point charges in PEECM^a

Cluster	B3LYP	PBE
T1-1CO ₂	−151.0 (−0.9)	−154.1 (−0.9)
T1-2CO ₂	−154.4 (+0.0)	
MS1-1CO ₂	−287.1 (+0.0)	−279.1 (+0.1)

^a In parentheses are the differences in adsorption energies compared with calculations including only 6 layers of point charges.

S1.2. Frequency scaling factors

We calculate frequencies of cluster-model adsorption structures in the harmonic approximation using finite differences, where all atoms that are allowed to relax during structure optimization are included in the construction of the partial hessian. We scale the resulting frequencies using a factor determined by averaging the ratios of the experimentally-observed anharmonic frequencies and the calculated harmonic frequencies for gas-phase CO₂ and CO₂[−], given in Table S2.

Table S2. Experimental and Calculated Vibrational Frequencies (cm^{−1}) and Calculated Harmonic Vibrational Scaling Factors (λ)

Experimental CO ₂	B3LYP	B3LYP λ	Scaled B3LYP ^a	ΔB3LYP^b	PBE	PBE λ
667	677.0	0.9852	663.5	−3.5	645.2	1.0338
1333	1371.6	0.9719	1344.2	11.2	1322.6	1.0079
2349	2409.3	0.9750	2361.1	12.1	2361.4	0.9947
Experimental CO ₂ ^{−c}	B3LYP	B3LYP λ	Scaled B3LYP ^a	ΔB3LYP^b	PBE	PBE λ
714	728.7	0.9798	714.1	0.1	701.1	1.0184
1254	1298.1	0.9660	1272.1	18.1	1252.8	1.0010
1658	1707.3	0.9711	1673.2	15.2	1677.5	0.9884
		B3LYP			PBE	
Average λ		0.9748			1.0074	
Global 6-311+G(2df,p) ^d		0.9686			0.9948	

^a Calculated B3LYP frequencies with $\lambda=0.9800$ applied.

^b Error in calculated scaled B3LYP frequencies.

^c Ref 1.

^d Ref 2.

The calculated harmonic frequencies with B3LYP are consistently overestimated, leading to scaling factors λ less than one. When an average $\lambda=0.9800$ is applied, the resulting scaled frequencies still have errors as high as 18 cm^{-1} . The average scaling factor λ for calculated PBE harmonic frequencies is nearly unity, and therefore calculated PBE frequencies are not scaled. We stress that scaled B3LYP and unscaled PBE frequencies can only be discussed qualitatively.

S1.3. Comparison of the PEECM results of MgO(001)

We compare the calculated adsorption energy and frequencies of CO₂ on MgO with previous calculations performed by Catlow and coworkers using an advanced embedding scheme.³ We find that despite the relatively small cluster T1-MgO (lattice constant $a=420.8$ pm), the adsorption energy of CO₂ calculated with PEECM matches closely with the much larger cluster employed by Catlow and coworkers, as shown in Table S3. We also performed calculations on cluster model MS1-MgO. The calculated frequencies for CO₂•MgO are given in Table S4. The agreement with the larger embedded cluster calculations implies confidence in our model to capture the physical nature of CO₂ adsorption as surface carbonate species.

Table S3. Calculated CO₂ adsorption energies, ΔE_{el} (kJ/mol), defined by the reaction $\text{CO}_2 + \text{MgO} \rightarrow \text{CO}_2\bullet\text{MgO}$

Cluster	B3LYP	B3LYP+D ^a
T1-MgO	-51.8	-73.0
MS1-MgO	-232.7	-249.8
Terrace-QM/MM ^b	-65.6	

^a DFT+D single point calculation at the DFT structure.

^b Ref 3.

Table S4. Calculated scaled frequencies and intensities of CO₂•MgO ^a

B3LYP	ν_3		ν_4		ν_5		ν_6	
Cluster	Freq.	Int.	Freq.	Int.	Freq.	Int.	Freq.	Int.
T1-MgO	822	20 (0)	873	261 (257)	1269	238 (236)	1690	636 (0)
MS1-MgO	843	45 (26)	1049	100 (31)	1331	437 (172)	1610	726 (0)
Terrace-QM/MM ^b			922		1291		1669	

^a Calculated frequencies are scaled according to $\lambda=0.9800$ and are in cm^{-1} . Calculated intensities are in km/mol . Values for intensities calculated with changes in the dipole gradient parallel to the surface projected out are shown in parentheses.

^b Unscaled B3LYP frequencies calculated with embedded QM/MM cluster, Ref 3.

S1.4. Periodic models

Models with periodic boundary conditions (shown in Figure S2) $T1_{\text{pbc}}$, $T2_{\text{pbc}}$, $T3_{\text{pbc}}$, $MS1_{\text{pbc}}$, $MS2_{\text{pbc}}$, and $MS3_{\text{pbc}}$, where $T1_{\text{pbc}}$, $T2_{\text{pbc}}$, $T3_{\text{pbc}}$ have clean terrace surfaces and $MS1_{\text{pbc}}$, $MS2_{\text{pbc}}$, and $MS3_{\text{pbc}}$ contain monatomic steps, were used to explore terrace- and step-adsorption from low to high coverage. Fully periodic calculations were performed with the Vienna *ab initio* simulation package (VASP).^{4,5} Structure optimization was performed with the projector augmented-wave method (PAW)^{6,7} using the PBE functional, a plane-wave kinetic energy cutoff of 400 eV, and sampling of the Brillouin zone at the Γ point, until the calculated forces on relaxed atoms fell below 0.2 eV/Å. The Ca pseudopotential includes ten valence electrons. Dispersion corrections to the DFT energy were calculated for the periodic calculations in the same manner as with PEECM. Vibrational frequencies were calculated numerically with central differences using atomic displacements of ± 0.02 Å, where only the atoms of the surface carbonate species were included in the construction of the partial hessian. To calculate adsorption energies in the periodic regime, CO_2 was optimized in vacuum with the same parameters as the CaO supercells.

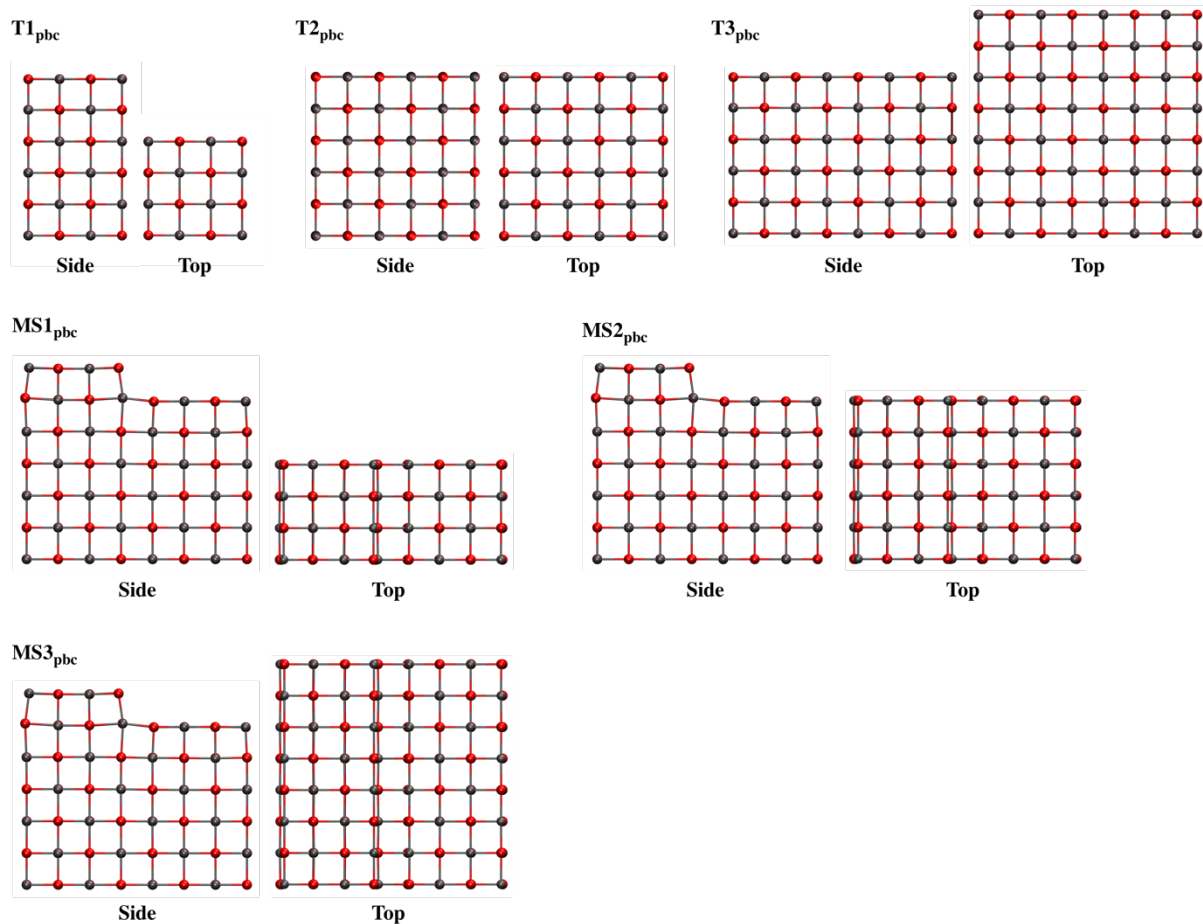


Figure S2. Periodic models (side view, left; top view, right) for different morphological sites of CaO(001) optimized with PBE: T1_{pbc} [terrace, $p(2 \times 2)$], T2_{pbc} [terrace, $p(3 \times 3)$], T3_{pbc} [terrace, $p(4 \times 4)$], MS1_{pbc} [monatomic step, $p(4 \times 2)$], MS2_{pbc} [monatomic step, $p(4 \times 3)$], and MS3_{pbc} [monatomic step, $p(4 \times 4)$]. Color code: red, O; gray, Ca.

The terrace model T1_{pbc}, a $p(2 \times 2)$ CaO supercell, was constructed by cutting CaO in the 001 direction with experimental lattice parameter $a=481.1$ pm extending 6 atomic layers. The bottom two layers were frozen to their lattice positions to maintain bulk geometry, and the z -direction cell vector was set to 2.4433 nm to allow for 10 Å of vacuum between the periodic images. Models T2_{pbc} and T3_{pbc} are $p(3 \times 3)$ and $p(4 \times 4)$ CaO supercells, respectively, with the same parameters as T1_{pbc}. The monatomic step models MS1_{pbc}, MS2_{pbc}, and MS3_{pbc} are constructed from a $p(2 \times 4)$, $p(3 \times 4)$, and $p(4 \times 4)$ CaO supercell, respectively. Each monatomic step model contains a 7th surface layer that covers half of the supercell: $p(2 \times 2)$, $p(3 \times 2)$, and $p(4 \times 2)$, for MS1_{pbc}, MS2_{pbc}, and MS3_{pbc}, respectively. The z -direction cell vector is 2.9244 nm, which provides the same 10 Å of vacuum between periodic images as in the terrace models.

The effects of the energy cutoff and k point sampling on the calculated adsorption energies and frequencies were tested, as shown in Tables S5-S6. While the adsorption energies did vary by ~ 8 kJ/mol with increased k sampling of T1_{pbc}, the difference dropped to less than

1 kJ/mol when considering the larger T2_{pbc} model. The difference in adsorption energies with the larger energy cutoff was also insignificant. In addition, the changes to the calculated frequencies were small. The ν_5 frequencies varied at most 3 cm⁻¹, which are the most relevant for comparing to experiment. We therefore use 400 eV energy cutoff and restrict sampling of the Brillouin zone to the Γ point for the remainder of the study.

Table S5. CO₂ adsorption energies, ΔE_{el} (kJ/mol), defined by the reaction $\text{CO}_2 + (\text{CO}_2)_{n-1} \bullet \text{CaO} \rightarrow (\text{CO}_2)_n \bullet \text{CaO}$, calculated with periodic boundary conditions^a

Energy cutoff →		400 eV	400 eV	600 eV	600 eV
k -point mesh →		2×2×1	1×1×1	2×2×1	1×1×1
Model	n				
T1 _{pbc} -1-CO ₂	1	−130.9	−138.4	−129.3	−136.9
T2 _{pbc} -1-CO ₂	1	−135.9	−136.6	−	−
T1 _{pbc} -2-CO ₂ (1,2)	2	−124.3	−132.4	−122.9	−131.0
T1 _{pbc} -2-CO ₂ (1,3)	2	−86.5	−93.8	−85.3	−92.6

^a Energy is PBE without dispersion

Table S6. Calculated, unscaled PBE frequencies (cm⁻¹) of CO₂•CaO with periodic boundary model T1_{pbc}

Energy cutoff	k -point mesh	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
400 eV	2×2×1	644	672	807	889	1253	1625
400 eV	1×1×1	646	672	809	901	1254	1616
600 eV	2×2×1	643	671	807	885	1251	1624
600 eV	1×1×1	645	670	809	895	1253	1618

S2. Detailed Discussion of DFT Results

S2.1. Adsorption of a single CO₂ molecule

For single CO₂ adsorption onto terrace and step sites of CaO(001), the T1 and MS1 models give similar frequencies compared to larger cluster models, as shown in Table S7. The calculated frequencies range at most 2 cm⁻¹, with the exception of T2. As will be discussed in detail below, the symmetry of the cluster models affects the adsorption structures and energies due to computational artifacts stemming from the proximity of the adsorbates to the surrounding periodic point charges. In the case of T2, which has C2 rotational symmetry about the z-axis, the isolated surface carbonate adsorbs at a 45° angle with respect to the surface lattice structure (see Figure S3 below). The oxygen atoms of CO₂ are positioned along the

longer side of the cluster. The rotated structure has higher frequency modes than the unrotated structure.

Table S7. Calculated scaled, surface-corrected frequencies (cm^{-1}) and intensities (km/mol) of $\text{CO}_2 \bullet \text{CaO}$

B3LYP	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
T1-1CO ₂	665 (0)	685 (1)	842 (0)	922 (200)	1274 (284)	1615 (0)
T2-1CO ₂	675 (1)	679 (0)	858 (0)	961 (153)	1281 (281)	1611 (1)
T3-1CO ₂	666 (0)	684 (1)	842 (0)	920 (196)	1273 (278)	1615 (0)
MS1-1CO ₂	678 (0)	695 (0)	843 (22)	1006 (20)	1294 (90)	1561 (0)
MS2-1CO ₂	676 (0)	696 (0)	842 (20)	1007 (22)	1293 (98)	1561 (1)
PBE	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
T1-1CO ₂	647 (0)	670 (2)	813 (0)	892 (194)	1249 (242)	1607 (0)
T2-1CO ₂	660 (1)	662 (0)	829 (0)	930 (147)	1254 (236)	1601 (1)
T3-1CO ₂	649 (0)	668 (2)	814 (0)	889 (188)	1248 (235)	1607 (0)
MS1-1CO ₂	662 (0)	680 (0)	814 (16)	983 (12)	1267 (54)	1549 (0)
MS2-1CO ₂	660 (0)	680 (0)	814 (14)	983 (13)	1266 (52)	1548 (1)

The adsorption energies of isolated adsorbed CO₂, unlike the frequencies, are slightly overestimated at the smaller cluster models, as shown in Table S8. The adsorption strength monotonically decreases with increasing cluster size, which correlates with the distance of the adsorbate from the embedded point charge array. The terrace and step cluster models are further used to evaluate adsorption of multiple CO₂ molecules, including adsorption on both step and terrace sites simultaneously. It is therefore important to evaluate the effect adsorption of CO₂ molecules on non-centered cluster adsorption sites has on adsorption energies and associated frequencies.

Table S8. Calculated CO₂ adsorption energies, ΔE_{el} (kJ/mol), defined by the reaction $\text{CO}_2 + \text{CaO} \rightarrow \text{CO}_2 \bullet \text{CaO}$, at centered surface oxygen atom sites

Model	B3LYP	B3LYP+D ^a	PBE	PBE+D ^a
T1-1CO ₂	−151.9	−171.5	−155.0	−169.2
T2-1CO ₂ ^b	−151.0	−170.3	−154.4	−168.3
T3-1CO ₂ ^c	−145.7	−165.5	−148.3	−162.6
T4-1CO ₂	−135.1	−155.3	—	—
T5-1CO ₂	−134.6	−154.8	−136.1	−150.6
MS1-1CO ₂	−287.1	−306.1	−279.0	−293.7
MS2-1CO ₂ ^c	−276.0	−295.2	−267.5	−283.0

^a DFT+D single point calculation at the DFT structure.

^b The center of the T2 surface falls between atoms. CO₂ adsorption therefore occurs at the closest surface atom, which is an oxygen atom. The surface carbonate is rotated 45° with respect to the surface lattice structure.

^c T3 and MS2 are calcium-centered, so the CO₂ adsorption site is the closest surface oxygen atom along the long edge of the cluster (T3) or on the rim of the step (MS2).

Adsorption is studied at the center surface oxygen atom of the cluster (position 1), as well as the nearest 5-coordinated neighbor (position 2) and next nearest neighbor (position 3) sites, as shown in Figure S3. Note that positions 1 and 2 are identical for T2 and positions 1 and 3 are identical for T3 due to symmetry of the cluster.

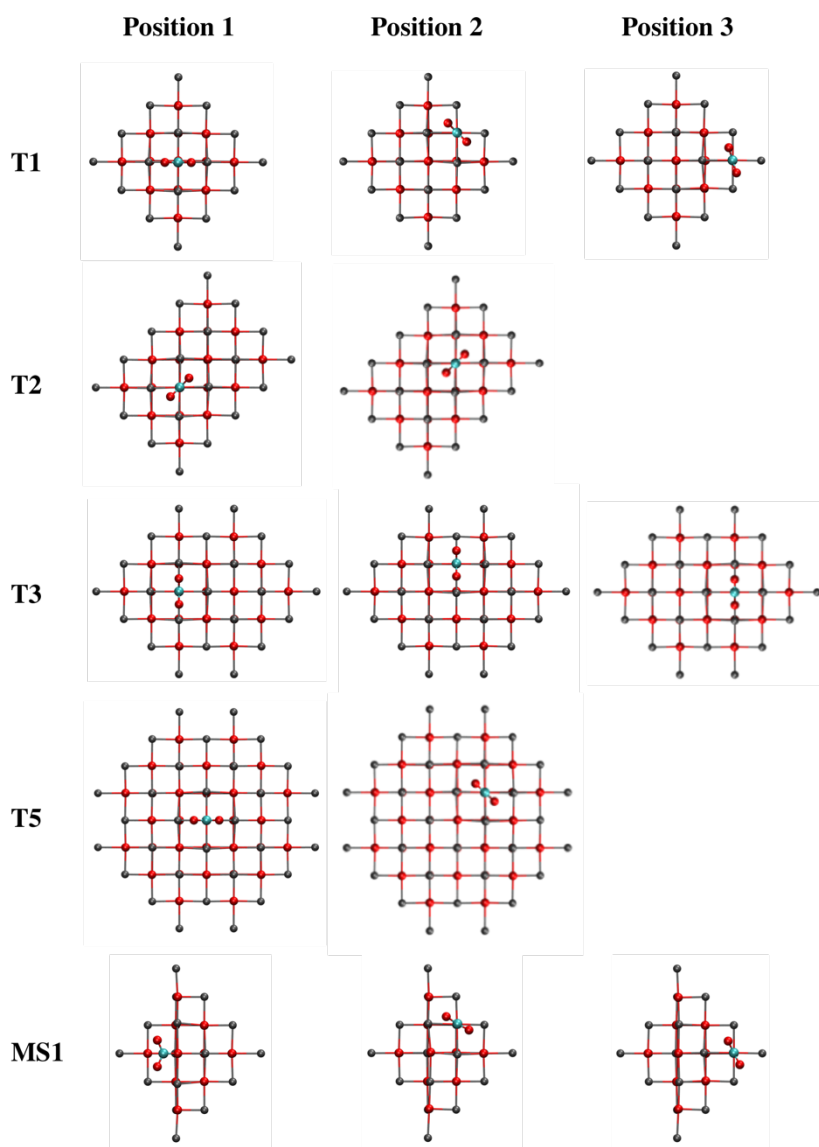


Figure S3. Structures of adsorbed CO₂ on cluster models T1, T2, T3, T5, and MS1 optimized with B3LYP at various oxygen sites from top views.

The calculated adsorption energies of single CO₂ adsorption are given in Table S8. Compared to adsorption at position 1 on terraces, the calculated adsorption energy at positions 2 and 3 are stronger by 6-20 kJ/mol. These changes can be rationalized by the distance of the adsorbate to the field of point charges, which is decreased upon adsorption at positions 2 and 3 compared to position 1. This trend is analogous to the trend in adsorption strength among the different terrace-site cluster models at position 1. It is worth noting that the adsorption structures in positions 2 and 3 often exhibit rotation with respect to the surface lattice structure. In position 2, the surface carbonate is typically rotated 45°. The exception is on T3, which has a mirror symmetry plane upon adsorption at position 2. The adsorption structure is also slightly rotated at position 3 on clusters T1 and MS1. These rotations are likely an artifact of being

close to the ends of the cluster surface and also have a stabilizing effect on the calculated adsorption energies.

Table S8. Calculated CO₂ adsorption energies, ΔE_{el} (kJ/mol), defined by the reaction $\text{CO}_2 + \text{CaO} \rightarrow \text{CO}_2 \bullet \text{CaO}$, at 5-coordinated sites

Model	Position	B3LYP	B3LYP+D ^a	PBE	PBE+D ^a
T1-1CO ₂	1	-151.9	-171.5	-155.0	-169.2
T1-1CO ₂	2	-163.5	-180.9	-172.1	-184.6
T1-1CO ₂	3	-166.0	-183.4	-174.5	-186.9
T2-1CO ₂	1,2	-151.0	-170.3	-154.4	-168.3
T3-1CO ₂	1,3	-145.7	-165.5	-148.3	-162.6
T3-1CO ₂	2	-165.7	-186.1	-170.6	-185.3
T5-1CO ₂	1	-134.6	-154.8	-136.1	-150.6
T5-1CO ₂	2	-141.9	-161.2	—	—
MS1-1CO ₂	2	-130.9	-148.1	-138.7	-150.9
MS1-1CO ₂	3	-174.1	-190.6	-185.9	-197.7

^a DFT+D single point calculation at the DFT structure

Calculated CO₂ adsorption energies can also be compared at positions 2 and 3 (5-coordinated sites) on T1 with MS1. The structures are very similar at positions 2 and 3 on T1 and MS1; however, the surface carbonate rotations are slightly greater on MS1 than T1, possibly due to the proximity to the monoatomic step edge: 61° versus 46° at position 2 and 27° versus 18° at position 3, respectively. At position 2, the calculated adsorption energy on MS1 is ca. +33 kJ/mol compared to T1. This implies that adsorption at a 5-coordinated site in close proximity to the step-edge is greatly disfavored. At position 3, the difference in calculated adsorption energy is ca. -10 kJ/mol on MS1 compared to T1, suggesting that the nearest neighbor position to step-edges is more favorable than isolated terrace sites. However, adsorption at step-edges (4-coordinated sites) is much more favorable than adsorption at terraces (5-coordinated sites). Therefore, we explore adsorption at 5-coordinated sites in proximity to filled CO₂ adsorption sites.

S2.2. Adsorption of a second CO₂ molecule

The optimized structures of CO₂ pairs on terrace and step cluster models are shown in Figure S4. The calculated adsorption energies for the CO₂ molecules adsorbed at positions 2

and 3, where position 1 is already filled, are given in Table S9. Adsorption of CO₂ at position 2 (nearest neighbor) on the terrace, forming the (1,2) pair, is favored compared to adsorption at position 3 (next nearest neighbor). Because the calculated isolated CO₂ adsorption energies at positions 2 and 3 are similar on T1, the presence of CO₂ already adsorbed at position 1 can be identified as the sole contributor to the difference in adsorption energies of the (1,2) and (1,3) pairs, rather than ascribed to an artifact of calculations due to the limited size of the T1 cluster. The difference in adsorption energies calculated on cluster T3 confirms the increased stability of the (1,2) pair compared with the (1,3) pair. On the monatomic step, however, adsorption at position 3 is more favorable than adsorption at position 2, when position 1 is already filled.

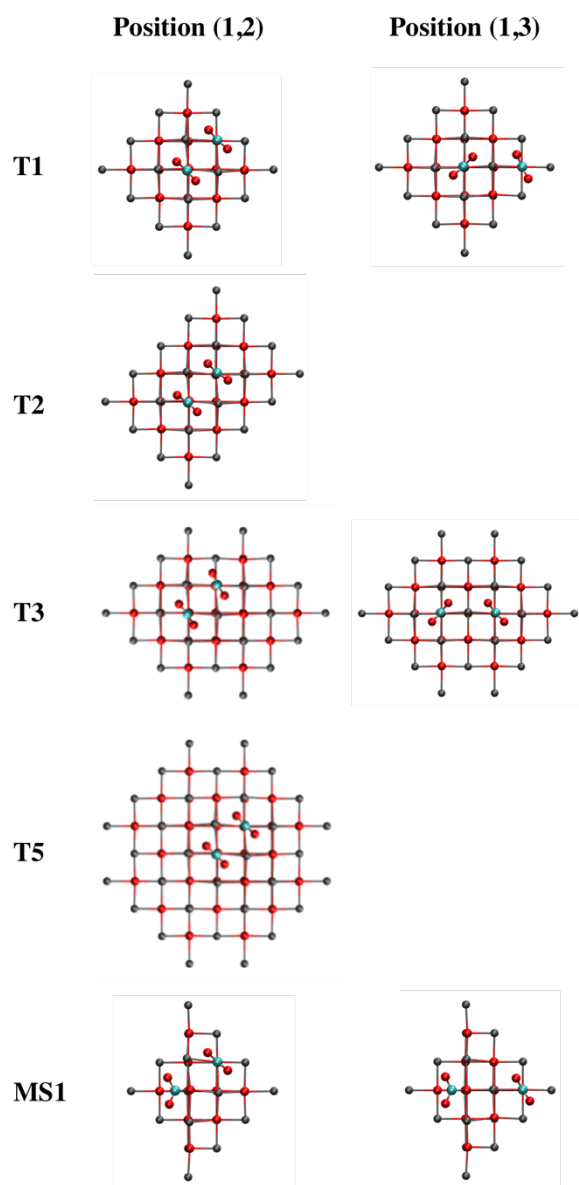


Figure S4. Structures of two adsorbed CO₂ molecules on cluster models T1, T2, T3, T5, and MS1 optimized with B3LYP at various oxygen sites from top views.

Table S9. Calculated CO₂ adsorption energies, ΔE_{el} (kJ/mol), defined by the reaction $\text{CO}_2 + \text{CO}_2 \bullet \text{CaO} \rightarrow (\text{CO}_2)_2 \bullet \text{CaO}$, where the first adsorbed CO₂ is at position 1

Model	Position	B3LYP	B3LYP+D ^a	PBE	PBE+D ^a
T1-2CO ₂ (1,2)	2	−154.4	−173.0	−164.2	−177.6
T1-2CO ₂ (1,3)	3	−128.8	−144.9	−140.6	−152.1
T2-2CO ₂ (1,2)	2	−137.8	−158.3	—	—
T3-2CO ₂ (1,2)	2	−157.3	−179.5	—	—
T3-2CO ₂ (1,3)	3	−116.1	−134.5	—	—
T5-2CO ₂ (1,2)	2	−141.6	−162.2	—	—
MS1-2CO ₂ (1,2 T) ^b	2	−141.6	−159.8	−150.5	−163.3
MS1-2CO ₂ (1,3 T) ^b	3	−152.1	−171.4	−165.6	−179.3

^a DFT+D single point calculation at the DFT structure

^b The “T” indicates adsorption at the nearest (1,2) or next nearest (1,3) 5-coordinated (“terrace”) surface oxygen atom

The differences in adsorption energies at positions 2 and 3 with and without CO₂ adsorbed at position 1, which quantitatively describe the effects of adsorption in proximity to CO₂ already adsorbed to position 1, are given in Table S10. In most cases, CO₂ adsorption at positions 2 and 3 are less favorable in proximity to CO₂ already bound to position 1. This would suggest that CO₂ prefers to bind as isolated molecules, rather than as pairs. However, there are two exceptions. First, the formation of the (1,2) pair is more slightly more favorable (−1 kJ/mol) on cluster T5 than two CO₂ molecules binding in isolation. This suggests that the smaller cluster models may not fully capture the necessary surface relaxation to stabilize adsorbed pairs. This will be analyzed further with periodic models in section S2.3. below. The second exception is for adsorption at the nearest neighbor (position 2) to a CO₂ bound to a monatomic step edge, where the calculated adsorption energy changes by ca. −11 kJ/mol compared to adsorption of an isolated CO₂ molecule at position 2. However, this site was highly disfavored for CO₂ adsorption compared to isolated terrace sites by ca. 33 kJ/mol. Therefore, even with the favorable adsorbate-adsorbate interaction of positions 1 and 2 on MS1, adsorption of CO₂ at 5-coordinated sites is unfavorable in proximity to step-edges.

Table S10. Calculated difference in CO₂ adsorption energies, ΔE_{el} (kJ/mol), for adsorption at 5-coordinated sites at positions 2 and 3 when position 1 is already filled (Table S9), subtracted by the adsorption energy of an isolated CO₂ molecule adsorbed at position 2 or 3 (Table S8)

Model	Position	B3LYP	B3LYP+D ^a	PBE	PBE+D ^a
T1-2CO ₂ (1,2)	2	9.1	7.9	7.9	7.0
T1-2CO ₂ (1,3)	3	37.2	38.5	33.9	34.8
T2-2CO ₂ (1,2)	2	13.2	12.0	—	—
T3-2CO ₂ (1,2)	2	8.4	6.6	—	—
T3-2CO ₂ (1,3)	3	29.6	31.0	—	—
T5-2CO ₂ (1,2)	2	0.3	−1.0	—	—
MS1-2CO ₂ (1,2 T) ^b	2	−10.7	−11.7	−11.8	−12.4
MS1-2CO ₂ (1,3 T) ^b	3	22.0	19.2	20.3	18.4

^a DFT+D single point calculation at the DFT structure

^b The “T” indicates adsorption at the nearest (1,2) or next nearest (1,3) 5-coordinated (“terrace”) surface oxygen atom

Having discussed the effects of the adsorption site on the calculated adsorption energy, we now turn to the associated frequencies. The scaled, surface-corrected frequencies and intensities of adsorbed CO₂ at 5-coordinated sites on T1, T2, T3, and MS1 are given in Table S11. Significant differences in the frequencies can be observed on cluster model T1, such as a $\sim 20 \text{ cm}^{-1}$ increase in ν_5 when CO₂ is bound to positions 2 and 3 compared to position 1. In ν_4 , a $\sim 20 \text{ cm}^{-1}$ increase is observed from position 1 to position 2, while a $\sim 20 \text{ cm}^{-1}$ decrease is observed from position 1 to position 3. Because positions 1 and 2 are identical on T2 and positions 1 and 3 are identical on T3 due to symmetry, no comparisons in the frequencies among these structures can be made. The ν_4 and ν_5 frequencies calculated on T3 in positions 1 and 2 only vary by 6 cm^{-1} , which is significantly less than the $\sim 20 \text{ cm}^{-1}$ differences calculated on T1. The differences in calculated frequencies in the various positions could be due to the partial rotation of the carbonate on the surface, the proximity to the embedded point charges, or a combination. Owing to the decreased change in frequencies on T3, in which the adsorbed structure does not rotate on the surface, the carbonate rotation is likely the primary cause for these differences. This will be investigated further when discussing the frequencies of CO₂ pairs and higher oligomers in section S2.4. below.

Table S11. Calculated scaled, surface-corrected frequencies (cm^{-1}) and intensities (km/mol) of $\text{CO}_2 \bullet \text{CaO}$

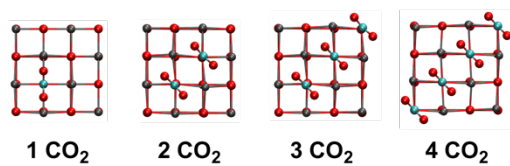
B3LYP	Position	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
T1-1CO ₂	1	665 (0)	685 (1)	842 (0)	922 (200)	1274 (284)	1615 (0)
T1-1CO ₂	2	683 (1)	684 (0)	864 (4)	946 (198)	1293 (306)	1655 (0)
T1-1CO ₂	3	682 (1)	694 (8)	851 (8)	900 (268)	1292 (313)	1693 (2)
T2-1CO ₂	1,2	675 (1)	679 (0)	858 (0)	961 (153)	1281 (281)	1611 (1)
T3-1CO ₂	1,3	666 (0)	684 (1)	842 (0)	920 (196)	1273 (278)	1615 (0)
T3-1CO ₂	2	669 (0)	691 (3)	845 (0)	923 (212)	1279 (302)	1633 (11)
MS1-1CO ₂	2	681 (3)	690 (1)	855 (7)	912 (236)	1290 (289)	1681 (9)
MS1-1CO ₂	3	692 (1)	702 (0)	865 (7)	927 (199)	1305 (289)	1698 (5)
PBE		ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
T1-1CO ₂	1	647 (0)	670 (2)	813 (0)	892 (194)	1249 (242)	1607 (0)
T1-1CO ₂	2	668 (0)	670 (2)	839 (4)	918 (192)	1268 (269)	1645 (0)
T1-1CO ₂	3	669 (1)	681 (11)	825 (9)	874 (256)	1270 (279)	1686 (3)
T2-1CO ₂	1,2	660 (1)	662 (0)	829 (0)	930 (147)	1254 (236)	1601 (1)
T3-1CO ₂	1,3	649 (0)	668 (2)	814 (0)	889 (188)	1248 (235)	1607 (0)
T3-1CO ₂	2	652 (0)	676 (5)	818 (0)	893 (205)	1254 (260)	1625 (12)
MS1-1CO ₂	2	665 (4)	675 (3)	828 (7)	882 (224)	1266 (253)	1674 (9)
MS1-1CO ₂	3	679 (2)	691 (0)	841 (7)	902 (188)	1282 (257)	1689 (5)

CO_2 adsorption at positions 2 and 3 on T1 and MS1 can also be compared to evaluate the effect the proximity of the monatomic step has on the calculated frequencies. At position 2, the ν_5 frequency is similar on T1 compared to MS1, while the ν_4 frequency decreases by $\sim 35 \text{ cm}^{-1}$. At position 3, the ν_5 frequency increases by $\sim 12 \text{ cm}^{-1}$ from T1 to MS1, while the ν_4 frequency increases by $\sim 27 \text{ cm}^{-1}$. From the calculated adsorption energies discussed above, we know that adsorption of CO_2 in the vicinity of a step-edge is thermodynamically unlikely, because the steps are likely to be populated first, and a populated step-edge disfavors adsorption at nearby 5-coordinated sites.

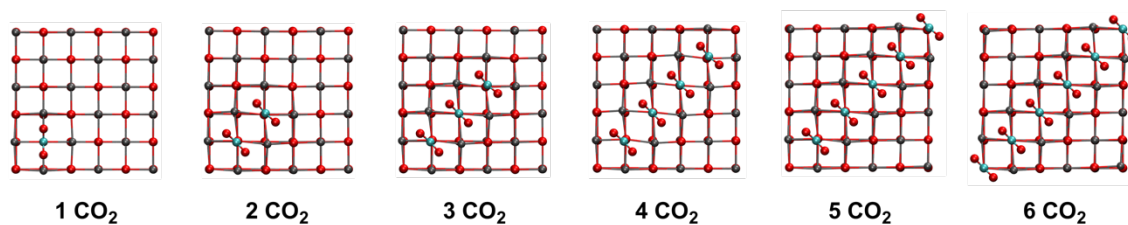
S2.3. Adsorption on periodic models

Due to the magnitude of the calculated adsorption energies on $\text{CaO}(001)$ sites, even low exposure can result in a relatively high surface coverage. Adsorption of two CO_2 molecules was only found more favorable as a pair when calculated on T5, the largest model we considered. Therefore, we used periodic models to determine the likelihood of CO_2 pairing and formation of higher oligomers on the $\text{CaO}(001)$ surface. Using the periodic models T1_{pbc}, T2_{pbc}, and T3_{pbc}, we calculated adsorption of one to eight CO_2 molecules in a diagonal stripe, the preferred binding motif, with PBE. The calculated adsorption structures are shown in Figure S5. The calculated energies and their associated coverages are given in Table S12.

T1_{pbc}



T2_{pbc}



T3_{pbc}

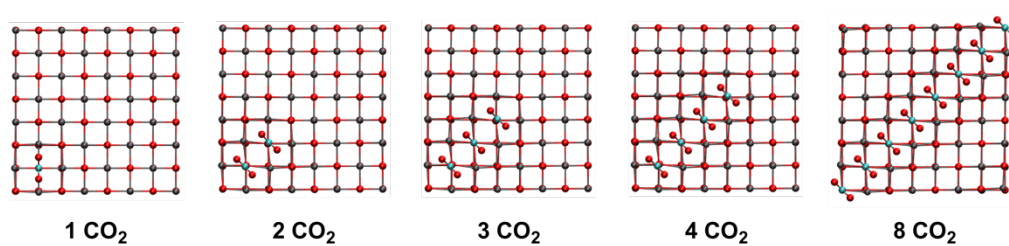


Figure S5. Structures of adsorbed CO₂ molecules on periodic models T1_{pbc}, T2_{pbc}, and T3_{pbc} optimized with PBE from top views forming a diagonal stripe.

Table S12. Calculated CO₂ adsorption energies per adsorbed CO₂, $\Delta E_{\text{el}}/n$ (kJ/mol), defined by the reaction $n\text{CO}_2 + \text{CaO} \rightarrow (\text{CO}_2)_n \bullet \text{CaO}$ on periodic terrace models, forming a diagonal stripe

Model	Θ^a	n	PBE	PBE+D ^b
T1 _{pbc}	0.125	1	-138.4	-152.4
T1 _{pbc}	0.250	2	-135.5	-150.4
T1 _{pbc}	0.375	3	-119.8	-135.6
T1 _{pbc}	0.500	4	-105.1	-122.5
T2 _{pbc}	0.056	1	-136.6	-148.8
T2 _{pbc}	0.111	2	-140.4	-155.0
T2 _{pbc}	0.167	3	-136.7	-152.0
T2 _{pbc}	0.222	4	-131.8	-147.4
T2 _{pbc}	0.278	5	-126.3	-142.3
T2 _{pbc}	0.333	6	-121.2	-138.0
T3 _{pbc}	0.031	1	-138.0	-146.3
T3 _{pbc}	0.063	2	-142.4	-154.4
T3 _{pbc}	0.094	3	-140.8	-154.6
T3 _{pbc}	0.125	4	-138.8	-153.5
T3 _{pbc}	0.250	8	-128.9	-145.1

^a Coverage is calculated as $n\text{CO}_2$ divided by the total surface oxygen atoms in the supercell, which are available adsorption sites.

^b DFT+D single point calculation at the DFT structure.

On T1_{pbc}, addition of a second, third, and fourth CO₂ molecule to the surface results in a decrease in calculated adsorption strength. However, the small $p(2 \times 2)$ supercell causes the diagonal stripe to be close to its image in the neighboring cells. By increasing the supercell to $p(3 \times 3)$ (T2_{pbc}) and $p(4 \times 4)$ (T3_{pbc}), the diagonal stripes form with greater separation, and the average CO₂ adsorption energies become more favorable. On T2_{pbc}, adsorption of two or three CO₂ molecules is more favorable than a single CO₂ molecule binding in isolation. On T3_{pbc}, the formation of an infinite diagonal stripe is only 1.2 kJ/mol less favorable than a single CO₂. Therefore, presuming an infinite terrace CaO(001) surface, CO₂ molecules will preferentially bind in infinite diagonal stripes that are separated by suitably large distance.

A similar analysis was performed on periodic models of monatomic step edges. Because the calculated CO₂ adsorption energy of the (1,2 S) pair on cluster step model MS2 is greater than adsorption at 5-coordinated sites, we hypothesize that step edges become completely filled prior to adsorption at terraces. The calculated CO₂ adsorption structures on periodic step models are shown in Figure S6. The calculated energies and their associated coverages are given in Table S13.

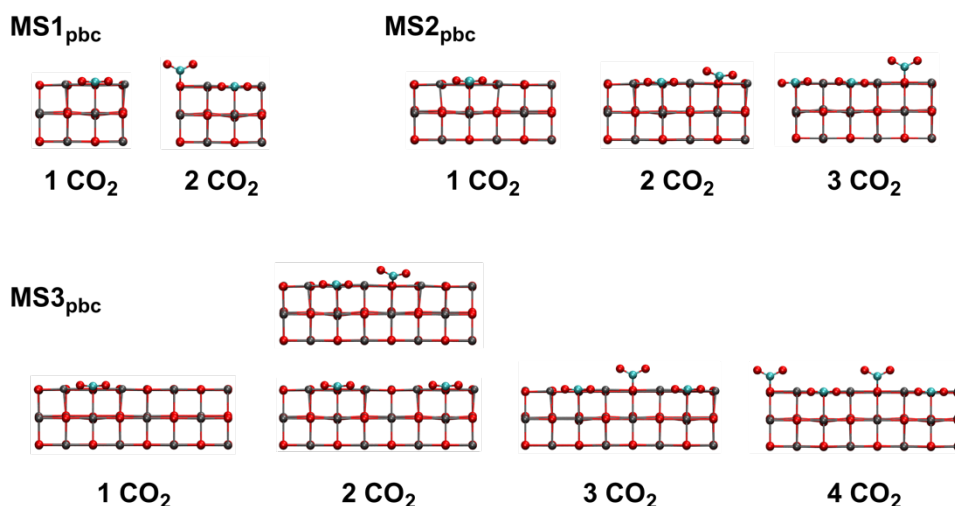


Figure S6. Structures of adsorbed CO₂ molecules on periodic models MS1_{pbc}, MS2_{pbc}, and MS3_{pbc} optimized with PBE, viewed from the side at the step-edge. On MS3_{pbc}, adsorption of two CO₂ molecules ($\theta=0.5$) can be as the (1,2 S) pair (top) or (1,3 S) pair (bottom).

Table S13. Calculated CO₂ adsorption energies per adsorbed CO₂, $\Delta E_{\text{el}}/n$ (kJ/mol), defined by the reaction $n\text{CO}_2 + \text{CaO} \rightarrow (\text{CO}_2)_n \bullet \text{CaO}$ on periodic step models

Model	θ^a	n	PBE	PBE+D ^b
MS1 _{pbc}	0.500	1	-253.2	-273.4
MS1 _{pbc}	1.000	2	-203.4	-218.9
MS2 _{pbc}	0.333	1	-252.3	-271.4
MS2 _{pbc}	0.667	2	-221.6	-238.7
MS2 _{pbc}	1.000	3	-195.8	-199.6
MS3 _{pbc}	0.250	1	-252.4	-271.2
MS3 _{pbc}	0.500	2 ^c	-224.9	-241.1
MS3 _{pbc}	0.500	2 ^d	-248.2	-266.6
MS3 _{pbc}	0.750	3	-217.5	-234.6
MS3 _{pbc}	1.000	4	-199.6	-215.5

^a Coverage is calculated as $n\text{CO}_2$ divided by the total surface oxygen atoms in step in the supercell, which are available adsorption sites.

^b DFT+D single point calculation at the DFT structure.

^c CO₂ molecules bind in the nearest neighbor position on the step: MS3_{pbc}-2CO₂ (1,2 S)

^d CO₂ molecules bind in the next-nearest neighbor position on the step: MS3_{pbc}-2CO₂ (1,3 S)

Similar to the cluster models, CO₂ adsorbed on the periodic monatomic step models leans toward the step surface layer. This structure is maintained upon adsorption of a second CO₂ molecule on the larger MS3_{pbc} model in the (1,3 S) position, with similar adsorption energy. However, when the two CO₂ molecules bind in the neighboring (1,2 S) positions, one surface carbonate is pushed up away from the step surface layer. The adsorption structure MS3_{pbc}-2CO₂ (1,2 S) is nearly identical to MS2-2CO₂ (1,2 S), indicating that the asymmetric adsorption structure is due to steric interaction of the adsorbates and not an artifact of the cluster

calculations. However, when every step adsorption site in the supercells is filled, the adsorbates form a zigzag pattern, in which every odd CO₂ leans down toward the step surface layer, and every even CO₂ is bent away from the step surface layer. This is evident in the adsorption structures MS1_{pbc}-2CO₂ and MS3_{pbc}-4CO₂ (Figure S6). The calculated adsorption energy of the completely filled MS2_{pbc}-3CO₂ is ca. 15-20 kJ/mol less favorable compared to MS1_{pbc} and MS3_{pbc}, because the three adsorption sites on the step in each supercell cause strain at the boundaries between supercell images. We note that the adsorption energy of the completely filled step is still more favorable than adsorption on terraces, confirming our hypothesis that step sites are completely filled prior to terrace-site adsorption.

S2.4. Analysis of calculated frequencies on terrace clusters

We assign the frequencies of adsorbed CO₂ pairs and higher oligomers to low-exposure IRA spectra. Therefore, it is important to test if the agreement is genuine or spurious. Specifically, we investigate the calculated frequencies of two, three, and four CO₂ molecules adsorbed in a diagonal stripe across the CaO(001) terrace, which is the lowest-energy configuration for adsorption of multiple CO₂ molecules in close proximity. The calculated optimized structures of two, three, and four CO₂ molecules adsorbed to cluster models T1 and T2 are given in Figure S7. The calculated scaled, surface-corrected frequencies and intensities are given in Table S14. The calculated ν_4 and ν_5 modes, which are most easily compared to the experimental spectra, are further detailed in Figure S8, which contains a normal mode diagram for each frequency.

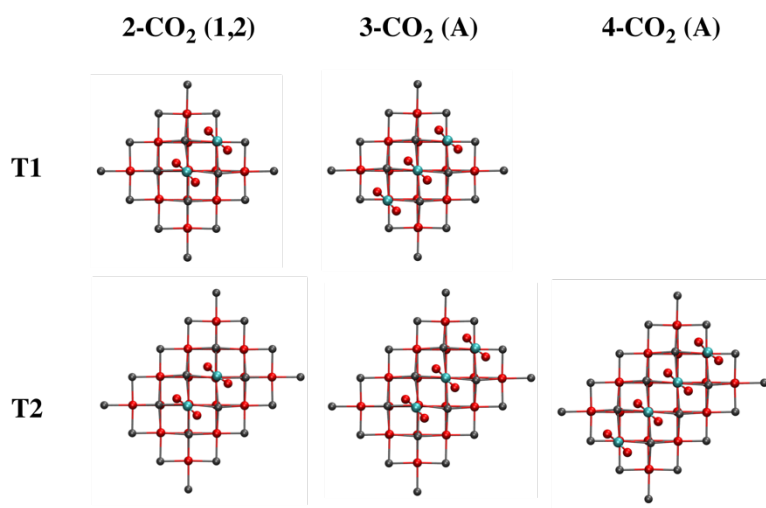


Figure S7. Structures of two, three, and four adsorbed CO₂ molecules on cluster models T1 and T2 optimized with B3LYP.

Table S14. Calculated B3LYP scaled, surface-corrected frequencies (cm⁻¹) and intensities (km/mol) of (CO₂)_n•CaO, for n=2,3,4, on cluster models T1 and T2

	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
T1-2CO ₂ (1,2)	675 (0)	678 (0)	858 (1)	946 (7)	1274 (45)	1612 (0)
	685 (1)	685 (0)	870 (2)	962 (316)	1300 (548)	1663 (0)
T1-3CO ₂ (A)	678 (0)	679 (0)	858 (0)	931 (244)	1272 (0)	1609 (0)
	682 (0)	685 (0)	867 (9)	933 (0)	1289 (0)	1671 (0)
	684 (0)	685 (3)	869 (0)	973 (248)	1302 (881)	1683 (0)
T2-2CO ₂ (1,2)	674 (0)	677 (1)	855 (0)	948 (0)	1270 (0)	1601 (1)
	675 (0)	679 (0)	863 (0)	963 (281)	1291 (546)	1629 (0)
T2-3CO ₂ (A)	674 (0)	680 (0)	855 (1)	937 (155)	1269 (23)	1601 (0)
	675 (0)	681 (0)	863 (1)	941 (59)	1283 (37)	1633 (0)
	680 (0)	685 (0)	869 (3)	978 (240)	1301 (772)	1674 (0)
T2-4CO ₂ (A)	675 (0)	682 (0)	854 (0)	924 (0)	1267 (0)	1604 (0)
	678 (0)	683 (0)	862 (5)	925 (268)	1279 (4)	1633 (0)
	679 (0)	685 (1)	866 (0)	959 (0)	1292 (0)	1680 (1)
	681 (0)	685 (4)	868 (6)	974 (385)	1302 (1107)	1686 (0)

Model	Mode	Diagram	Frequency	Intensity	Model	Mode	Diagram	Frequency	Intensity
T1	ν_4		946	7	T2	ν_4		937	155
T1	ν_4		962	316	T2	ν_4		941	59
T1	ν_5		1274	45	T2	ν_4		978	240
T1	ν_5		1300	548	T2	ν_5		1269	23
T1	ν_4		931	244	T2	ν_5		1283	37
T1	ν_4		933	0	T2	ν_5		1301	772
T1	ν_4		973	248	T2	ν_4		924	0
T1	ν_5		1272	0	T2	ν_4		925	268
T1	ν_5		1289	0	T2	ν_4		959	0
T1	ν_5		1302	881	T2	ν_4		974	385
T2	ν_4		948	0	T2	ν_5		1267	0
T2	ν_4		963	281	T2	ν_5		1279	4
T2	ν_5		1270	0	T2	ν_5		1292	0
T2	ν_5		1291	546	T2	ν_5		1302	1107

Figure S8. Calculated B3LYP scaled, surface-corrected ν_4 and ν_5 frequencies (cm^{-1}), intensities (km/mol), and normal mode diagrams of $(\text{CO}_2)_n \cdot \text{CaO}$, for $n=2,3,4$, on cluster models T1 and T2. In the normal mode diagrams, the gray dots represent surface oxygen atoms of the T1 and T2 cluster along the diagonal. The vertical lines represent bound CO_2 molecules as surface carbonates, viewed from the side. The arrows represent the direction and magnitude of the atomic displacements within the carbonate (including the surface oxygen atom) in each normal mode. Symmetry planes can be inferred from the normal mode diagrams: on T1, symmetry exists upon adsorption of 3 CO_2 molecules (center left); on T2, symmetry exists upon adsorption of 2 CO_2 molecules (bottom left) or 4 CO_2 molecules (bottom right).

First we compare the calculated ν_4 and ν_5 modes of the adsorbed CO_2 pair on clusters T1 and T2. On T1, the second CO_2 molecule is on the edge of the cluster (position 2), which

results in ν_4 and ν_5 frequencies calculated ca. $+20\text{ cm}^{-1}$ compared to the center (position 1; see above). On T2, the resulting structure with two bound CO_2 molecules has symmetry in the form of a reflection plane. Therefore, for each of the two ν_4 and ν_5 modes, the calculated intensity of one mode interferes constructively while the intensity of the other mode interferes destructively. This is demonstrated in Figure S8 by the normal mode diagrams of ν_4 and ν_5 of the CO_2 pairs on model T2 that show atomic displacements occurring symmetrically (constructive) or asymmetrically (destructive). Therefore, on T2, there are only two symmetric stretching frequencies in the simulated IRA spectrum of the adsorbed CO_2 pair. On T1, the structure with two bound CO_2 molecules has no symmetry. The calculated normal mode intensities do not perfectly cancel from destructive interference, resulting in two low-frequency shoulders to the two symmetric stretching peaks in the simulated IRA spectrum of the adsorbed CO_2 pair. These shoulders are artifacts of the asymmetry of the cluster. While the calculated ν_4 frequencies are similar between the CO_2 pair on T1 and T2, the calculated ν_5 frequencies are slightly overestimated by $\sim 10\text{ cm}^{-1}$.

Next we compare the calculated ν_4 and ν_5 modes of T1 and T2 with three CO_2 molecules bound in a diagonal stripe. Unlike the previous case in which T2 had symmetry in the form of a reflection plane and T1 had no symmetry, when three CO_2 molecules are bound, T1 has symmetry and T2 is asymmetric. A similar analysis of the ν_4 and ν_5 modes follows. With three CO_2 adsorbates, there are three ν_4 and ν_5 modes each. The atomic displacements with the outer surface carbonates differ from the atomic displacements of the center molecule. As depicted in Figure S8, the constructive and destructive interference of the calculated normal mode intensities yields two ν_4 modes and one ν_5 mode with positive intensity. In the case of adsorption on T2, all six ν_4 and ν_5 modes have nonzero calculated intensities. The qualitative picture, however, is similar, as the modes with the largest intensities are analogous to the nonzero intensity modes on T1. The simulated IRA spectra look nearly identical because the two low-frequency ν_4 modes overlap, erasing the effect of the artifact of the calculation. There are some minor differences in the calculated frequencies of ν_4 , but those of ν_5 are quantitatively equivalent.

The final comparison of the ν_4 and ν_5 modes that is required is between the fully-filled diagonal stripe of both the T1 and T2 cluster models. As discussed above, the ν_4 band splits into two distinct peaks in the simulated IRA spectrum, due to the outer adsorbed CO_2 molecules being distinct from the inner adsorbed CO_2 molecule. As shown in Figure S8, the fully-adsorbed diagonal stripe on T2 behaves similarly. Just as with the adsorbed carbonate pair on T2, the same reflection plane of symmetry exists in the case of four adsorbed CO_2 molecules.

Two of the four ν_4 modes have zero calculated intensity due to destructive interference across the plane of symmetry. Additionally, three of the four ν_5 modes also vanish, leaving only a single ν_5 peak. These calculations imply that a diagonal stripe, regardless of its composition, will have only a single ν_5 peak, and that its frequency remains constant at $\sim 1302 \text{ cm}^{-1}$. The ν_5 frequency of the stripes is ca -10 cm^{-1} from that of the CO_2 pair. These two frequencies are herein assigned as appearing in the observed IRA spectra after adsorption at low-coordinated sites.

S2.5. Comparison of calculated frequencies on periodic versus cluster models

We can directly compare the calculated frequencies of adsorbed CO_2 on periodic and cluster models optimized with PBE. In Table S15, the calculated frequencies of one and two CO_2 molecules bound to $\text{CaO}(001)$ are listed. Selected cluster models have been included according to the analysis performed in section S2.4 (see above) for an accurate comparison. First, we note that utilizing all of the optimized atoms in the construction of the partial hessian of model T1_{pbc} , rather than only the surface carbonate atoms, has negligible effects. We also observe that ν_4 and ν_5 frequencies calculated with cluster models are less than those calculated with periodic models. In the case of an isolated adsorbed CO_2 molecule, the difference is $3\text{-}10 \text{ cm}^{-1}$. However, the difference is more pronounced when considering the (1,2) CO_2 pair: ν_4 is $\sim 40 \text{ cm}^{-1}$ less and ν_5 is $\sim 10 \text{ cm}^{-1}$ less.

Table S15. Calculated surface-corrected PBE frequencies (cm^{-1}) and intensities (km/mol) of $(\text{CO}_2)_n \bullet \text{CaO}$, for $n=1,2$ on terrace models

	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
$\text{T1}_{\text{pbc}}\text{-1CO}_2$	648	673	810	903	1255	1617
$\text{T1}_{\text{pbc}}\text{-1CO}_2^a$	646	672	809	901	1254	1616
$\text{T2}_{\text{pbc}}\text{-1CO}_2^a$	644	672	808	897	1251	1617
$\text{T3}_{\text{pbc}}\text{-1CO}_2^a$	644	673	808	899	1252	1616
$\text{T1}\text{-1CO}_2$	647 (0)	670 (2)	813 (0)	892 (194)	1249 (242)	1607 (0)
$\text{T3}\text{-1CO}_2$	649 (0)	668 (2)	814 (0)	889 (188)	1248 (235)	1607 (0)
$\text{T1}_{\text{pbc}}\text{-2CO}_2(1,2)^a$	658	662	828	948	1249	1594
	660	665	834	961	1271	1610
$\text{T2}_{\text{pbc}}\text{-2CO}_2(1,2)^a$	659	660	824	959	1251	1582
	660	664	830	969	1271	1605
$\text{T3}_{\text{pbc}}\text{-2CO}_2(1,2)^a$	659	661	824	963	1252	1581
	660	664	830	973	1272	1605
$\text{T2}\text{-2CO}_2(1,2)$	657 (0)	662 (2)	828 (0)	918 (0)	1243 (0)	1591 (0)
	660 (0)	662 (0)	834 (0)	934 (272)	1263 (465)	1618 (0)

^a Calculated frequencies with finite differences of only surface carbonate atoms.

We also compare calculated PBE frequencies for adsorption of three or more CO₂ molecules, forming a diagonal stripe across the CaO(001) terrace, in Table S16. For a valid comparison, we consider only the cases in which the diagonal stripe crosses the entire unit cell of the periodic models. While we did not explicitly calculate frequency intensities with periodic models, we can infer from the cluster calculations and normal mode analysis performed in section S2.4. that the largest ν_5 frequency will dominate the observed spectrum. We can also infer that both the largest and smallest ν_4 frequencies will be visible. The ν_4 frequencies calculated with periodic models increase from the smaller T1_{pbc} to the larger T3_{pbc}, with the frequencies calculated with the T1 cluster model falling in between. The ν_5 frequencies calculated with periodic models also increase, albeit to a lesser degree; again, the largest ν_5 frequency calculated with the T1 cluster model falls in between the calculations with the smallest and largest periodic models.

Table S16. Calculated surface-corrected PBE frequencies (cm⁻¹) and intensities (km/mol) of (CO₂)_n•CaO, for n=3,4,6,8 on terrace models

	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
T1-3CO ₂ (A)	660 (0)	664 (0)	832 (0)	899 (222)	1245 (2)	1602 (0)
	665 (0)	670 (0)	842 (12)	901 (0)	1264 (0)	1663 (0)
	667 (0)	671 (7)	843 (0)	941 (288)	1275 (764)	1674 (0)
T1 _{pbc} -4CO ₂ (A) ^a	658	662	821	891	1236	1622
	660	662	828	903	1247	1652
	661	663	828	903	1247	1652
	661	664	834	927	1271	1665
T2 _{pbc} -6CO ₂ (A) ^a	659	663	821	935	1239	1592
	660	663	825	940	1245	1604
	660	664	825	940	1245	1604
	661	664	832	951	1261	1635
	662	665	832	951	1261	1636
	662	666	834	960	1275	1647
T3 _{pbc} -8CO ₂ (A) ^a	659	663	821	955	1241	1580
	660	664	824	957	1245	1587
	660	665	824	957	1245	1587
	661	665	829	963	1256	1606
	662	665	829	964	1257	1606
	662	666	833	971	1270	1631
	662	666	833	971	1270	1631
	662	667	834	976	1279	1640

^a Calculated frequencies with finite differences of only surface carbonate atoms.

We compare calculated PBE frequencies with periodic and cluster models of monatomic step sites in Table S17. Similar to adsorption of a single CO₂ at terrace sites, the calculated ν_4 and ν_5 frequencies of isolated carbonates at steps are 4-9 cm⁻¹ of each other. Most important, however, is the comparison of the (1,2 S) pair between the cluster and periodic models. Because the adsorption energy on step sites is so strong, the steps are favored to

become completely filled prior to adsorption at terraces. Therefore, it is important to test if the frequencies of the (1,2 S) pair on the MS2 cluster are similar to the frequencies of completely filled steps. First, comparing the frequencies of the (1,2 S) pair on MS2 with periodic models MS2_{pb}c and MS3_{pb}c, in which some step adsorption sites remain empty, the calculated largest ν_5 frequencies are identical. The calculated ν_4 frequencies, however, are again underestimated on the cluster model compared to the periodic models. Now comparing the calculated frequencies of the partially filled with the completely filled steps, there is a 4-6 cm⁻¹ decrease in the ν_5 frequencies. This shift in the ν_5 frequencies can be applied to the (1,2 S) pair on the MS2 cluster to better compare with the experimental IRA spectra.

Table S17. Calculated surface-corrected PBE frequencies (cm⁻¹) and intensities (km/mol) of (CO₂)_n•CaO, for n=1,2,4 on step models

	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
MS1 _{pb} c-1CO ₂ ^a	662	669	805	992	1265	1528
MS2 _{pb} c-1CO ₂ ^a	658	670	806	991	1262	1532
MS3 _{pb} c-1CO ₂ ^a	658	671	806	992	1262	1533
MS1-1CO ₂	662 (0)	680 (0)	814 (16)	983 (12)	1267 (54)	1549 (0)
MS2-1CO ₂	660 (0)	680 (0)	814 (14)	983 (13)	1266 (52)	1548 (1)
MS1 _{pb} c-2CO ₂ ^a	661	679	795	905	1255	1562
	663	681	798	949	1262	1635
MS2 _{pb} c-2CO ₂ ^a	657	674	801	954	1255	1560
	663	688	802	965	1265	1604
MS3 _{pb} c-2CO ₂ (1,2 S) ^{a,b}	656	672	802	957	1256	1553
	660	689	804	971	1266	1602
MS2-2CO ₂	659 (0)	675 (0)	806 (16)	950 (99)	1254 (1)	1564 (4)
	664 (0)	687 (0)	816 (2)	954 (40)	1266 (291)	1595 (1)
MS3 _{pb} c-4CO ₂	660	674	794	899	1251	1567
	662	678	794	901	1253	1578
	664	681	797	941	1258	1637
	667	682	797	942	1260	1640

^a Calculated frequencies with finite differences of only surface carbonate atoms.

^b The “S” indicates adsorption at the nearest (1,2) 4-coordinated (“step”) surface oxygen atom.

S3. Discussion of HF, MP2, and CCSD(T) Results

While DFT provides qualitative results, we performed high-level *ab initio* calculations to accurately calculate the adsorption energy of CO₂ on a terrace. Our goal is to ascertain the relative errors in adsorption energy as calculated by DFT to better compare with the experimentally-determined adsorption energies from TPD and microcalorimetry.

We first calculated CCSD(T) corrections to the DFT results, denoted $\Delta_{CC}B3LYP+D$ and $\Delta_{CC}PBE+D$ for the two functionals utilized, of a 3×3×2 Ca₉O₉ cluster. The Ca₉O₉ cluster was constructed from the T1 cluster optimized with B3LYP at the triple-zeta (TZ) level within

the PEECM formalism, shown in Figure S9. DFT, HF, MP2, and CCSD(T) calculations were performed on the Ca_9O_9 cluster without point charge embedding at the TZ and quadruple-zeta (QZ) levels, given in Table S18. Basis set extrapolation to the complete basis set (CBS) limit was performed with an exponential function for HF and with a cubic function for correlation energies. The extrapolated MP2 and CCSD(T) energies are therefore a sum of the cubic-extrapolated correlation energy and the exponential-extrapolated HF energy.

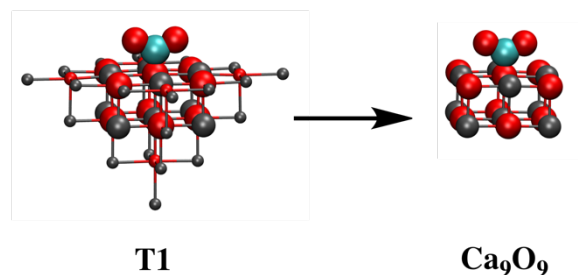


Figure S9. Optimized T1 with B3LYP (left) and $3 \times 3 \times 2$ Ca_9O_9 cluster (right).

Table S18. CO_2 adsorption energies, ΔE_{el} (kJ/mol), defined by the reaction $\text{CO}_2 + \text{CaO} \rightarrow \text{CO}_2 \bullet \text{CaO}$, calculated with the Ca_9O_9 nonembedded cluster ^a

Method	TZ	QZ	CBS
HF	-137.4	-138.9	-139.0 ^d
MP2	-137.4	-134.8	-131.9
$\delta\text{CCSD(T)}$ ^b	-16.1	-17.7	-19.0 ^e
CCSD(T)	-153.5	-152.6	-150.9
B3LYP+D	-120.6		
PBE+D	-119.0		
$\Delta_{\text{CC}}\text{B3LYP+D}$ ^c	-32.9		-30.3
$\Delta_{\text{CC}}\text{PBE+D}$ ^c	-34.5		-31.9

^a TZ=triple zeta, the def2-TZVP basis; All calculations performed on a Ca_9O_9 $3 \times 3 \times 2$ nonembedded cluster taken from the optimized T1 structure at the B3LYP//TZ level.

^b $\delta\text{CCSD(T)} = \Delta E_{\text{el}}[\text{CCSD(T)}] - \Delta E_{\text{el}}[\text{MP2}]$.

^c Δ_{CC} is the coupled-cluster correction to the DFT adsorption energy defined by $\Delta_{\text{CC}}\text{DFT+D} = \Delta E_{\text{el}}[\text{CCSD(T)}] - \Delta E_{\text{el}}[\text{DFT+D}]$.

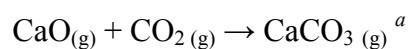
^d Extrapolation with the equation $\Delta E_{\text{el}}(x) = \Delta E_{\text{el}}(\text{CBS}) + A e^{-2.9x}$, where $x = 3$ for TZ and $x = 4$ for QZ. The factor -2.9 is the optimized exponential parameter for the Ahlrichs basis sets for two-point extrapolation of HF energies, from ref 8.

^e Extrapolation with the equation $\Delta E_{\text{el}}(x) = \Delta E_{\text{el}}(\text{CBS}) + A x^{-3}$, where $x = 3$ for TZ and $x = 4$ for QZ.

The coupled-cluster correction to DFT+D, $\Delta_{\text{CC}}\text{DFT+D}$, calculated for B3LYP+D and PBE+D from both the TZ Ca_9O_9 results as well as CBS, was found to be ~ 30 kJ/mol. This correction is similar to $\Delta_{\text{CC}}\text{DFT+D}$ calculated for the analogous gas-phase reaction, calculated

to be ~40-50 kJ/mol (see Table S19). When $\Delta_{\text{CCDFT+D}}$ of the Ca_9O_9 cluster is added to the adsorption energies calculated with the converged DFT+D adsorption energy on the largest T5 cluster, we calculated a final adsorption energy of –185.1 kJ/mol for B3LYP and –182.5 kJ/mol for PBE, or –184 kJ/mol on average.

Table S19. Calculated reaction energy, ΔE_{el} (kJ/mol), defined by the reaction



Method	TZ	QZ	CBS
HF	–313.0	–308.8	–308.5 ^e
MP2 _{corr} ^b	83.6	83.4	83.2 ^f
MP2	–229.5	–225.4	–225.3
$\delta\text{CCSD(T)}$ ^c	–25.8	–31.2	–35.1 ^f
CCSD(T)	–255.3	–256.6	–260.4
B3LYP+D	–224.4	–220.1	–219.9 ^e
PBE+D	–215.5	–211.8	–211.6 ^e
Δ_{CCB3LYP} ^d	–30.9	–36.5	–40.5
Δ_{CCPBE} ^d	–39.8	–44.8	–48.8

^a TZ=triple zeta, the def2-TZVP basis; QZ=quadruple zeta, the def2-QZVP basis; CBS=complete basis set limit. HF, MP2, and CCSD(T) calculations were performed on structures optimized with HF. DFT calculations were performed on structures optimized with DFT.

^b The MP2 correlation energy.

^c $\delta\text{CCSD(T)} = \Delta E_{\text{el}}[\text{CCSD(T)}] - \Delta E_{\text{el}}[\text{MP2}]$.

^d $\Delta_{\text{CCDFT}} = \Delta E_{\text{el}}[\text{CCSD(T)}] - \Delta E_{\text{el}}[\text{DFT+D}]$.

^e Extrapolation with the equation $\Delta E_{\text{el}}(x) = \Delta E_{\text{el}}(\text{CBS}) + A e^{-2.9x}$, where $x = 3$ for TZ and $x = 4$ for QZ. The factor –2.9 is the optimized exponential parameter for the Ahlrichs basis sets for two-point extrapolation of HF energies, from ref 8.

^f Extrapolation with the equation $\Delta E_{\text{el}}(x) = \Delta E_{\text{el}}(\text{CBS}) + A x^{-3}$, where $x = 3$ for TZ and $x = 4$ for QZ.

We also calculated the adsorption energy of CO_2 on T1 with CCSD(T) at the B3LYP//TZVP level within the PEECM formalism. The calculated CCSD(T) adsorption energy, –194.3 kJ/mol, gives a coupled-cluster correction, Δ_{CCB3LYP} , of –22.8 kJ/mol.

S4. Additional DFT Adsorption Structures, Energies, and Frequencies

S4.1. Adsorption structures and structural parameters

Optimized structures of adsorption of a single CO_2 are shown in Figure S10. Optimized structures of adsorption of two CO_2 molecules are shown in Figure S11. Optimized structures of adsorbed CO_2 onto 5-coordinated sites in proximity to filled low-coordinated sites are given in Figure S12. Optimized structures of adsorption of one, two, three, four, and five CO_2

molecules on cluster T1 are shown in Figure S13. Structural parameters for the adsorption of one or two CO₂ molecules are given in Tables S20-S23, where bond distances and angles are annotated in Figures S14-S17.

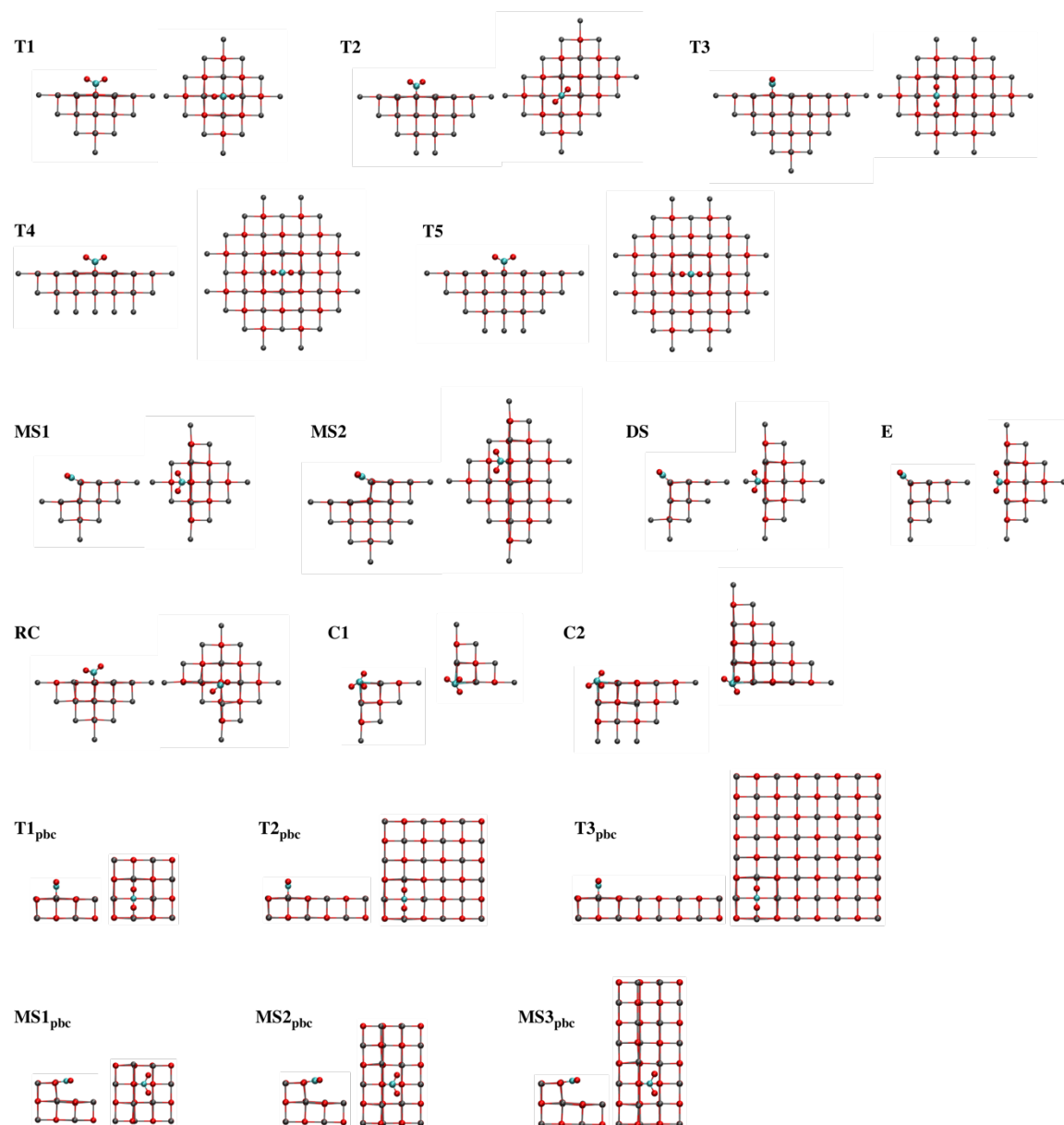


Figure S10. Structures of adsorbed CO₂ on cluster models T1, T2, T3, T4, T5, RC, MS1, MS2, DS, E, C1, and C2 optimized with B3LYP and periodic models T1_{pbc}, T2_{pbc}, T3_{pbc}, MS1_{pbc}, MS2_{pbc}, and MS3_{pbc} optimized with PBE from side (left) and top (right) views. The top views of periodic step models and side views of all periodic models are truncated for clarity.

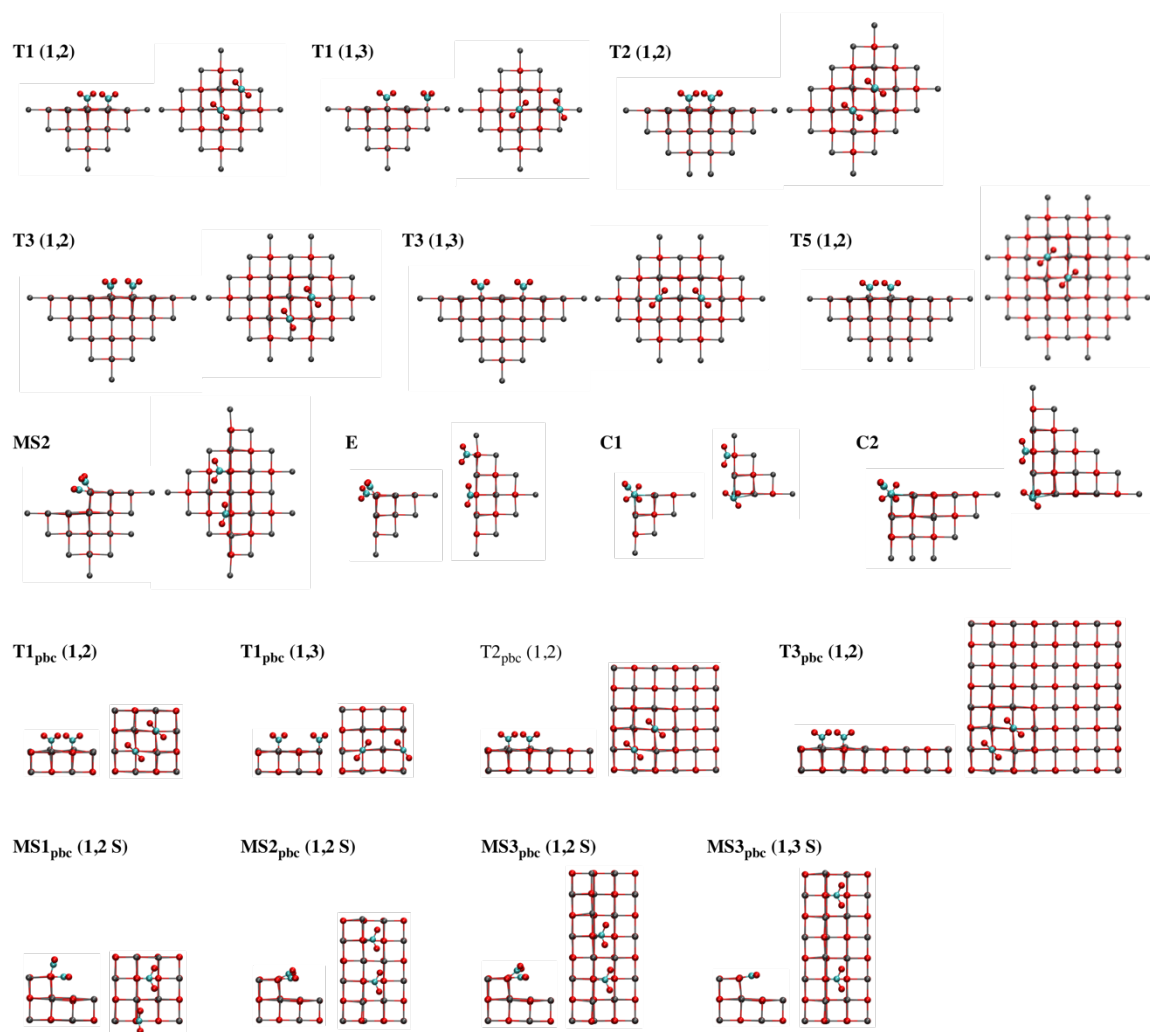


Figure S11. Structures of two adsorbed CO_2 on cluster models T1, T2, T3, MS2, E, C1, and C2 optimized with B3LYP and periodic models T1_{pbc} , T2_{pbc} , T3_{pbc} , MS1_{pbc} , MS2_{pbc} , and MS3_{pbc} optimized with PBE from side (left) and top (right) views. The top views of periodic step models and side views of all periodic models are truncated for clarity.

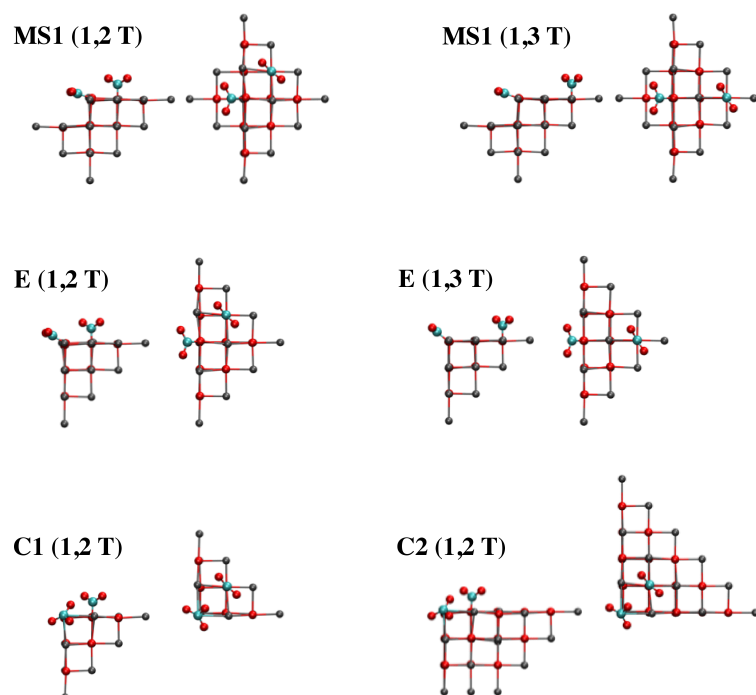


Figure S12. Structures of two adsorbed CO₂ molecules on cluster models MS1, E, C1, and C2 optimized with B3LYP from side (left) and top (right) views, in which one CO₂ binds to a 5-coordinated site in close proximity to a CO₂ bound to a low-coordinated site.

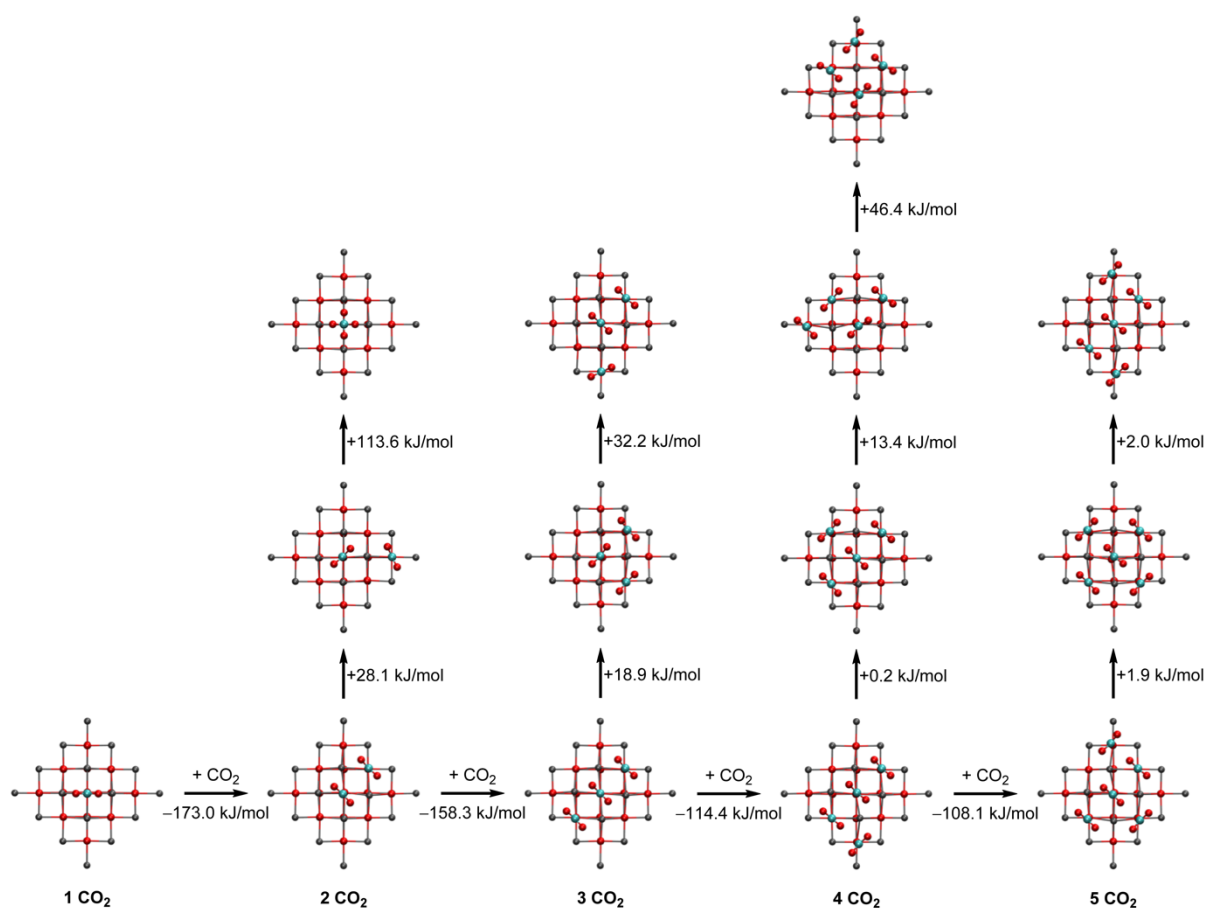


Figure S13. Flowchart of top views of structures for the adsorption of $n\text{CO}_2$ on T1 optimized with B3LYP. Energies are single point DFT+D calculations at the DFT structure. The lowest energy structures (bottom row) are denoted as “A”; the structures in the next row are denoted “B” and so on.

Table S20. Selected bond distances (pm) of adsorption of one or two CO₂ molecules on terrace sites

B3LYP	r_1	r_2	r_3	r_{CC}	r_{11}	r_{21}	r_{31}	r_{12}	r_{22}	r_{32}
T1-nCO ₂	139.1	125.6	125.6	364.2	137.7	125.7	125.7	138.4	125.2	125.2
T2-nCO ₂	137.4	125.8	125.7	363.0	137.7	125.5	125.9	137.7	125.9	125.5
T3-nCO ₂	139.2	125.5	125.5	368.7	137.7	126.0	125.4	138.0	125.1	126.0

PBE	r_1	r_2	r_3	r_{CC}	r_{11}	r_{21}	r_{31}	r_{12}	r_{22}	r_{32}
T1 _{pbc} -nCO ₂	140.5	126.9	126.9	351.8	138.3	127.2	127.2	138.3	127.2	127.2
T2 _{pbc} -nCO ₂	140.7	126.9	126.8	354.4	137.9	127.4	127.4	137.9	127.4	127.4
T3 _{pbc} -nCO ₂	140.7	126.9	126.9	354.2	137.8	127.4	127.4	137.8	127.4	127.4
T1-nCO ₂	140.6	126.5	126.5	363.8	139.2	126.7	126.7	140.0	126.2	126.2
T2-nCO ₂	138.9	126.7	126.8	—	—	—	—	—	—	—
T3-nCO ₂	140.7	126.5	126.5	—	—	—	—	—	—	—

Table S21. Selected bond distances (pm) and angles (degrees) of adsorption of CO₂ on monatomic step (MS1, MS2, MS1_{pbc}, MS2_{pbc}, MS3_{pbc}), diatomic step (DS), and edge (E) sites

B3LYP	r_1	r_2	r_3	θ
MS1-1CO ₂	135.3	126.6	126.6	157.8
MS2-1CO ₂	135.3	126.6	126.6	156.2
DS-1CO ₂	136.5	126.1	126.1	136.0
E-1CO ₂	136.3	126.2	126.2	133.0

PBE	r_1	r_2	r_3	θ
MS1 _{pbc} -1CO ₂	136.2	128.2	128.2	176.0
MS2 _{pbc} -1CO ₂	136.5	128.2	128.3	175.5
MS3 _{pbc} -1CO ₂	136.4	128.2	128.2	174.1
MS1-1CO ₂	136.6	127.6	127.6	163.5
MS2-1CO ₂	136.6	127.6	127.6	163.5
DS-1CO ₂	137.9	127.0	127.0	136.0
E-1CO ₂	137.7	127.1	127.1	132.3

Table S22. Selected bond distances (pm) of adsorption of CO₂ on reverse corner (RC) and corner sites (C1 and C2)

B3LYP	r_1	r_2	r_3
RC-1CO ₂	134.6	129.2	124.4
C1-1CO ₂	129.1	129.4	129.4
C2-1CO ₂	129.3	129.3	129.3

PBE	r_1	r_2	r_3
RC-1CO ₂	136.1	129.9	125.6
C1-1CO ₂	130.2	130.5	130.5

Table S23. Selected bond distances (pm) and angles (degrees) of adsorption of two CO₂ molecules on monatomic step (MS2), edge (E), and corner sites (C1 and C2)

B3LYP	r_{11}	r_{21}	r_{31}	r_{12}	r_{22}	r_{32}	θ_1	θ_2
MS2-2CO ₂	136.9	125.8	126.2	136.7	126.6	125.9	120.9	173.2
E-2CO ₂	137.7	125.8	125.7	138.1	124.6	126.0	118.7	175.1
C1-2CO ₂	129.7	130.0	128.1	138.3	125.3	125.2	–	130.1
C2-2CO ₂	129.8	129.8	128.3	136.2	126.5	126.1	–	132.3

PBE	r_{11}	r_{21}	r_{31}	r_{12}	r_{22}	r_{32}	θ_1	θ_2
MS1 _{pb} c-2CO ₂	140.4	126.7	126.7	138.1	127.7	127.2	107.8	177.7
MS2 _{pb} c-2CO ₂	138.4	126.6	127.9	137.6	128.5	127.0	154.8	178.9
MS3 _{pb} c-2CO ₂	138.3	126.8	127.7	137.3	128.5	127.2	141.8	178.9
MS2-2CO ₂	138.2	126.8	127.0	137.9	127.6	127.0	119.5	175.9
E-2CO ₂	139.0	126.8	126.6	139.3	125.4	127.3	117.5	176.9
C1-2CO ₂	130.8	131.1	129.3	139.7	126.2	126.2	–	126.9

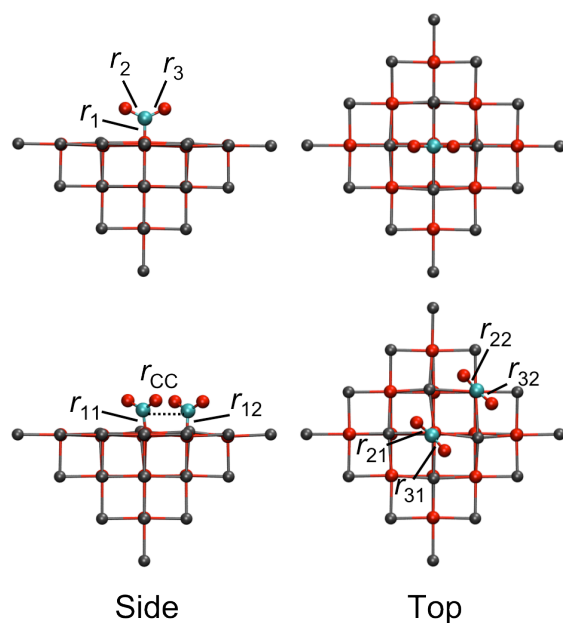


Figure S14. Side (left) and top (right) views of structures for the adsorption of CO₂ on a terrace site (T1) optimized with B3LYP.

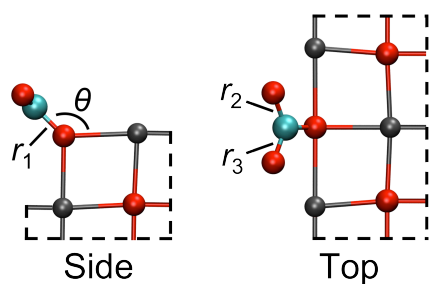


Figure S15. Side (left) and top (right) views of structures for the adsorption of CO₂ on a monatomic step (MS1, MS2), a diatomic step (DS), and an edge (E) site. Dashed lines truncate the clusters for clarity.

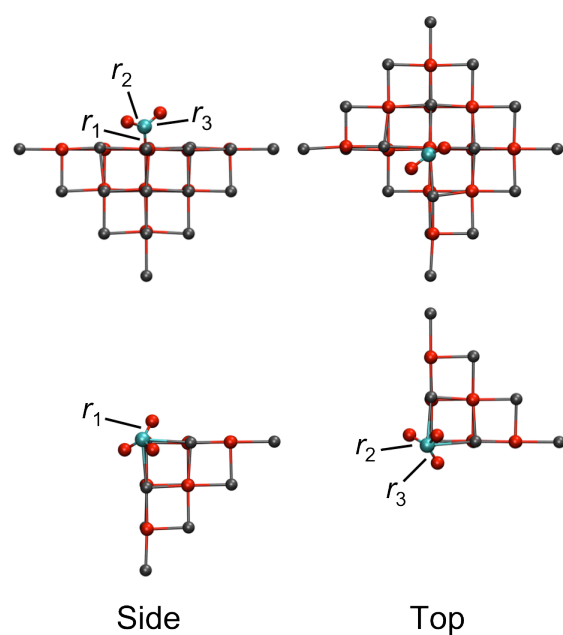


Figure S16. Side (left) and top (right) views of structures for the adsorption of CO₂ on a reverse corner (RC, top) and corner (C1, bottom) optimized with B3LYP.

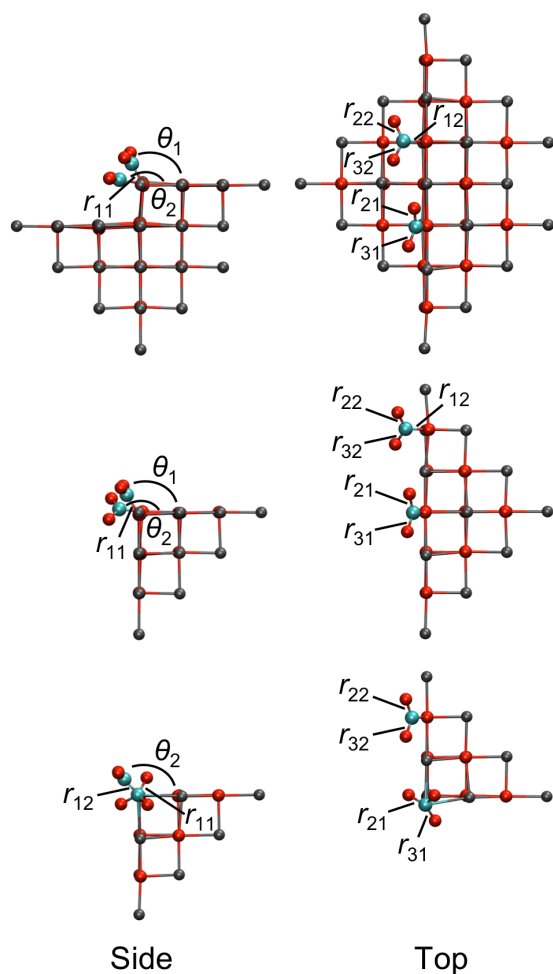


Figure S17. Side (left) and top (right) views of structures for the adsorption of 2CO₂ on a monatomic step (MS2, top), edge (E, middle), and corner (C1, bottom) optimized with B3LYP.

S4.2. Adsorption energies

The calculated energies for adsorbing a second CO₂ molecule to a surface pre-adsorbed with a single CO₂ are given in Table S24. The calculated adsorption energies per CO₂ molecule for adsorption of three or more CO₂ molecules are given in Table S25.

Table S24. Calculated CO₂ adsorption energies, ΔE_{el} (kJ/mol), defined by the reaction $\text{CO}_2 + \text{CO}_2 \cdot \text{CaO} \rightarrow (\text{CO}_2)_2 \cdot \text{CaO}$

Model	B3LYP	B3LYP+D ^a	PBE	PBE+D ^a
T1 _{pbc} -2CO ₂ (1,2)	—	—	−132.4	−148.5
T1 _{pbc} -2CO ₂ (1,3)	—	—	−93.8	−108.3
T2 _{pbc} -2CO ₂ (1,2)	—	—	−144.3	−161.2
T3 _{pbc} -2CO ₂ (1,2)	—	—	−146.7	−162.5
MS1 _{pbc} -2CO ₂ (1,2 S) ^b	—	—	−153.6	−164.4
MS2 _{pbc} -2CO ₂ (1,2 S) ^b	—	—	−191.0	−206.1
MS3 _{pbc} -2CO ₂ (1,2 S) ^b	—	—	−197.4	−211.0
MS3 _{pbc} -2CO ₂ (1,3 S) ^b	—	—	−243.9	−262.1
T1-2CO ₂ (phys) ^c	−20.6	−31.3	−22.5	−30.3
T1-2CO ₂ (1,2)	−154.4	−173.0	−164.2	−177.6
T1-2CO ₂ (1,3)	−128.8	−144.9	−140.6	−152.1
T2-2CO ₂ (1,2)	−137.8	−158.3	−142.0	−157.0
T3-2CO ₂ (1,2)	−157.3	−179.5	—	—
T3-2CO ₂ (1,3)	−116.1	−134.5	—	—
T5-2CO ₂ (1,2)	−141.6	−162.2	—	—
MS2-2CO ₂ (1,2 S) ^b	−213.3	−233.0	−210.8	−223.9
E-2CO ₂	−179.6	−191.9	−184.8	−193.5
MS1-2CO ₂ (1,2 T) ^d	−141.6	−159.8	−150.5	−163.3
MS1-2CO ₂ (1,3 T) ^d	−152.1	−171.4	−165.6	−179.3
E-2CO ₂ (1,2 T) ^d	−143.3	−160.8	−151.2	−163.7
E-2CO ₂ (1,3 T) ^d	−149.0	−165.6	−161.5	−173.4
C1-2CO ₂	−234.5	−244.5	−235.5	−242.7
C2-2CO ₂	−240.3	−250.7	—	—
C1-2CO ₂ (1,2 T) ^d	−144.5	−163.1	−149.1	−162.3
C2-2CO ₂ (1,2 T) ^d	−155.2	−175.3	—	—

^a DFT+D single point calculation at the DFT structure.

^b The “S” indicates adsorption at the nearest (1,2) or next nearest (1,3) 4-coordinated (“step”) surface oxygen atom.

^c Basis set superposition error (BSSE) is not included; however, BSSE was calculated to be 2.6 kJ/mol for the physisorbed structure with B3LYP using the counterpoise correction method.

^d The “T” indicates adsorption at the nearest (1,2) or next nearest (1,3) 5-coordinated (“terrace”) surface oxygen atom.

Table S25. Calculated adsorption energies per adsorbed CO₂, $\Delta E_{\text{el}}/n$ (kJ/mol), defined by the reaction $n\text{CO}_2 + \text{CaO} \rightarrow (\text{CO}_2)_n \bullet \text{CaO}^a$

Model	B3LYP	B3LYP+D ^b	PBE	PBE+D ^a
T1 _{pbc} -3CO ₂ (A)	—	—	−88.5	−105.9
T1 _{pbc} -3CO ₂ (B)	—	—	−71.7	−89.2
T2 _{pbc} -3CO ₂	—	—	−129.2	−146.1
T3 _{pbc} -3CO ₂	—	—	−137.6	−155.0
T1 _{pbc} -4CO ₂	—	—	−61.1	−83.2
T2 _{pbc} -4CO ₂	—	—	−116.9	−133.5
T3 _{pbc} -4CO ₂	—	—	−132.9	−150.3
T2 _{pbc} -5CO ₂	—	—	−104.7	−121.7
T2 _{pbc} -6CO ₂	—	—	−95.7	−116.5
T3 _{pbc} -8CO ₂	—	—	−128.9	−145.1
MS2 _{pbc} -3CO ₂	—	—	−195.8	−212.9
MS3 _{pbc} -3CO ₂	—	—	−217.5	−234.6
MS3 _{pbc} -4CO ₂	—	—	−199.6	−215.5
T1-3CO ₂ (A)	−148.4	−167.7	−156.0	−169.9
T1-3CO ₂ (B)	−142.4	−161.4	−150.1	−163.8
T1-3CO ₂ (C)	−141.5	−160.0	−149.7	−163.1
T2-3CO ₂ (A)	−143.6	−163.6	—	—
T5-3CO ₂ (A)	−135.1	−156.9	—	—
T1-4CO ₂ (A)	−135.4	−154.4	−143.6	−157.3
T1-4CO ₂ (B)	−136.0	−154.4	−144.4	−157.7
T1-4CO ₂ (C)	−132.3	−151.0	−140.5	−154.1
T1-4CO ₂ (D)	−119.3	−139.4	−127.7	−142.3
T2-4CO ₂ (A)	−134.0	−153.8	—	—
T1-5CO ₂ (A)	−126.8	−145.2	−135.6	−149.0
T1-5CO ₂ (B)	−127.0	−144.9	−135.9	−149.0
T1-5CO ₂ (C)	−125.5	−144.4	−134.4	−148.1

^a Global minima are specified by structure A, while local minima are denoted B, C, and D, in increasing DFT+D energy as calculated by B3LYP.

^b DFT+D single point calculation at the DFT structure.

S4.3. Frequencies

The calculated scaled, surface-corrected frequencies and intensities of a single adsorbed CO₂ molecule are given in Table S26. The calculated scaled, surface-corrected B3LYP frequencies and intensities of two adsorbed CO₂ molecules are given in Table S27. The calculated surface-corrected PBE frequencies and intensities of two adsorbed CO₂ molecules are given in Table S28. The calculated scaled, surface-corrected B3LYP frequencies and intensities of three or more adsorbed CO₂ molecules with cluster models are given in Table S29. The calculated surface-corrected PBE frequencies and intensities of three or more adsorbed CO₂ molecules with cluster models are given in Table S30. Calculated PBE frequencies of three or more adsorbed CO₂ molecules on periodic terrace models are given in Table S31. Calculated PBE frequencies of three or four adsorbed CO₂ molecules on periodic step models are given in Table S32.

Table S26. Calculated scaled, surface-corrected frequencies (cm⁻¹) and intensities (km/mol) of CO₂•CaO

B3LYP	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
T1-1CO ₂	665 (0)	685 (1)	842 (0)	922 (200)	1274 (284)	1615 (0)
T2-1CO ₂	675 (1)	679 (0)	858 (0)	961 (153)	1281 (281)	1611 (1)
T3-1CO ₂	666 (0)	684 (1)	842 (0)	920 (196)	1273 (278)	1615 (0)
MS1-1CO ₂	678 (0)	695 (0)	843 (22)	1006 (20)	1294 (90)	1561 (0)
MS2-1CO ₂	676 (0)	696 (0)	842 (20)	1007 (22)	1293 (98)	1561 (1)
DS-1CO ₂	674 (0)	700 (0)	844 (10)	987 (90)	1290 (229)	1591 (0)
E-1CO ₂	676 (0)	699 (0)	845 (9)	989 (90)	1292 (253)	1587 (0)
RC-1CO ₂	673 (0)	687 (1)	868 (1)	1014 (75)	1271 (274)	1584 (97)
C1-1CO ₂	681 (0)	684 (4)	875 (9)	1038 (0)	1418 (342)	1407 (0)
C2-1CO ₂	680 (0)	680 (2)	875 (9)	1037 (0)	1408 (188)	1410 (30)
PBE	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
T1 _{pbc} -1CO ₂	648	673	810	903	1255	1617
T1 _{pbc} -1CO ₂ ^a	646	672	809	901	1254	1616
T2 _{pbc} -1CO ₂ ^a	644	672	808	897	1251	1617
T3 _{pbc} -1CO ₂ ^a	644	673	808	899	1252	1616
T1-1CO ₂	647 (0)	670 (2)	813 (0)	892 (194)	1249 (242)	1607 (0)
T2-1CO ₂	660 (1)	662 (0)	829 (0)	930 (147)	1254 (236)	1601 (1)
T3-1CO ₂	649 (0)	668 (2)	814 (0)	889 (188)	1248 (235)	1607 (0)
MS1 _{pbc} -1CO ₂ ^a	662	669	805	992	1265	1528
MS2 _{pbc} -1CO ₂ ^a	658	670	806	991	1262	1532
MS3 _{pbc} -1CO ₂ ^a	658	671	806	992	1262	1533
MS1-1CO ₂	662 (0)	680 (0)	814 (16)	983 (12)	1267 (54)	1549 (0)
MS2-1CO ₂	660 (0)	680 (0)	814 (14)	983 (13)	1266 (52)	1548 (1)
DS-1CO ₂	657 (0)	686 (0)	819 (6)	960 (95)	1266 (204)	1587 (0)
E-1CO ₂	660 (0)	686 (0)	820 (5)	964 (94)	1268 (229)	1582 (0)
RC-1CO ₂	659 (0)	670 (1)	838 (0)	989 (82)	1244 (250)	1571 (68)
C1-1CO ₂	667 (0)	670 (4)	849 (5)	1018 (0)	1399 (300)	1387 (0)

^a Calculated frequencies with finite differences of only surface carbonate atoms.

Table S27. Calculated scaled, surface-corrected B3LYP frequencies (cm^{-1}) and intensities (km/mol) of $(\text{CO}_2)_2 \cdot \text{CaO}$

	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
T1-2CO ₂ (1,2)	675 (0) 685 (1)	678 (0) 685 (0)	858 (1) 870 (2)	946 (7) 962 (316)	1274 (45) 1300 (548)	1612 (0) 1663 (0)
T2-2CO ₂ (1,2)	674 (0) 675 (0)	677 (1) 679 (0)	855 (0) 863 (0)	948 (0) 963 (281)	1270 (0) 1291 (546)	1601 (1) 1629 (0)
T3-2CO ₂ (1,2)	675 (0) 677 (0)	687 (1) 679 (0)	854 (0) 860 (0)	947 (0) 962 (299)	1272 (12) 1293 (563)	1608 (6) 1638 (16)
T1-2CO ₂ (phys)	668 (0) 634 (105)	691 (1) 662 (0)	843 (0)	946 (187)	1285 (351) 1342 (2)	1601 (0) 2354 (0)
T1-2CO ₂ (1,3)	672 (1) 684 (0)	687 (0) 692 (9)	854 (2) 856 (6)	890 (221) 931 (230)	1276 (135) 1294 (417)	1636 (0) 1714 (5)
T3-2CO ₂ (1,3)	672 (0) 672 (1)	680 (0) 684 (0)	855 (0) 857 (0)	935 (0) 941 (340)	1274 (0) 1282 (524)	1622 (0) 1639 (3)
MS2-2CO ₂	674 (0) 679 (0)	692 (0) 701 (0)	836 (23) 842 (5)	974 (61) 978 (78)	1277 (1) 1290 (327)	1577 (5) 1603 (1)
E-2CO ₂	680 (0) 687 (3)	699 (3) 703 (0)	838 (4) 867 (14)	962 (149) 972 (16)	1285 (286) 1301 (17)	1615 (7) 1664 (238)
C1-2CO ₂	682 (2) 686 (3)	690 (1) 711 (0)	879 (8) 844 (12)	1039 (0) 975 (102)	1389 (218) 1310 (208)	1446 (120) 1660 (20)
C2-2CO ₂	680 (1) 675 (0)	685 (2) 701 (0)	877 (8) 843 (6)	1038 (0) 988 (106)	1390 (158) 1295 (315)	1437 (61) 1584 (1)

Table S28. Calculated surface-corrected PBE frequencies (cm^{-1}) and intensities (km/mol) of $(\text{CO}_2)_2 \bullet \text{CaO}$

	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
$\text{T1}_{\text{pbc}}\text{-2CO}_2$ (1,2) ^a	658 660	662 665	828 834	948 961	1249 1271	1594 1610
$\text{T1}_{\text{pbc}}\text{-2CO}_2$ (1,3) ^a	660 661	665 671	821 824	911 923	1250 1263	1625 1651
T1-2CO_2 (1,2)	660 (0) 661 (1)	668 (0) 671 (2)	830 (0) 845 (3)	915 (5) 932 (313)	1248 (48) 1273 (467)	1601 (0) 1653 (0)
T1-2CO_2 (phys)	651 (0) 602 (103)	678 (1) 636 (0)	815 (0)	921 (184)	1260 (306) 1318 (4)	1589 (0) 2350 (0)
T1-2CO_2 (1,3)	657 (2) 667 (0)	671 (0) 677 (14)	824 (0) 830 (11)	858 (207) 899 (226)	1249 (129) 1269 (349)	1626 (0) 1708 (6)
$\text{T2}_{\text{pbc}}\text{-2CO}_2$ (1,2) ^a	659 660	660 664	824 830	959 969	1251 1271	1582 1605
$\text{T3}_{\text{pbc}}\text{-2CO}_2$ (1,2) ^a	659 660	661 664	824 830	963 973	1252 1272	1581 1605
T2-2CO_2 (1,2)	657 (0) 660 (0)	662 (2) 662 (0)	828 (0) 834 (0)	918 (0) 934 (272)	1243 (0) 1263 (465)	1591 (0) 1618 (0)
$\text{MS1}_{\text{pbc}}\text{-2CO}_2$ ^a	661 663	679 681	795 798	905 949	1255 1262	1562 1635
$\text{MS2}_{\text{pbc}}\text{-2CO}_2$ ^a	657 663	674 688	801 802	954 965	1255 1265	1560 1604
$\text{MS3}_{\text{pbc}}\text{-2CO}_2$ (1,2 S) ^{a,b}	656 660	672 689	802 804	957 971	1256 1266	1553 1602
$\text{MS3}_{\text{pbc}}\text{-2CO}_2$ (1,3 S) ^{a,b}	660 661	673 673	804 804	985 986	1261 1263	1541 1548
MS2-2CO_2	659 (0) 664 (0)	675 (0) 687 (0)	806 (16) 816 (2)	950 (99) 954 (40)	1254 (1) 1266 (291)	1564 (4) 1595 (1)
E-2CO_2	665 (0) 674 (2)	686 (4) 689 (0)	814 (2) 849 (8)	937 (159) 952 (7)	1263 (262) 1278 (8)	1609 (4) 1655 (232)
C1-2CO_2	668 (1) 673 (4)	676 (0) 700 (0)	854 (5) 821 (8)	1019 (0) 952 (109)	1369 (187) 1289 (200)	1426 (111) 1655 (24)

^a Calculated frequencies with finite differences of only surface carbonate atoms.

^b The “S” indicates adsorption at the nearest (1,2) or next nearest (1,3) 4-coordinated (“step”) surface oxygen atom.

Table S29. Calculated scaled, surface-corrected B3LYP frequencies (cm^{-1}) and intensities (km/mol) of $(\text{CO}_2)_n \bullet \text{CaO}$ with cluster models

	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
T1-3CO ₂ (A)	678 (0)	679 (0)	858 (0)	931 (244)	1272 (0)	1609 (0)
	682 (0)	685 (0)	867 (9)	933 (0)	1289 (0)	1671 (0)
	684 (0)	685 (3)	869 (0)	973 (248)	1302 (881)	1683 (0)
T1-3CO ₂ (B)	674 (6)	684 (0)	857 (15)	887 (162)	1282 (23)	1609 (2)
	678 (1)	690 (0)	863 (3)	938 (150)	1284 (22)	1677 (1)
	681 (1)	694 (3)	870 (2)	988 (187)	1306 (799)	1713 (7)
T1-3CO ₂ (C)	673 (0)	685 (1)	853 (12)	877 (241)	1272 (17)	1632 (0)
	682 (0)	687 (1)	858 (2)	931 (0)	1290 (59)	1676 (0)
	683 (0)	691 (12)	869 (3)	949 (384)	1298 (763)	1723 (4)
T2-3CO ₂ (A)	674 (0)	680 (0)	855 (1)	937 (155)	1269 (23)	1601 (0)
	675 (0)	681 (0)	863 (1)	941 (59)	1283 (37)	1633 (0)
	680 (0)	685 (0)	869 (3)	978 (240)	1301 (772)	1674 (0)
T1-4CO ₂ (A)	668 (15)	686 (0)	847 (177)	874 (2)	1272 (1)	1620 (0)
	675 (0)	691 (0)	858 (10)	916 (142)	1282 (79)	1669 (1)
	681 (0)	691 (3)	861 (28)	960 (117)	1292 (268)	1693 (0)
	684 (3)	697 (1)	867 (11)	990 (259)	1316 (744)	1751 (33)
T1-4CO ₂ (B)	677 (2)	686 (0)	857 (9)	883 (134)	1279 (58)	1599 (2)
	677 (0)	687 (0)	862 (0)	920 (1)	1285 (30)	1683 (0)
	679 (7)	691 (3)	866 (11)	921 (388)	1287 (0)	1694 (4)
	682 (0)	693 (0)	871 (0)	1009 (162)	1311 (1033)	1722 (0)
T1-4CO ₂ (C)	668 (13)	691 (0)	852 (45)	875 (7)	1278 (34)	1625 (5)
	673 (8)	692 (6)	853 (116)	880 (172)	1282 (33)	1670 (0)
	677 (2)	694 (0)	861 (1)	968 (88)	1288 (265)	1720 (10)
	699 (1)	699 (1)	865 (69)	993 (237)	1319 (708)	1746 (37)
T1-4CO ₂ (D)	665 (0)	689 (1)	843 (19)	868 (45)	1275 (26)	1650 (3)
	667 (3)	691 (0)	852 (0)	899 (98)	1283 (63)	1705 (52)
	669 (3)	695 (3)	858 (20)	911 (161)	1287 (44)	1716 (17)
	676 (2)	701 (10)	862 (10)	937 (429)	1299 (774)	1752 (38)
T2-4CO ₂ (A)	675 (0)	682 (0)	854 (0)	924 (0)	1267 (0)	1604 (0)
	678 (0)	683 (0)	862 (5)	925 (268)	1279 (4)	1633 (0)
	679 (0)	685 (1)	866 (0)	959 (0)	1292 (0)	1680 (1)
	681 (0)	685 (4)	868 (6)	974 (385)	1302 (1107)	1686 (0)
T1-5CO ₂ (A)	665 (19)	688 (0)	839 (198)	875 (5)	1280 (151)	1611 (4)
	676 (2)	691 (2)	856 (17)	878 (139)	1281 (7)	1677 (0)
	679 (8)	692 (0)	859 (13)	905 (222)	1285 (28)	1704 (3)
	682 (2)	694 (2)	862 (2)	979 (94)	1298 (128)	1727 (0)
	688 (4)	697 (1)	869 (5)	1002 (229)	1320 (996)	1757 (37)
T1-5CO ₂ (B)	680 (10)	687 (0)	856 (0)	884 (0)	1284 (1)	1584 (0)
	680 (0)	690 (2)	858 (14)	885 (253)	1287 (0)	1679 (0)
	683 (7)	691 (0)	864 (4)	910 (273)	1290 (248)	1702 (0)
	685 (0)	692 (0)	870 (5)	940 (211)	1292 (237)	1722 (0)
	685 (2)	695 (0)	876 (1)	1039 (94)	1336 (868)	1725 (0)
T1-5CO ₂ (C)	665 (0)	690 (0)	835 (0)	869 (7)	1272 (4)	1634 (0)
	665 (40)	690 (8)	836 (420)	872 (0)	1281 (0)	1679 (3)
	679 (0)	691 (0)	857 (0)	943 (19)	1282 (216)	1693 (0)
	681 (0)	697 (0)	857 (16)	970 (0)	1306 (0)	1759 (1)
	688 (3)	698 (4)	861 (0)	976 (531)	1315 (1060)	1759 (66)

Table S30. Calculated surface-corrected PBE frequencies (cm^{-1}) and intensities (km/mol) of $(\text{CO}_2)_n \bullet \text{CaO}$ with cluster models

	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
T1-3CO ₂ (A)	660 (0)	664 (0)	832 (0)	899 (222)	1245 (2)	1602 (0)
	665 (0)	670 (0)	842 (12)	901 (0)	1264 (0)	1663 (0)
	667 (0)	671 (7)	843 (0)	941 (288)	1275 (764)	1674 (0)
T1-3CO ₂ (B)	658 (8)	670 (1)	828 (18)	855 (148)	1256 (1)	1599 (2)
	660 (1)	674 (1)	835 (2)	907 (142)	1261 (22)	1668 (0)
	665 (2)	678 (5)	845 (3)	956 (197)	1279 (711)	1705 (6)
T1-3CO ₂ (C)	657 (1)	669 (0)	827 (21)	846 (218)	1246 (23)	1623 (0)
	665 (0)	672 (3)	830 (3)	897 (5)	1266 (20)	1666 (0)
	667 (0)	676 (19)	843 (2)	917 (375)	1273 (687)	1717 (5)
T1-4CO ₂ (A)	650 (22)	670 (2)	813 (193)	846 (2)	1245 (6)	1613 (0)
	659 (1)	672 (0)	831 (7)	884 (125)	1261 (54)	1661 (0)
	664 (0)	674 (8)	833 (0)	925 (111)	1267 (222)	1684 (0)
	668 (2)	683 (2)	842 (10)	955 (287)	1288 (666)	1748 (30)
T1-4CO ₂ (B)	660 (3)	670 (0)	827 (15)	847 (128)	1253 (25)	1589 (2)
	661 (0)	672 (0)	836 (0)	888 (0)	1262 (11)	1676 (0)
	663 (10)	676 (7)	842 (9)	889 (366)	1263 (0)	1686 (3)
	665 (2)	676 (0)	843 (0)	976 (176)	1283 (938)	1716 (0)
T1-4CO ₂ (C)	650 (20)	674 (1)	818 (173)	846 (156)	1255 (1)	1616 (4)
	656 (10)	675 (9)	825 (38)	849 (0)	1261 (31)	1664 (0)
	661 (3)	677 (0)	832 (0)	932 (69)	1264 (231)	1713 (8)
	669 (2)	684 (2)	834 (15)	958 (268)	1291 (644)	1744 (34)
T1-4CO ₂ (D)	647 (1)	673 (1)	810 (32)	836 (11)	1252 (39)	1640 (1)
	650 (5)	675 (0)	819 (1)	865 (93)	1261 (73)	1699 (50)
	652 (3)	679 (7)	828 (14)	877 (142)	1266 (11)	1708 (13)
	659 (3)	685 (15)	831 (36)	906 (430)	1276 (660)	1749 (32)
T1-5CO ₂ (A)	646 (26)	672 (2)	806 (190)	841 (86)	1255 (31)	1603 (4)
	660 (2)	674 (4)	826 (32)	848 (1)	1260 (62)	1672 (0)
	662 (14)	675 (0)	830 (3)	872 (198)	1262 (1)	1696 (2)
	664 (2)	676 (4)	835 (6)	941 (100)	1270 (151)	1722 (0)
	670 (3)	683 (2)	840 (43)	967 (252)	1290 (892)	1754 (33)
T1-5CO ₂ (B)	662 (0)	669 (14)	824 (0)	842 (51)	1258 (13)	1580 (0)
	662 (25)	671 (0)	826 (62)	844 (0)	1263 (214)	1683 (0)
	664 (0)	672 (0)	838 (0)	880 (0)	1263 (0)	1696 (0)
	666 (0)	674 (0)	839 (0)	882 (451)	1264 (0)	1721 (0)
	668 (0)	679 (2)	840 (179)	1006 (128)	1295 (944)	1723 (0)
T1-5CO ₂ (C)	647 (0)	671 (0)	801 (0)	843 (6)	1245 (14)	1625 (0)
	647 (58)	673 (15)	802 (393)	844 (0)	1261 (0)	1671 (1)
	662 (0)	673 (0)	828 (0)	904 (19)	1261 (161)	1684 (0)
	665 (0)	683 (0)	829 (2)	934 (0)	1279 (0)	1757 (0)
	669 (3)	684 (5)	835 (0)	941 (545)	1287 (934)	1757 (60)

Table S31. Calculated PBE frequencies (cm^{-1}) of $(\text{CO}_2)_n \bullet \text{CaO}$ on terraces with periodic boundary conditions ^a

	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
T1 _{pbc} -3CO ₂ (A)	657	663	825	910	1245	1601
	658	663	828	914	1249	1635
	660	665	836	964	1273	1638
T1 _{pbc} -3CO ₂ (B)	660	664	810	895	1245	1600
	661	669	827	915	1252	1633
	662	670	834	980	1280	1661
T2 _{pbc} -3CO ₂	658	662	824	949	1249	1576
	659	663	827	949	1257	1606
	660	665	834	987	1277	1616
T3 _{pbc} -3CO ₂	659	662	823	960	1251	1569
	660	663	826	961	1259	1597
	660	666	833	994	1279	1610
T1 _{pbc} -4CO ₂	658	662	821	891	1236	1622
	660	662	828	903	1247	1652
	661	663	828	903	1247	1652
	661	664	834	927	1271	1665
T2 _{pbc} -4CO ₂	658	662	823	934	1247	1578
	658	663	825	935	1251	1599
	659	664	830	972	1261	1620
	660	666	834	982	1278	1624
T3 _{pbc} -4CO ₂	659	663	823	953	1250	1567
	659	664	825	954	1255	1586
	660	664	830	986	1266	1607
	661	667	835	994	1283	1615
T2 _{pbc} -5CO ₂	658	662	822	921	1243	1584
	658	662	823	923	1246	1598
	659	664	827	956	1254	1618
	659	664	831	961	1262	1632
	661	666	834	971	1275	1634
T2 _{pbc} -6CO ₂	659	663	821	935	1239	1592
	660	663	825	940	1245	1604
	660	664	825	940	1245	1604
	661	664	832	951	1261	1635
	662	665	832	951	1261	1636
	662	666	834	960	1275	1647
T3 _{pbc} -8CO ₂	659	663	821	955	1241	1580
	660	664	824	957	1245	1587
	660	665	824	957	1245	1587
	661	665	829	963	1256	1606
	662	665	829	964	1257	1606
	662	666	833	971	1270	1631
	662	666	833	971	1270	1631
	662	667	834	976	1279	1640

^a Calculated frequencies with finite differences of only surface carbonate atoms.

Table S32. Calculated PBE frequencies (cm^{-1}) of $(\text{CO}_2)_n \bullet \text{CaO}$ on steps with periodic boundary conditions ^a

	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
MS2 _{pbc} -3CO ₂	660	676	793	890	1254	1578
	669	676	794	936	1257	1609
	673	680	797	943	1266	1642
MS3 _{pbc} -3CO ₂	658	670	799	916	1253	1551
	665	671	800	962	1254	1559
	665	683	800	963	1261	1628
MS3 _{pbc} -4CO ₂	660	674	794	899	1251	1567
	662	678	794	901	1253	1578
	664	681	797	941	1258	1637
	667	682	797	942	1260	1640

^a Calculated frequencies with finite differences of only surface carbonate atoms.

The calculated frequencies provided in this work have been corrected for surface selection rules in accordance with experimental IRAS. These effects are demonstrated for select simulated IRA spectra shown in Figure S18. Most noticeable are the changes in intensity for the asymmetric ν_6 mode, which would ordinarily have the greatest measurable intensity. For the ν_4 and ν_5 modes, a significant decrease in intensity is only expected on step sites in which the adsorbed CO_2 is bending toward the surface step layer, which results in a nonzero component of the change in dipole parallel to the $\text{CaO}(001)$ surface.

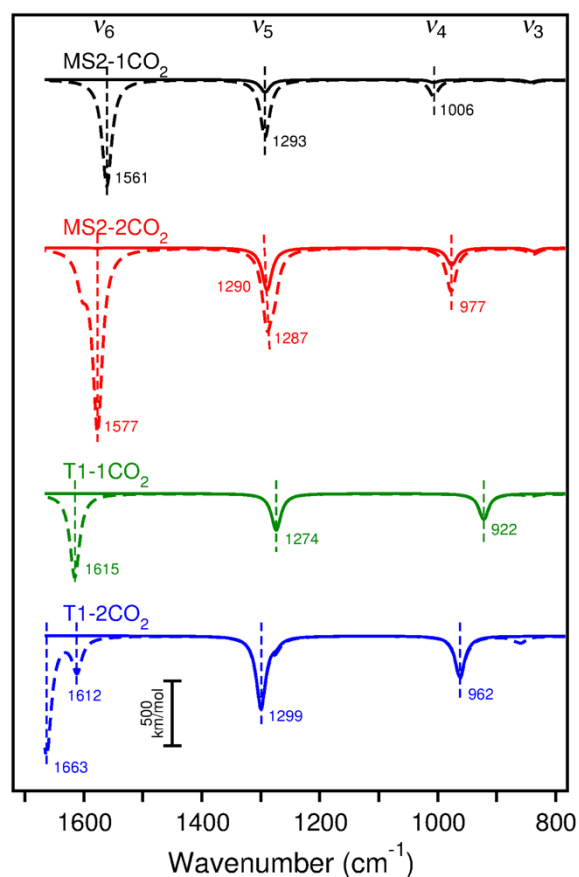


Figure S18. Calculated IRA spectra of one and two CO_2 molecules adsorbed on cluster models MS2 (black and red) and T1 (green and blue) before (dashed lines) and after (solid lines) correction for surface dipole selection rules. Spectra are plotted with Lorentzian broadening of B3LYP frequencies scaled by $\lambda=0.9800$.

S5. References

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S6. Coordinates and Energies of Optimized Structures

S6.1. Cluster models

T1	T1-1CO ₂ (position 1)
O 0.0000000 -0.0000000 0.0032881	O -0.0000001 -0.0000003 0.0287425
O -0.0000000 -0.0000000 4.7851347	O 0.0000194 0.0000090 4.9580942
O -0.0000000 2.4274301 2.4121371	O -0.0000040 2.3978932 2.4275305
O 0.0000000 4.7761813 4.8229830	O 0.0000097 4.7951046 4.8174717
O 0.0000000 -2.4274301 2.4121371	O 0.0000155 -2.3978936 2.4275321
O 0.0000000 -4.7761813 4.8229830	O -0.0000113 -4.7951036 4.8174737
O 2.4274301 0.0000000 2.4121371	O 2.4129226 -0.0000128 2.4356431
O 2.3957144 2.3957144 4.8059373	O 2.4105283 2.3808984 4.7605967
O 2.3957144 -2.3957144 4.8059373	O 2.4104376 -2.3808103 4.7607798
O 4.7761813 -0.0000000 4.8229830	O 4.7873009 0.0000108 4.8123917
O -2.4274301 -0.0000000 2.4121371	O -2.4129203 0.0000104 2.4356408
O -2.3957144 2.3957144 4.8059373	O -2.4104519 2.3808193 4.7607393
O -2.3957144 -2.3957144 4.8059373	O -2.4105394 -2.3809070 4.7605628
O -4.7761813 -0.0000000 4.8229830	O -4.7873044 -0.0000109 4.8123927
Ca 0.0000000 2.4159993 0.0000000	Ca 0.0000000 2.4159979 0.0000000
Ca 0.0000000 -2.4159993 0.0000000	Ca 0.0000000 -2.4159979 0.0000000
Ca 0.0000000 7.2479980 4.8319986	Ca 0.0000000 7.2479940 4.8319958
Ca 0.0000000 -7.2479980 4.8319986	Ca 0.0000000 -7.2479940 4.8319958
Ca 2.4159993 0.0000000 0.0000000	Ca 2.4159979 0.0000000 0.0000000
Ca 2.4159993 4.8319986 4.8319986	Ca 2.4159979 4.8319958 4.8319958
Ca 2.4159993 -4.8319986 4.8319986	Ca 2.4159979 -4.8319958 4.8319958
Ca 4.8319986 2.4159993 4.8319986	Ca 4.8319958 2.4159979 4.8319958
Ca 4.8319986 -2.4159993 4.8319986	Ca 4.8319958 -2.4159979 4.8319958
Ca -2.4159993 0.0000000 0.0000000	Ca -2.4159979 0.0000000 0.0000000
Ca -2.4159993 4.8319986 4.8319986	Ca -2.4159979 4.8319958 4.8319958
Ca -2.4159993 -4.8319986 4.8319986	Ca -2.4159979 -4.8319958 4.8319958
Ca -4.8319986 2.4159993 4.8319986	Ca -4.8319958 2.4159979 4.8319958
Ca -4.8319986 -2.4159993 4.8319986	Ca -4.8319958 -2.4159979 4.8319958
Ca 7.2479980 0.0000000 4.8319986	Ca 7.2479940 0.0000000 4.8319958
Ca -7.2479980 0.0000000 4.8319986	Ca -7.2479940 0.0000000 4.8319958
Ca 0.0000001 -0.0000000 2.4330032	Ca -0.0000055 -0.0000010 2.4156573
Ca 0.0000000 0.0000000 -2.4159993	Ca 0.0000000 0.0000000 -2.4159979
Ca -0.0000000 2.4064839 4.8020348	Ca 0.0000756 2.5160525 4.9197772
Ca 0.0000000 4.8319986 2.4159993	Ca 0.0000000 4.8319958 2.4159979
Ca -0.0000000 -2.4064840 4.8020348	Ca -0.0001087 -2.5160500 4.9197816
Ca 0.0000000 -4.8319986 2.4159993	Ca 0.0000000 -4.8319958 2.4159979
Ca 2.4064840 0.0000000 4.8020348	Ca 2.5233389 0.0001015 4.8139894
Ca 2.4159993 2.4159993 2.4159993	Ca 2.4159979 2.4159979 2.4159979
Ca 2.4159993 -2.4159993 2.4159993	Ca 2.4159979 -2.4159979 2.4159979
Ca 4.8319986 0.0000000 2.4159993	Ca 4.8319958 0.0000000 2.4159979
Ca -2.4064839 0.0000001 4.8020348	Ca -2.5233583 -0.0001001 4.8140002
Ca -2.4159993 2.4159993 2.4159993	Ca -2.4159979 2.4159979 2.4159979
Ca -2.4159993 -2.4159993 2.4159993	Ca -2.4159979 -2.4159979 2.4159979
Ca -4.8319986 0.0000000 2.4159993	Ca -4.8319958 0.0000000 2.4159979
-10600.86796585 Hartrees	O 0.0009262 1.1274436 6.9018078
	O -0.0014674 -1.1274310 6.9018033
	C -0.0001708 0.0000065 6.3493121
	-10789.51314910 Hartrees

T1-2CO₂ (1,2)	T1-2CO₂ (phys)
O 0.0029142 0.0029010 0.0356723	O -0.0000002 0.0000032 0.0302624
O 0.0896144 0.0886132 4.8800072	O 0.0000011 0.0000306 4.9641517
O 0.0372103 2.4014723 2.4709955	O -0.0000062 2.3973870 2.4287046
O -0.0476985 4.7853369 4.7198868	O 0.0000072 4.7940852 4.8165024
O 0.0047989 -2.4070177 2.4464439	O 0.0000101 -2.3973727 2.4287018
O 0.0041607 -4.7851284 4.8161834	O -0.0000083 -4.7940778 4.8164833
O 2.4016253 0.0372683 2.4709941	O 2.4110655 -0.0000030 2.4359648
O 2.4374110 2.4379315 4.8051915	O 2.4080027 2.3798828 4.7603372
O 2.4430417 -2.4400547 4.7348225	O 2.4079402 -2.3798122 4.7604576
O 4.7856083 -0.0475490 4.7197291	O 4.7865920 0.0000089 4.8079508
O -2.4070133 0.0047231 2.4466632	O -2.4110680 0.0000139 2.4359626
O -2.4402982 2.4429511 4.7344937	O -2.4079514 2.3798231 4.7604519
O -2.3665499 -2.3663466 4.7967284	O -2.4080130 -2.3798795 4.7603029
O -4.7850072 0.0042105 4.8162163	O -4.7865967 -0.0000064 4.8079555
Ca 0.0000000 2.4159972 0.0000000	Ca 0.0000000 2.4159972 0.0000000
Ca 0.0000000 -2.4159972 0.0000000	Ca 0.0000000 -2.4159972 0.0000000
Ca 0.0000000 7.2479920 4.8319944	Ca 0.0000000 7.2479920 4.8319944
Ca 0.0000000 -7.2479920 4.8319944	Ca 0.0000000 -7.2479920 4.8319944
Ca 2.4159972 0.0000000 0.0000000	Ca 2.4159972 0.0000000 0.0000000
Ca 2.4159972 4.8319944 4.8319944	Ca 2.4159972 4.8319944 4.8319944
Ca 2.4159972 -4.8319944 4.8319944	Ca 2.4159972 -4.8319944 4.8319944
Ca 4.8319944 2.4159972 4.8319944	Ca 4.8319944 2.4159972 4.8319944
Ca 4.8319944 -2.4159972 4.8319944	Ca 4.8319944 -2.4159972 4.8319944
Ca -2.4159972 0.0000000 0.0000000	Ca -2.4159972 0.0000000 0.0000000
Ca -2.4159972 4.8319944 4.8319944	Ca -2.4159972 4.8319944 4.8319944
Ca -2.4159972 -4.8319944 4.8319944	Ca -2.4159972 -4.8319944 4.8319944
Ca -4.8319944 2.4159972 4.8319944	Ca -4.8319944 2.4159972 4.8319944
Ca -4.8319944 -2.4159972 4.8319944	Ca -4.8319944 -2.4159972 4.8319944
Ca 7.2479920 0.0000000 4.8319944	Ca 7.2479920 0.0000000 4.8319944
Ca -7.2479920 0.0000000 4.8319944	Ca -7.2479920 0.0000000 4.8319944
Ca 0.0115021 0.0113698 2.4381964	Ca -0.0000029 0.0000122 2.4119436
Ca 0.0000000 0.0000000 -2.4159972	Ca 0.0000000 0.0000000 -2.4159972
Ca -0.2033860 2.5771999 4.9944583	Ca 0.0000561 2.5194527 4.9156791
Ca 0.0000000 4.8319944 2.4159972	Ca 0.0000000 4.8319944 2.4159972
Ca 0.0398488 -2.5322402 4.8829461	Ca -0.0000752 -2.5194379 4.9156353
Ca 0.0000000 -4.8319944 2.4159972	Ca 0.0000000 -4.8319944 2.4159972
Ca 2.5775709 -0.2031187 4.9944551	Ca 2.5283711 0.0000756 4.8138841
Ca 2.4159972 2.4159972 2.4159972	Ca 2.4159972 2.4159972 2.4159972
Ca 2.4159972 -2.4159972 2.4159972	Ca 2.4159972 -2.4159972 2.4159972
Ca 4.8319944 0.0000000 2.4159972	Ca 4.8319944 0.0000000 2.4159972
Ca -2.5322148 0.0399448 4.8826008	Ca -2.5283855 -0.0000656 4.8138816
Ca -2.4159972 2.4159972 2.4159972	Ca -2.4159972 2.4159972 2.4159972
Ca -2.4159972 -2.4159972 2.4159972	Ca -2.4159972 -2.4159972 2.4159972
Ca -4.8319944 0.0000000 2.4159972	Ca -4.8319944 0.0000000 2.4159972
O -0.9393391 0.6646953 6.7719780	O 0.0006199 1.1251123 6.9065958
O 0.6588555 -0.9427205 6.7729422	O -0.0009485 -1.1251334 6.9065432
C -0.0682241 -0.0678147 6.2387375	C -0.0001096 0.0000030 6.3443249
O 1.7573096 3.3595350 6.7130846	C 0.0006542 -0.0002427 9.5856282
O 3.3562105 1.7529128 6.7125059	O 1.1601155 0.0012261 9.6360488
C 2.5071252 2.5071012 6.1859002	O -1.1587647 -0.0017149 9.6369769
-10978.15927907 Hartrees	-10978.10831401 Hartrees

T1-2CO₂ (1,3)	T1-3CO₂ (A)
O 0.0035444 -0.0009983 0.0352124	O 0.0000194 0.0000117 0.0450811
O -0.0437370 -0.0176885 4.8505310	O 0.0000978 0.0002022 4.8583695
O -0.0104940 2.3985910 2.4278957	O 0.0303167 2.3999689 2.4834233
O -0.0021358 4.7900469 4.8105828	O -0.0469028 4.7809684 4.7172542
O 0.0098465 -2.4017463 2.4341506	O -0.0303140 -2.3999152 2.4833854
O -0.0026004 -4.7754736 4.8127455	O 0.0469045 -4.7810211 4.7172258
O 2.4617154 0.0007767 2.4668521	O 2.3999550 0.0302937 2.4833757
O 2.3935454 2.4082059 4.6569660	O 2.4197784 2.4198741 4.8126680
O 2.3795148 -2.3052803 4.7898889	O 2.4518941 -2.4519558 4.7524010
O 4.8263153 0.0367164 4.7949230	O 4.7809942 -0.0469073 4.7172039
O -2.4062598 0.0012394 2.4279618	O -2.3999179 -0.0303125 2.4833866
O -2.3757890 2.3773247 4.7963405	O -2.4519592 2.4519310 4.7523408
O -2.4207620 -2.4283213 4.7107042	O -2.4198698 -2.4197265 4.8127812
O -4.7941441 -0.0069522 4.8131664	O -4.7810013 0.0469178 4.7172443
Ca 0.0000000 2.4159972 0.0000000	Ca 0.0000000 2.4159972 0.0000000
Ca 0.0000000 -2.4159972 0.0000000	Ca 0.0000000 -2.4159972 0.0000000
Ca 0.0000000 7.2479920 4.8319944	Ca 0.0000000 7.2479920 4.8319944
Ca 0.0000000 -7.2479920 4.8319944	Ca 0.0000000 -7.2479920 4.8319944
Ca 2.4159972 0.0000000 0.0000000	Ca 2.4159972 0.0000000 0.0000000
Ca 2.4159972 4.8319944 4.8319944	Ca 2.4159972 4.8319944 4.8319944
Ca 2.4159972 -4.8319944 4.8319944	Ca 2.4159972 -4.8319944 4.8319944
Ca 4.8319944 2.4159972 4.8319944	Ca 4.8319944 2.4159972 4.8319944
Ca 4.8319944 -2.4159972 4.8319944	Ca 4.8319944 -2.4159972 4.8319944
Ca -2.4159972 0.0000000 0.0000000	Ca -2.4159972 0.0000000 0.0000000
Ca -2.4159972 4.8319944 4.8319944	Ca -2.4159972 4.8319944 4.8319944
Ca -2.4159972 -4.8319944 4.8319944	Ca -2.4159972 -4.8319944 4.8319944
Ca -4.8319944 2.4159972 4.8319944	Ca -4.8319944 2.4159972 4.8319944
Ca -4.8319944 -2.4159972 4.8319944	Ca -4.8319944 -2.4159972 4.8319944
Ca 7.2479920 0.0000000 4.8319944	Ca 7.2479920 0.0000000 4.8319944
Ca -7.2479920 0.0000000 4.8319944	Ca -7.2479920 0.0000000 4.8319944
Ca -0.0210771 0.0043056 2.3998485	Ca 0.0000174 0.0000096 2.4598241
Ca 0.0000000 0.0000000 -2.4159972	Ca 0.0000000 0.0000000 -2.4159972
Ca 0.0170164 2.5439910 4.8661251	Ca -0.1855197 2.5907461 4.9961849
Ca 0.0000000 4.8319944 2.4159972	Ca 0.0000000 4.8319944 2.4159972
Ca -0.0679150 -2.5116984 4.8616855	Ca 0.1854078 -2.5907991 4.9963636
Ca 0.0000000 -4.8319944 2.4159972	Ca 0.0000000 -4.8319944 2.4159972
Ca 2.3381144 0.1350741 4.9369713	Ca 2.5907208 -0.1854267 4.9962447
Ca 2.4159972 2.4159972 2.4159972	Ca 2.4159972 2.4159972 2.4159972
Ca 2.4159972 -2.4159972 2.4159972	Ca 2.4159972 -2.4159972 2.4159972
Ca 4.8319944 0.0000000 2.4159972	Ca 4.8319944 0.0000000 2.4159972
Ca -2.5425142 -0.0529025 4.8727046	Ca -2.5907946 0.1854390 4.9962058
Ca -2.4159972 2.4159972 2.4159972	Ca -2.4159972 2.4159972 2.4159972
Ca -2.4159972 -2.4159972 2.4159972	Ca -2.4159972 -2.4159972 2.4159972
Ca -4.8319944 0.0000000 2.4159972	Ca -4.8319944 0.0000000 2.4159972
O 0.6845747 0.8781793 6.7531988	O -0.8028017 0.8016930 6.7724311
O -0.9679740 -0.6730182 6.7797241	O 0.8019141 -0.8021899 6.7725219
C -0.1179157 0.0640940 6.2328963	C -0.0002629 -0.0001094 6.2309935
O 4.3986772 1.0705492 6.7349694	O 1.7890470 3.3919633 6.7149765
O 5.3714062 -0.9729338 6.7141727	O 3.3917432 1.7884436 6.7147834
C 4.8610532 0.0416420 6.2095394	C 2.5258063 2.5257178 6.1974485
-10978.14955045 Hartrees	O -1.7886909 -3.3918473 6.7149156
	O -3.3922592 -1.7891909 6.7150229
	C -2.5259127 -2.5258729 6.1975751
	-11166.79954052 Hartrees

T1-3CO₂ (B)	T1-3CO₂ (C)
O 0.0049711 0.0008360 0.0436766	O 0.0022022 -0.0004984 0.0460877
O 0.1478620 -0.0851295 4.8604607	O 0.0572785 0.0983857 4.8531930
O 0.0471066 2.4009092 2.4867755	O 0.0357372 2.3991636 2.4653486
O -0.0401543 4.7750432 4.7162381	O -0.0483097 4.7886865 4.7147217
O 0.0464577 -2.3999420 2.4772173	O 0.0092962 -2.4607108 2.4784217
O -0.0481773 -4.7751589 4.7199014	O 0.0342252 -4.8182321 4.7929215
O 2.4080118 0.0078637 2.4627230	O 2.3916857 0.0441642 2.4644515
O 2.4509960 2.4958977 4.8673152	O 2.4328658 2.4298010 4.8060973
O 2.4255536 -2.4515378 4.8491330	O 2.4200545 -2.4044803 4.6731282
O 4.7815019 0.0033292 4.6686017	O 4.7880234 -0.0401395 4.7152636
O -2.4025836 0.0054929 2.4590960	O -2.3974750 -0.0012377 2.4436792
O -2.3794272 2.3739109 4.8089950	O -2.4401544 2.4418460 4.7271430
O -2.4450125 -2.4380794 4.7242701	O -2.2956102 -2.3733844 4.7792824
O -4.7781227 -0.0063506 4.8132824	O -4.7714933 0.0015521 4.8088995
Ca 0.0000000 2.4159972 0.0000000	Ca 0.0000000 2.4159972 0.0000000
Ca 0.0000000 -2.4159972 0.0000000	Ca 0.0000000 -2.4159972 0.0000000
Ca 0.0000000 7.2479920 4.8319944	Ca 0.0000000 7.2479920 4.8319944
Ca 0.0000000 -7.2479920 4.8319944	Ca 0.0000000 -7.2479920 4.8319944
Ca 2.4159972 0.0000000 0.0000000	Ca 2.4159972 0.0000000 0.0000000
Ca 2.4159972 4.8319944 4.8319944	Ca 2.4159972 4.8319944 4.8319944
Ca 2.4159972 -4.8319944 4.8319944	Ca 2.4159972 -4.8319944 4.8319944
Ca 4.8319944 2.4159972 4.8319944	Ca 4.8319944 2.4159972 4.8319944
Ca 4.8319944 -2.4159972 4.8319944	Ca 4.8319944 -2.4159972 4.8319944
Ca -2.4159972 0.0000000 0.0000000	Ca -2.4159972 0.0000000 0.0000000
Ca -2.4159972 4.8319944 4.8319944	Ca -2.4159972 4.8319944 4.8319944
Ca -2.4159972 -4.8319944 4.8319944	Ca -2.4159972 -4.8319944 4.8319944
Ca -4.8319944 2.4159972 4.8319944	Ca -4.8319944 2.4159972 4.8319944
Ca -4.8319944 -2.4159972 4.8319944	Ca -4.8319944 -2.4159972 4.8319944
Ca 7.2479920 0.0000000 4.8319944	Ca 7.2479920 0.0000000 4.8319944
Ca -7.2479920 0.0000000 4.8319944	Ca -7.2479920 0.0000000 4.8319944
Ca 0.0383144 -0.0058308 2.4563670	Ca 0.0124782 0.0337319 2.4232751
Ca 0.0000000 0.0000000 -2.4159972	Ca 0.0000000 0.0000000 -2.4159972
Ca -0.1010952 2.5849799 4.9683860	Ca -0.1995562 2.5976213 4.9905220
Ca 0.0000000 4.8319944 2.4159972	Ca 0.0000000 4.8319944 2.4159972
Ca -0.2078618 -2.5733312 4.9799841	Ca 0.1132390 -2.3516679 4.9178479
Ca 0.0000000 -4.8319944 2.4159972	Ca 0.0000000 -4.8319944 2.4159972
Ca 2.7006592 0.0639087 5.2520991	Ca 2.6048117 -0.1636734 4.9896957
Ca 2.4159972 2.4159972 2.4159972	Ca 2.4159972 2.4159972 2.4159972
Ca 2.4159972 -2.4159972 2.4159972	Ca 2.4159972 -2.4159972 2.4159972
Ca 4.8319944 0.0000000 2.4159972	Ca 4.8319944 0.0000000 2.4159972
Ca -2.5396918 -0.0578565 4.8743198	Ca -2.5234523 0.0565976 4.8790157
Ca -2.4159972 2.4159972 2.4159972	Ca -2.4159972 2.4159972 2.4159972
Ca -2.4159972 -2.4159972 2.4159972	Ca -2.4159972 -2.4159972 2.4159972
Ca -4.8319944 0.0000000 2.4159972	Ca -4.8319944 0.0000000 2.4159972
O 0.5818087 0.9773399 6.7599569	O -0.8884199 0.7664132 6.7634002
O -0.8848402 -0.7463396 6.7201741	O 0.7930050 -0.7564399 6.7692959
C -0.0595099 0.0514262 6.2026518	C -0.0154281 0.0404174 6.2349534
O 2.0295829 3.6155802 6.7693195	O 1.7492190 3.3645826 6.7073459
O 3.4996089 1.8939067 6.7333468	O 3.3968240 1.8071108 6.7137314
C 2.6420617 2.6734077 6.2540474	C 2.5180518 2.5249963 6.1901141
O 3.3725576 -1.7964130 6.7459828	O 1.0777323 -4.4137909 6.7351657
O 1.8527951 -3.4768302 6.7505883	O -0.9825698 -5.3505687 6.7147908
C 2.5372072 -2.5799454 6.2282391	C 0.0406164 -4.8571551 6.2135086
-11166.79267357 Hartrees	-11166.79167714 Hartrees

T1-4CO₂ (A)	T1-4CO₂ (B)
O 0.0066859 -0.0002206 0.0603949	O -0.0024204 0.0024266 0.0513522
O 0.0372474 -0.0540784 4.9008963	O -0.0149794 0.0129428 4.8528236
O -0.0401740 2.3926912 2.4860221	O -0.0105429 2.4063672 2.4851360
O 0.0327362 4.7955268 4.7100876	O -0.0041595 4.7821104 4.6719702
O 0.0319302 -2.3892331 2.4850599	O -0.0397779 -2.3972465 2.4953818
O -0.0511994 -4.7777091 4.7136518	O 0.0464968 -4.7711214 4.7178018
O 2.4756035 -0.0241712 2.4933615	O 2.3971641 0.0398364 2.4955274
O 2.3996188 2.4728651 4.6960479	O 2.4352949 2.4055764 4.8557112
O 2.4446164 -2.4644546 4.7492678	O 2.4522459 -2.4522183 4.7404575
O 4.8455048 0.0438852 4.8237518	O 4.7710995 -0.0464594 4.7177750
O -2.3899393 0.0300969 2.4931759	O -2.4064279 0.0105771 2.4850282
O -2.4125804 2.4136233 4.8148984	O -2.4838523 2.4839516 4.8804102
O -2.4543002 -2.4515071 4.7469994	O -2.4057737 -2.4355821 4.8555347
O -4.7864519 -0.0473484 4.7121200	O -4.7819837 0.0041623 4.6719545
Ca 0.0000000 2.4159972 0.0000000	Ca 0.0000000 2.4159972 0.0000000
Ca 0.0000000 -2.4159972 0.0000000	Ca 0.0000000 -2.4159972 0.0000000
Ca 0.0000000 7.2479920 4.8319944	Ca 0.0000000 7.2479920 4.8319944
Ca 0.0000000 -7.2479920 4.8319944	Ca 0.0000000 -7.2479920 4.8319944
Ca 2.4159972 0.0000000 0.0000000	Ca 2.4159972 0.0000000 0.0000000
Ca 2.4159972 4.8319944 4.8319944	Ca 2.4159972 4.8319944 4.8319944
Ca 2.4159972 -4.8319944 4.8319944	Ca 2.4159972 -4.8319944 4.8319944
Ca 4.8319944 2.4159972 4.8319944	Ca 4.8319944 2.4159972 4.8319944
Ca 4.8319944 -2.4159972 4.8319944	Ca 4.8319944 -2.4159972 4.8319944
Ca -2.4159972 0.0000000 0.0000000	Ca -2.4159972 0.0000000 0.0000000
Ca -2.4159972 4.8319944 4.8319944	Ca -2.4159972 4.8319944 4.8319944
Ca -2.4159972 -4.8319944 4.8319944	Ca -2.4159972 -4.8319944 4.8319944
Ca -4.8319944 2.4159972 4.8319944	Ca -4.8319944 2.4159972 4.8319944
Ca -4.8319944 -2.4159972 4.8319944	Ca -4.8319944 -2.4159972 4.8319944
Ca 7.2479920 0.0000000 4.8319944	Ca 7.2479920 0.0000000 4.8319944
Ca -7.2479920 0.0000000 4.8319944	Ca -7.2479920 0.0000000 4.8319944
Ca 0.0125050 0.0004094 2.4719401	Ca -0.0246480 0.0244936 2.4808501
Ca 0.0000000 0.0000000 -2.4159972	Ca 0.0000000 0.0000000 -2.4159972
Ca 0.1288293 2.6383961 4.9765183	Ca -0.0505019 2.7099332 5.2450666
Ca 0.0000000 4.8319944 2.4159972	Ca 0.0000000 4.8319944 2.4159972
Ca -0.2014915 -2.5922680 4.9848987	Ca 0.1926941 -2.5855875 4.9715734
Ca 0.0000000 -4.8319944 2.4159972	Ca 0.0000000 -4.8319944 2.4159972
Ca 2.4323291 0.3560257 5.2732044	Ca 2.5856115 -0.1926674 4.9714325
Ca 2.4159972 2.4159972 2.4159972	Ca 2.4159972 2.4159972 2.4159972
Ca 2.4159972 -2.4159972 2.4159972	Ca 2.4159972 -2.4159972 2.4159972
Ca 4.8319944 0.0000000 2.4159972	Ca 4.8319944 0.0000000 2.4159972
Ca -2.6141315 -0.1810876 4.9883670	Ca -2.7095607 0.0505467 5.2448248
Ca -2.4159972 2.4159972 2.4159972	Ca -2.4159972 2.4159972 2.4159972
Ca -2.4159972 -2.4159972 2.4159972	Ca -2.4159972 -2.4159972 2.4159972
Ca -4.8319944 0.0000000 2.4159972	Ca -4.8319944 0.0000000 2.4159972
O -0.9258325 -0.7375981 6.7931990	O -0.7907031 0.7921060 6.7759324
O 0.5983077 0.9423406 6.8045175	O 0.8111575 -0.8095323 6.7447286
C -0.1120545 0.0511402 6.2650109	C 0.0050639 -0.0046423 6.2092878
O 5.9221519 -0.4414755 6.7441273	O 1.8149978 3.3996819 6.7423999
O 4.2922314 1.1277634 6.6930527	O 3.4899274 1.8723459 6.7552131
C 5.0337919 0.2285519 6.2289373	C 2.5863992 2.5483350 6.2379990
O -1.8375381 3.4291018 6.7137229	O -1.8717874 -3.4895937 6.7551192
O -3.4050602 1.7902318 6.7111520	O -3.3992010 -1.8147356 6.7423833
C -2.5452602 2.5378542 6.2033513	C -2.5480550 -2.5862726 6.2378371
O 3.2164244 -1.6178055 6.6396690	O -1.9638503 3.5688491 6.7590025
O 1.7571931 -3.3471962 6.6697519	O -3.5686315 1.9637597 6.7589955
C 2.4579727 -2.4709833 6.1211793	C -2.6713961 2.6714747 6.2680538
-11355.42365739 Hartrees	-11355.42448089 Hartrees

T1-4CO₂ (C)	T1-4CO₂ (D)
O -0.0061000 0.0073595 0.0626458	O 0.0026210 0.0117072 0.0579687
O -0.0807956 0.1865086 4.9759391	O -0.0136788 -0.0844472 4.9320028
O 0.0069970 2.3981671 2.4929239	O 0.0005439 2.4737636 2.4705040
O 0.0081728 4.7883222 4.6567307	O -0.0184814 4.8341981 4.8221517
O 0.0119693 -2.3906978 2.4582617	O 0.0045024 -2.3922235 2.4353188
O 0.0059345 -4.7908257 4.8002034	O -0.0007846 -4.8109809 4.7887083
O 2.3886309 0.0495799 2.4942647	O 2.3930973 0.0597112 2.4799601
O 2.4955880 2.4356569 4.8593670	O 2.4851343 2.4252109 4.8394560
O 2.3808990 -2.3896312 4.7880622	O 2.4073588 -2.4001301 4.7663724
O 4.7841352 -0.0395714 4.7117744	O 4.7838102 -0.0410211 4.7089571
O -2.4717022 0.0445510 2.4741161	O -2.3790359 0.0484791 2.4779493
O -2.4639618 2.4750870 4.7706247	O -2.4491534 2.4279260 4.8901015
O -2.3900663 -2.4640391 4.6775699	O -2.4275880 -2.4661873 4.7192446
O -4.8492359 -0.0474068 4.8390021	O -4.7212462 -0.0318257 4.7523211
Ca 0.0000000 2.4159972 0.0000000	Ca 0.0000000 2.4159972 0.0000000
Ca 0.0000000 -2.4159972 0.0000000	Ca 0.0000000 -2.4159972 0.0000000
Ca 0.0000000 7.2479920 4.8319944	Ca 0.0000000 7.2479920 4.8319944
Ca 0.0000000 -7.2479920 4.8319944	Ca 0.0000000 -7.2479920 4.8319944
Ca 2.4159972 0.0000000 0.0000000	Ca 2.4159972 0.0000000 0.0000000
Ca 2.4159972 4.8319944 4.8319944	Ca 2.4159972 4.8319944 4.8319944
Ca 2.4159972 -4.8319944 4.8319944	Ca 2.4159972 -4.8319944 4.8319944
Ca 4.8319944 2.4159972 4.8319944	Ca 4.8319944 2.4159972 4.8319944
Ca 4.8319944 -2.4159972 4.8319944	Ca 4.8319944 -2.4159972 4.8319944
Ca -2.4159972 0.0000000 0.0000000	Ca -2.4159972 0.0000000 0.0000000
Ca -2.4159972 4.8319944 4.8319944	Ca -2.4159972 4.8319944 4.8319944
Ca -2.4159972 -4.8319944 4.8319944	Ca -2.4159972 -4.8319944 4.8319944
Ca -4.8319944 2.4159972 4.8319944	Ca -4.8319944 2.4159972 4.8319944
Ca -4.8319944 -2.4159972 4.8319944	Ca -4.8319944 -2.4159972 4.8319944
Ca 7.2479920 0.0000000 4.8319944	Ca 7.2479920 0.0000000 4.8319944
Ca -7.2479920 0.0000000 4.8319944	Ca -7.2479920 0.0000000 4.8319944
Ca -0.0260335 0.0282356 2.4796150	Ca 0.0093963 0.0154365 2.4573042
Ca 0.0000000 0.0000000 -2.4159972	Ca 0.0000000 0.0000000 -2.4159972
Ca 0.0730048 2.7029850 5.1751095	Ca -0.0163357 2.3132818 5.5667976
Ca 0.0000000 4.8319944 2.4159972	Ca 0.0000000 4.8319944 2.4159972
Ca -0.0066902 -2.5874276 4.8611704	Ca -0.0195909 -2.6040918 4.8432502
Ca 0.0000000 -4.8319944 2.4159972	Ca 0.0000000 -4.8319944 2.4159972
Ca 2.6119942 -0.1108197 4.9474975	Ca 2.6113378 -0.1391321 4.9326043
Ca 2.4159972 2.4159972 2.4159972	Ca 2.4159972 2.4159972 2.4159972
Ca 2.4159972 -2.4159972 2.4159972	Ca 2.4159972 -2.4159972 2.4159972
Ca 4.8319944 0.0000000 2.4159972	Ca 4.8319944 0.0000000 2.4159972
Ca -2.4186949 -0.3914471 5.3345366	Ca -2.4883506 -0.2654887 4.9320743
Ca -2.4159972 2.4159972 2.4159972	Ca -2.4159972 2.4159972 2.4159972
Ca -2.4159972 -2.4159972 2.4159972	Ca -2.4159972 -2.4159972 2.4159972
Ca -4.8319944 0.0000000 2.4159972	Ca -4.8319944 0.0000000 2.4159972
O -0.5773814 -1.0405901 6.7662759	O -0.2664503 -1.3101973 6.8065934
O 1.1617424 0.3995020 6.8193573	O 1.0736817 0.5050723 6.7712238
C 0.1863934 -0.1566196 6.2786460	C 0.2541039 -0.3192553 6.2710426
O 1.8433066 3.4611248 6.7204974	O 1.8203907 3.4245286 6.6981584
O 3.6277370 2.0685009 6.7693264	O 3.6284698 2.0720637 6.7451591
C 2.6622331 2.6352321 6.2508546	C 2.6586151 2.6198325 6.2174022
O -1.7894128 3.3420831 6.6940264	O -3.6732379 2.6070510 6.7770313
O -3.2902072 1.6492761 6.6524077	O -1.8378598 1.3108740 6.7229660
C -2.5102715 2.4787610 6.1391052	C -2.6792770 2.1215503 6.2405376
O -4.2931689 -1.1365953 6.7042381	O -1.0626747 4.2052563 6.6808900
O -5.9473864 0.4042800 6.7565555	O 0.3437479 5.9683456 6.7426919
C -5.0454941 -0.2437111 6.2378593	C -0.2287213 5.0231881 6.2164360
-11355.41892826 Hartrees	-11355.39913394 Hartrees

T1-5CO₂ (A)	-11544.04613070 Hartrees
O -0.0041690 0.0029251 0.0681951	
O -0.0883957 0.1273517 4.8941891	
O 0.0120702 2.3984382 2.4885370	
O 0.0100403 4.7784475 4.6659175	
O 0.0508488 -2.3882775 2.4998185	
O -0.0324695 -4.7871756 4.7109886	
O 2.3957494 0.0096265 2.5029707	
O 2.4913917 2.4784777 4.8745428	
O 2.3986950 -2.4261980 4.8618321	
O 4.7980258 0.0035961 4.6707769	
O -2.4778533 0.0328095 2.5108570	
O -2.4528275 2.4599899 4.7730675	
O -2.4032430 -2.4708009 4.6848403	
O -4.8504626 -0.0411852 4.8261754	
Ca 0.0000000 2.4159972 0.0000000	
Ca 0.0000000 -2.4159972 0.0000000	
Ca 0.0000000 7.2479920 4.8319944	
Ca 0.0000000 -7.2479920 4.8319944	
Ca 2.4159972 0.0000000 0.0000000	
Ca 2.4159972 4.8319944 4.8319944	
Ca 2.4159972 -4.8319944 4.8319944	
Ca 4.8319944 2.4159972 4.8319944	
Ca 4.8319944 -2.4159972 4.8319944	
Ca -2.4159972 0.0000000 0.0000000	
Ca -2.4159972 4.8319944 4.8319944	
Ca -2.4159972 -4.8319944 4.8319944	
Ca -4.8319944 2.4159972 4.8319944	
Ca -4.8319944 -2.4159972 4.8319944	
Ca 7.2479920 0.0000000 4.8319944	
Ca -7.2479920 0.0000000 4.8319944	
Ca 0.0103648 0.0254063 2.4969351	
Ca 0.0000000 0.0000000 -2.4159972	
Ca 0.0723061 2.7006262 5.2028814	
Ca 0.0000000 4.8319944 2.4159972	
Ca -0.1419839 -2.6344988 4.9537511	
Ca 0.0000000 -4.8319944 2.4159972	
Ca 2.7515291 0.0455487 5.2577158	
Ca 2.4159972 2.4159972 2.4159972	
Ca 2.4159972 -2.4159972 2.4159972	
Ca 4.8319944 0.0000000 2.4159972	
Ca -2.4493610 -0.3498603 5.2420176	
Ca -2.4159972 2.4159972 2.4159972	
Ca -2.4159972 -2.4159972 2.4159972	
Ca -4.8319944 0.0000000 2.4159972	
O -0.5890218 -0.9704151 6.7563664	
O 0.9090497 0.7255781 6.7846904	
C 0.0903239 -0.0457505 6.2305975	
O 1.9545793 3.5555150 6.7529853	
O 3.5836571 1.9744976 6.7539310	
C 2.6761517 2.6690638 6.2646546	
O -1.8071379 3.3556183 6.6959268	
O -3.3015470 1.6555126 6.6529279	
C -2.5173021 2.4823422 6.1459341	
O -4.2731379 -1.1261457 6.6876594	
O -5.9419405 0.4003382 6.7535871	
C -5.0380078 -0.2409758 6.2335838	
O 3.4233688 -1.8249820 6.7405034	
O 1.9139485 -3.5168455 6.7562077	
C 2.5684513 -2.5971040 6.2462636	

T1-5CO₂ (B) O -0.0020331 0.0020809 0.0607935 O 0.2533121 -0.2525592 4.8721446 O -0.0029947 2.4005549 2.5301089 O 0.0022031 4.8025354 4.6733351 O -0.0090787 -2.4094586 2.4843296 O -0.0045600 -4.7838487 4.6691477 O 2.4094429 0.0090811 2.4841246 O 2.4803662 2.4925176 4.8705023 O 2.4617057 -2.4616789 4.8563261 O 4.7838800 0.0045601 4.6691746 O -2.4005254 0.0030071 2.5299380 O -2.4121822 2.4121514 4.8843630 O -2.4925413 -2.4803823 4.8704907 O -4.8026085 -0.0021848 4.6734165 Ca 0.0000000 2.4159972 0.0000000 Ca 0.0000000 -2.4159972 0.0000000 Ca 0.0000000 7.2479920 4.8319944 Ca 0.0000000 -7.2479920 4.8319944 Ca 2.4159972 0.0000000 0.0000000 Ca 2.4159972 4.8319944 4.8319944 Ca 2.4159972 -4.8319944 4.8319944 Ca 4.8319944 2.4159972 4.8319944 Ca 4.8319944 -2.4159972 4.8319944 Ca -2.4159972 0.0000000 0.0000000 Ca -2.4159972 4.8319944 4.8319944 Ca -2.4159972 -4.8319944 4.8319944 Ca -4.8319944 2.4159972 4.8319944 Ca -4.8319944 -2.4159972 4.8319944 Ca 7.2479920 0.0000000 4.8319944 Ca -7.2479920 0.0000000 4.8319944 Ca 0.0158829 -0.0158854 2.5178458 Ca 0.0000000 0.0000000 -2.4159972 Ca 0.0520891 2.7544625 5.2397108 Ca 0.0000000 4.8319944 2.4159972 Ca -0.0573175 -2.7099276 5.2222452 Ca 0.0000000 -4.8319944 2.4159972 Ca 2.7101736 0.0573784 5.2227960 Ca 2.4159972 2.4159972 2.4159972 Ca 2.4159972 -2.4159972 2.4159972 Ca 4.8319944 0.0000000 2.4159972 Ca -2.7547758 -0.0520489 5.2405725 Ca -2.4159972 2.4159972 2.4159972 Ca -2.4159972 -2.4159972 2.4159972 Ca -4.8319944 0.0000000 2.4159972 O -0.9136929 -0.6810790 6.7061995 O 0.6799491 0.9143384 6.7067149 C -0.0041735 0.0042629 6.1616726 O 3.5449064 1.9467702 6.7526093 O 1.9645864 3.5763103 6.7498116 C 2.6618251 2.6704458 6.2595874 O -1.8749036 3.4808451 6.7629000 O -3.4807131 1.8749044 6.7629844 C -2.5922041 2.5922849 6.2645137 O -1.9469535 -3.5451055 6.7525621 O -3.5761628 -1.9644480 6.7498244 C -2.6704204 -2.6618940 6.2595539 O 3.4312028 -1.8266949 6.7527305 O 1.8267606 -3.4313067 6.7526942 C 2.5734398 -2.5734730 6.2359810	-11544.04660271 Hartrees
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T1-5CO₂ (C) O 0.0000068 0.0000056 0.0750549 O 0.0000668 0.0000605 4.9134476 O -0.0420208 2.3801351 2.4819157 O 0.0371190 4.7883820 4.7079716 O 0.0420025 -2.3801256 2.4819353 O -0.0370932 -4.7884116 4.7079738 O 2.4685456 -0.0230404 2.5143907 O 2.4032424 2.4696298 4.6873746 O 2.4290971 -2.4523682 4.7520100 O 4.8484629 0.0406061 4.8151460 O -2.4685018 0.0230511 2.5143885 O -2.4289975 2.4523451 4.7520716 O -2.4032430 -2.4695839 4.6873619 O -4.8484281 -0.0405218 4.8150130 Ca 0.0000000 2.4159972 0.0000000 Ca 0.0000000 -2.4159972 0.0000000 Ca 0.0000000 7.2479920 4.8319944 Ca 0.0000000 -7.2479920 4.8319944 Ca 2.4159972 0.0000000 0.0000000 Ca 2.4159972 4.8319944 4.8319944 Ca 2.4159972 -4.8319944 4.8319944 Ca 4.8319944 2.4159972 4.8319944 Ca 4.8319944 -2.4159972 4.8319944 Ca -2.4159972 0.0000000 0.0000000 Ca -2.4159972 4.8319944 4.8319944 Ca -2.4159972 -4.8319944 4.8319944 Ca -4.8319944 2.4159972 4.8319944 Ca -4.8319944 -2.4159972 4.8319944 Ca 7.2479920 0.0000000 4.8319944 Ca -7.2479920 0.0000000 4.8319944 Ca 0.0000111 0.0000162 2.4783679 Ca 0.0000000 0.0000000 -2.4159972 Ca 0.1462415 2.6319896 4.9724057 Ca 0.0000000 4.8319944 2.4159972 Ca -0.1462509 -2.6319819 4.9723693 Ca 0.0000000 -4.8319944 2.4159972 Ca 2.4584101 0.3390002 5.2196524 Ca 2.4159972 2.4159972 2.4159972 Ca 2.4159972 -2.4159972 2.4159972 Ca 4.8319944 0.0000000 2.4159972 Ca -2.4583505 -0.3389451 5.2195206 Ca -2.4159972 2.4159972 2.4159972 Ca -2.4159972 -2.4159972 2.4159972 Ca -4.8319944 0.0000000 2.4159972 O -0.6879783 -0.9031560 6.8267888 O 0.6879738 0.9031595 6.8269019 C 0.0000160 0.0000188 6.2954051 O 5.9221787 -0.4365837 6.7425312 O 4.2849820 1.1255629 6.6817583 C 5.0331143 0.2293036 6.2266585 O -1.8195435 3.3896131 6.6752028 O -3.2308328 1.6195259 6.6373057 C -2.4798074 2.4833172 6.1312258 O -4.2850098 -1.1254634 6.6816296 O -5.9219749 0.4369442 6.7423797 C -5.0330294 -0.2291209 6.2265178 O 3.2310356 -1.6195756 6.6372108 O 1.8192109 -3.3892223 6.6751798 C 2.4797930 -2.4831957 6.1311497	-11544.04368058 Hartrees
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T2	O -4.8431089 2.4173148 2.4126039 -15140.87408971 Hartrees
O -0.0042170 0.0042179 -0.0003573	
O -0.0097031 0.0097037 4.7840464	
O 0.0086263 2.4246280 2.4037399	
O -0.0109702 4.8064249 4.8099479	
O 0.0013153 -2.4271104 2.4126029	
O 0.0001777 -4.7740277 4.8223835	
O 2.4271108 -0.0013146 2.4126027	
O 2.3904252 2.4050306 4.8099483	
O 2.3959849 -2.3959844 4.8063930	
O 4.7740281 -0.0001775 4.8223837	
O -2.4246275 -0.0086263 2.4037393	
O -2.4062986 2.4062980 4.7840474	
O -2.4050310 -2.3904256 4.8099491	
O -4.8064257 0.0109696 4.8099502	
Ca 0.0000000 -2.4159993 0.0000000	
Ca 0.0000000 7.2479979 4.8319986	
Ca 0.0000000 -7.2479979 4.8319986	
Ca 2.4159993 0.0000000 0.0000000	
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Ca -2.4168103 4.8218948 4.8013007	
Ca -2.4159993 -4.8319986 4.8319986	
Ca -4.8218959 2.4168080 4.8013018	
Ca -4.8319986 -2.4159993 4.8319986	
Ca 7.2479979 0.0000000 4.8319986	
Ca -7.2479979 0.0000000 4.8319986	
Ca -0.0014825 0.0014810 2.4269211	
Ca 0.0000000 0.0000000 -2.4159993	
Ca -0.0032931 2.4127044 4.8015387	
Ca 0.0000000 4.8319986 2.4159993	
Ca 0.0008086 -2.4058935 4.8013007	
Ca 0.0000000 -4.8319986 2.4159993	
Ca 2.4058937 -0.0008096 4.8013009	
Ca 2.4159993 2.4159993 2.4159993	
Ca 2.4159993 -2.4159993 2.4159993	
Ca 4.8319986 0.0000000 2.4159993	
Ca -2.4127067 0.0032910 4.8015381	
Ca -2.4145183 2.4145153 2.4269198	
Ca -2.4159993 -2.4159993 2.4159993	
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Ca 0.0000000 2.4159993 0.0000000	
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O -2.4117818 2.4117820 -0.0003565	
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Ca -4.8319986 2.4159993 0.0000000	
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Ca -4.8319986 7.2479979 4.8319986	
O -2.4161763 7.1900262 4.8223831	
O -4.8119833 4.8119837 4.8063932	
O -2.4173144 4.8431087 2.4126029	
Ca -2.4159993 7.2479979 2.4159993	
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Ca -9.6639972 2.4159993 4.8319986	
O -7.1900267 2.4161770 4.8223833	
Ca -7.2479979 2.4159993 2.4159993	

T2-1CO₂ O -0.0038049 0.0038069 0.0198194 O -0.0152814 0.0152798 4.8313334 O 0.0028723 2.4115366 2.4250650 O -0.0098092 4.8232062 4.8096160 O -0.0047808 -2.4102626 2.4327237 O 0.0041892 -4.7858344 4.8215996 O 2.4103025 0.0047842 2.4327748 O 2.3649657 2.3863043 4.8114111 O 2.4255594 -2.4254526 4.7167861 O 4.7857840 -0.0041953 4.8215863 O -2.4115610 -0.0028580 2.4251128 O -2.4615885 2.4614908 4.7003005 O -2.3864059 -2.3648785 4.8113841 O -4.8231747 0.0098031 4.8095951 Ca 0.0000000 -2.4159993 0.0000000 Ca 0.0000000 7.2479979 4.8319986 Ca 0.0000000 -7.2479979 4.8319986 Ca 2.4159993 0.0000000 0.0000000 Ca 2.4159993 4.8319986 4.8319986 Ca 2.4159993 -4.8319986 4.8319986 Ca 4.8319986 2.4159993 4.8319986 Ca 4.8319986 -2.4159993 4.8319986 Ca -2.4159993 0.0000000 0.0000000 Ca -2.4507248 4.8451671 4.7887512 Ca -2.4159993 -4.8319986 4.8319986 Ca -4.8451779 2.4507489 4.7887384 Ca -4.8319986 -2.4159993 4.8319986 Ca 7.2479979 0.0000000 4.8319986 Ca -7.2479979 0.0000000 4.8319986 Ca -0.0044459 0.0044348 2.4017171 Ca 0.0000000 0.0000000 -2.4159993 Ca -0.0694271 2.5398531 4.8844168 Ca 0.0000000 4.8319986 2.4159993 Ca 0.0531022 -2.5104670 4.8757160 Ca 0.0000000 -4.8319986 2.4159993 Ca 2.5104464 -0.0531539 4.8754131 Ca 2.4159993 2.4159993 2.4159993 Ca 2.4159993 -2.4159993 2.4159993 Ca 4.8319986 0.0000000 2.4159993 Ca -2.5398837 0.0694544 4.8840797 Ca -2.4198130 2.4198726 2.4171695 Ca -2.4159993 -2.4159993 2.4159993 Ca -4.8319986 0.0000000 2.4159993 Ca 0.0000000 2.4159993 0.0000000 Ca -2.4159993 4.8319986 0.0000000 O -2.4086394 2.4086398 -0.0083984 Ca -2.4159993 2.4159993 -2.4159993 Ca -4.8319986 2.4159993 0.0000000 Ca -2.4159993 9.6639972 4.8319986 Ca -4.8319986 7.2479979 4.8319986 O -2.4214818 7.1908196 4.8182708 O -4.8242525 4.8242532 4.7998560 O -2.4157241 4.8538031 2.4051543 Ca -2.4159993 7.2479979 2.4159993 Ca -4.8319986 4.8319986 2.4159993 Ca -7.2479979 4.8319986 4.8319986 Ca -9.6639972 2.4159993 4.8319986 O -7.1908265 2.4214755 4.8182768 Ca -7.2479979 2.4159993 2.4159993	O -4.8538078 2.4157211 2.4051516 C -0.0133673 0.0132090 6.2055123 O 0.7872884 -0.7899515 6.7490281 O -0.8133216 0.8155262 6.7509022 -15329.51894068 Hartrees
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T2-2CO₂ (1,2) O -0.0083232 0.0081614 0.0232594 O -0.0838868 0.0559420 4.8753148 O -0.0107211 2.4019840 2.4586633 O 0.0416410 4.8434287 4.7437733 O -0.0022061 -2.4088153 2.4384585 O -0.0049657 -4.7887003 4.8153826 O 2.4097129 0.0018480 2.4436036 O 2.4360326 2.4539777 4.7334774 O 2.3746622 -2.3668774 4.7958780 O 4.7849059 0.0057701 4.8171495 O -2.4052172 0.0140273 2.4585562 O -2.3317144 2.3600169 4.8755333 O -2.4576795 -2.4275479 4.7437362 O -4.8520147 -0.0379431 4.7335172 Ca 0.0000000 -2.4159993 0.0000000 Ca 0.0000000 7.2479979 4.8319986 Ca 0.0000000 -7.2479979 4.8319986 Ca 2.4159993 0.0000000 0.0000000 Ca 2.4159993 4.8319986 4.8319986 Ca 2.4159993 -4.8319986 4.8319986 Ca 4.8319986 2.4159993 4.8319986 Ca 4.8319986 -2.4159993 4.8319986 Ca -2.4159993 0.0000000 0.0000000 Ca -2.3749429 4.9445292 4.8870467 Ca -2.4159993 -4.8319986 4.8319986 Ca -4.9435369 2.3724670 4.8761945 Ca -4.8319986 -2.4159993 4.8319986 Ca 7.2479979 0.0000000 4.8319986 Ca -7.2479979 0.0000000 4.8319986 Ca -0.0135646 0.0088047 2.4342764 Ca 0.0000000 0.0000000 -2.4159993 Ca 0.1789030 2.5820319 4.9970669 Ca 0.0000000 4.8319986 2.4159993 Ca -0.0411355 -2.5285685 4.8870187 Ca 0.0000000 -4.8319986 2.4159993 Ca 2.5275530 0.0434685 4.8763030 Ca 2.4159993 2.4159993 2.4159993 Ca 2.4159993 -2.4159993 2.4159993 Ca 4.8319986 0.0000000 2.4159993 Ca -2.5947767 -0.1661244 4.9975637 Ca -2.4024112 2.4071098 2.4343398 Ca -2.4159993 -2.4159993 2.4159993 Ca -4.8319986 0.0000000 2.4159993 Ca 0.0000000 2.4159993 0.0000000 Ca -2.4159993 4.8319986 0.0000000 O -2.4076711 2.4078334 0.0232673 Ca -2.4159993 2.4159993 -2.4159993 Ca -4.8319986 2.4159993 0.0000000 Ca -2.4159993 9.6639972 4.8319986 Ca -4.8319986 7.2479979 4.8319986 O -2.4110544 7.2046994 4.8153473 O -4.7906982 4.7828252 4.7957867 O -2.4137827 4.8247843 2.4384242 Ca -2.4159993 7.2479979 2.4159993 Ca -4.8319986 4.8319986 2.4159993 Ca -7.2479979 4.8319986 4.8319986 Ca -9.6639972 2.4159993 4.8319986 O -7.2008794 2.4102149 4.8171607 Ca -7.2479979 2.4159993 2.4159993	O -4.8257117 2.4141058 2.4436297 C 0.0818421 -0.0690005 6.2361961 O -0.5586827 -0.9983603 6.7853961 O 0.8829646 0.7489286 6.7587644 C -2.4979980 2.4849341 6.2363794 O -1.8587715 3.4150645 6.7857398 O -3.2983695 1.6661287 6.7587525 -15518.15877371 Hartrees
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T3	
O 0.0000000 -0.0037706 -0.0041424	Ca 2.4159993 9.6639972 4.8319986
O -0.0000000 0.0095061 4.7784065	Ca -2.4159993 9.6639972 4.8319986
O 0.0000001 2.4159993 2.4269211	Ca -4.8319986 7.2479979 4.8319986
O -0.0000001 4.8224926 4.7784066	O 4.7802934 4.8107182 4.8178648
O 0.0000001 -2.4280118 2.4073139	O 2.4029930 7.2247913 4.8069018
O 0.0000000 -4.7729101 4.8208813	O -0.0000000 9.6049091 4.8208813
O 2.4297766 -0.0099579 2.3930508	O -2.4029930 7.2247913 4.8069018
O 2.4016299 2.4159993 4.7944550	O -4.7802935 4.8107183 4.8178645
O 2.4029930 -2.3927926 4.8069018	O -2.4297766 4.8419565 2.3930508
O 4.7802934 0.0212804 4.8178648	O 2.4297766 4.8419565 2.3930508
O -2.4297766 -0.0099579 2.3930508	O -0.0000000 7.2600104 2.4073139
O -2.4016299 2.4159993 4.7944549	Ca 4.8319986 4.8319986 2.4159993
O -2.4029929 -2.3927927 4.8069018	Ca 2.4159993 7.2479979 2.4159993
O -4.7802933 0.0212804 4.8178647	Ca 0.0000000 9.6639972 2.4159993
Ca 0.0000000 -2.4159993 0.0000000	Ca -2.4159993 7.2479979 2.4159993
Ca 0.0000001 7.2399352 4.7954968	Ca -4.8319986 4.8319986 2.4159993
Ca 0.0000000 -7.2479959 4.8319986	O 2.3995923 2.4159993 -0.0074885
Ca 2.4159993 0.0000000 0.0000000	Ca 4.8319986 2.4159993 0.0000000
Ca 2.4011370 4.8352740 4.7930971	-19692.62787637 Hartrees
Ca 2.4159993 -4.8319986 4.8319986	
Ca 4.8319986 2.4159993 4.8319986	
Ca 4.8319986 -2.4159993 4.8319986	
Ca -2.4159993 0.0000000 0.0000000	
Ca -2.4011371 4.8352740 4.7930970	
Ca -2.4159993 -4.8319986 4.8319986	
Ca -4.8319986 2.4159993 4.8319986	
Ca -4.8319986 -2.4159993 4.8319986	
Ca 7.2479979 0.0000000 4.8319986	
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Ca -0.0000000 0.0093894 2.4112970	
Ca 0.0000000 0.0000000 -2.4159993	
Ca -0.0000000 2.4159994 4.8197291	
Ca -0.0000000 4.8226093 2.4112970	
Ca 0.0000000 -2.4079363 4.7954968	
Ca 0.0000000 -4.8319986 2.4159993	
Ca 2.4011370 -0.0032753 4.7930971	
Ca 2.4159993 2.4159993 2.4159993	
Ca 2.4159993 -2.4159993 2.4159993	
Ca 4.8319986 0.0000000 2.4159993	
Ca -2.4011371 -0.0032753 4.7930971	
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Ca -4.8319986 0.0000000 2.4159993	
Ca 0.0000000 2.4159993 0.0005868	
O 0.0000000 4.8357692 -0.0041424	
Ca -2.4159993 4.8319986 0.0000000	
Ca 2.4159993 4.8319986 0.0000000	
Ca 0.0000000 4.8319986 -2.4159993	
Ca 0.0000000 7.2479979 0.0000000	
O -2.3995923 2.4159993 -0.0074885	
O -0.0000000 2.4159993 -2.4140652	
Ca 0.0000000 2.4159993 -4.8319986	
Ca 2.4159993 2.4159993 -2.4159993	
Ca -2.4159993 2.4159993 -2.4159993	
Ca -4.8319986 2.4159993 0.0000000	
Ca -7.2479984 4.8319996 4.8319976	
Ca 7.2479979 4.8319986 4.8319986	
Ca 0.0000000 12.0799965 4.8319986	
Ca 4.8319986 7.2479979 4.8319986	

T3-1CO₂ (position 1)	
O -0.0000039 -0.0071005 0.0217566	Ca 2.4159993 9.6639972 4.8319986
O 0.0000463 0.0146054 4.9502874	Ca -2.4159993 9.6639972 4.8319986
O 0.0000218 2.4013765 2.4564912	Ca -4.8319986 7.2479979 4.8319986
O 0.0000948 4.8436524 4.7699108	O 4.7807962 4.8141046 4.8109328
O 0.0000690 -2.4144224 2.4307483	O 2.4048160 7.2263565 4.8030921
O -0.0000618 -4.7849474 4.8112981	O -0.0000016 9.6030206 4.8177417
O 2.4043771 -0.0068854 2.4073891	O -2.4047837 7.2262540 4.8031118
O 2.3958209 2.4414150 4.7556371	O -4.7806683 4.8139924 4.8109122
O 2.3880176 -2.4072699 4.7621140	O -2.4249713 4.8483959 2.3864235
O 4.7994824 0.0195072 4.8144389	O 2.4249665 4.8485544 2.3862959
O -2.4043661 -0.0068258 2.4073897	O -0.0000322 7.2578223 2.4042100
O -2.3951862 2.4407299 4.7566069	Ca 4.8319986 4.8319986 2.4159993
O -2.3885005 -2.4078058 4.7611276	Ca 2.4159993 7.2479979 2.4159993
O -4.7994947 0.0193930 4.8144809	Ca 0.0000000 9.6639972 2.4159993
Ca 0.0000000 -2.4159993 0.0000000	Ca -2.4159993 7.2479979 2.4159993
Ca 0.0000483 7.2483103 4.7969760	Ca -4.8319986 4.8319986 2.4159993
Ca 0.0000000 -7.2479959 4.8319986	O 2.3940393 2.4146753 -0.0121966
Ca 2.4159993 0.0000000 0.0000000	Ca 4.8319986 2.4159993 0.0000000
Ca 2.4235829 4.8499492 4.7858740	C 0.0000410 0.0055307 6.3419809
Ca 2.4159993 -4.8319986 4.8319986	O 1.1273464 0.0089170 6.8944406
Ca 4.8319986 2.4159993 4.8319986	O -1.1272410 -0.0042164 6.8944178
Ca 4.8319986 -2.4159993 4.8319986	-19881.27071745 Hartrees
Ca -2.4159993 0.0000000 0.0000000	
Ca -2.4232899 4.8497891 4.7860076	
Ca -2.4159993 -4.8319986 4.8319986	
Ca -4.8319986 2.4159993 4.8319986	
Ca -4.8319986 -2.4159993 4.8319986	
Ca 7.2479979 0.0000000 4.8319986	
Ca -7.2479979 0.0000000 4.8319986	
Ca 0.0000214 0.0136457 2.3907953	
Ca 0.0000000 0.0000000 -2.4159993	
Ca 0.0005959 2.5622056 4.8347031	
Ca 0.0000249 4.8401122 2.4006528	
Ca -0.0005586 -2.5211581 4.8078595	
Ca 0.0000000 -4.8319986 2.4159993	
Ca 2.5094863 -0.0013814 4.9131503	
Ca 2.4159993 2.4159993 2.4159993	
Ca 2.4159993 -2.4159993 2.4159993	
Ca 4.8319986 0.0000000 2.4159993	
Ca -2.5094677 -0.0023750 4.9130949	
Ca -2.4159993 2.4159993 2.4159993	
Ca -2.4159993 -2.4159993 2.4159993	
Ca -4.8319986 0.0000000 2.4159993	
Ca 0.0000271 2.4224381 0.0007149	
O -0.0000132 4.8328472 -0.0030369	
Ca -2.4159993 4.8319986 0.0000000	
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Ca 0.0000000 4.8319986 -2.4159993	
Ca 0.0000000 7.2479979 0.0000000	
O -2.3940642 2.4146892 -0.0121074	
O -0.0000201 2.4102749 -2.4091778	
Ca 0.0000000 2.4159993 -4.8319986	
Ca 2.4159993 2.4159993 -2.4159993	
Ca -2.4159993 2.4159993 -2.4159993	
Ca -4.8319986 2.4159993 0.0000000	
Ca -7.2479984 4.8319996 4.8319976	
Ca 7.2479979 4.8319986 4.8319986	
Ca 0.0000000 12.0799965 4.8319986	
Ca 4.8319986 7.2479979 4.8319986	

T3-2CO₂ (1,2) O -0.0026014 -0.0006447 0.0243978 O -0.0305551 0.1035288 4.8696716 O -0.0199744 2.4092963 2.4939665 O 0.0649092 4.9006789 4.7120513 O -0.0007772 -2.4091540 2.4409148 O -0.0033323 -4.7826673 4.8166808 O 2.4146470 -0.0009868 2.4181610 O 2.4590940 2.4846281 4.7364114 O 2.3752239 -2.3744279 4.7928604 O 4.7967720 0.0216973 4.8105975 O -2.3990987 0.0128862 2.4461894 O -2.4280337 2.3468685 4.8588668 O -2.4384269 -2.4471229 4.7256457 O -4.7766707 -0.0287871 4.7348289 Ca 0.0000000 -2.4159993 0.0000000 Ca 0.0425361 7.2765166 4.7869909 Ca 0.0000000 -7.2479959 4.8319986 Ca 2.4159993 0.0000000 0.0000000 Ca 2.4659845 4.8952134 4.7655714 Ca 2.4159993 -4.8319986 4.8319986 Ca 4.8319986 2.4159993 4.8319986 Ca 4.8319986 -2.4159993 4.8319986 Ca -2.4159993 0.0000000 0.0000000 Ca -2.3433862 4.9972422 4.8636839 Ca -2.4159993 -4.8319986 4.8319986 Ca -4.8319986 2.4159993 4.8319986 Ca -4.8319986 -2.4159993 4.8319986 Ca 7.2479979 0.0000000 4.8319986 Ca -7.2479979 0.0000000 4.8319986 Ca -0.0046329 0.0285261 2.4144681 Ca 0.0000000 0.0000000 -2.4159993 Ca 0.1979595 2.6313818 5.0234274 Ca 0.0103852 4.8285990 2.4092325 Ca -0.0374702 -2.5286292 4.8657332 Ca 0.0000000 -4.8319986 2.4159993 Ca 2.5278095 0.0337092 4.8816785 Ca 2.4159993 2.4159993 2.4159993 Ca 2.4159993 -2.4159993 2.4159993 Ca 4.8319986 0.0000000 2.4159993 Ca -2.5416347 -0.1978596 4.9538620 Ca -2.4159993 2.4159993 2.4159993 Ca -2.4159993 -2.4159993 2.4159993 Ca -4.8319986 0.0000000 2.4159993 Ca 0.0044023 2.4230927 0.0081290 O -0.0025254 4.8277136 -0.0089569 Ca -2.4159993 4.8319986 0.0000000 Ca 2.4159993 4.8319986 0.0000000 Ca 0.0000000 4.8319986 -2.4159993 Ca 0.0000000 7.2479979 0.0000000 O -2.3976933 2.4138447 0.0232531 O -0.0069898 2.4088109 -2.4041656 Ca 0.0000000 2.4159993 -4.8319986 Ca 2.4159993 2.4159993 -2.4159993 Ca -2.4159993 2.4159993 -2.4159993 Ca -4.8319986 2.4159993 0.0000000 Ca -7.2479984 4.8319996 4.8319976 Ca 7.2479979 4.8319986 4.8319986 Ca 0.0000000 12.0799965 4.8319986 Ca 4.8319986 7.2479979 4.8319986	Ca 2.4159993 9.6639972 4.8319986 Ca -2.4159993 9.6639972 4.8319986 Ca -4.8319986 7.2479979 4.8319986 O 4.7921566 4.8270671 4.8080466 O 2.4219132 7.2463824 4.7958175 O 0.0069291 9.6062385 4.8151619 O -2.3976600 7.2502761 4.8049299 O -4.7181629 4.8170167 4.7660594 O -2.4116302 4.8246311 2.4228944 O 2.4380893 4.8529173 2.3757407 O -0.0032219 7.2669548 2.4013055 Ca 4.8319986 4.8319986 2.4159993 Ca 2.4159993 7.2479979 2.4159993 Ca 0.0000000 9.6639972 2.4159993 Ca -2.4159993 7.2479979 2.4159993 Ca -4.8319986 4.8319986 2.4159993 O 2.3917672 2.4124476 -0.0091390 Ca 4.8319986 2.4159993 0.0000000 C 0.0738005 -0.0749386 6.2311462 O 1.0431658 0.4919999 6.7896859 O -0.8032867 -0.8195461 6.7441809 C -2.5075093 2.5581983 6.2198078 O -3.5459337 2.1454912 6.7816416 O -1.5418553 3.1917389 6.7234203 -20069.91796684 Hartrees
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T3-2CO₂ (1,3) O 0.0007202 -0.0025746 0.0186740 O 0.0047246 -0.0067008 4.8417949 O -0.0134918 2.4159998 2.4831910 O 0.0047182 4.8386945 4.8417968 O -0.0019683 -2.4110137 2.4257303 O 0.0070041 -4.7897956 4.8156965 O 2.4105352 0.0004898 2.4159108 O 2.3508942 2.4159974 4.8278644 O 2.4327912 -2.4230750 4.7133933 O 4.7869899 0.0179236 4.8142550 O -2.4126108 -0.0168697 2.4045236 O -2.4748251 2.4159975 4.6675867 O -2.3848359 -2.3779230 4.7975601 O -4.8053253 0.0149765 4.8109393 Ca 0.0000000 -2.4159993 0.0000000 Ca 0.0564633 7.3629860 4.8610703 Ca 0.0000000 -7.2479959 4.8319986 Ca 2.4159993 0.0000000 0.0000000 Ca 2.5018985 4.8884827 4.8748482 Ca 2.4159993 -4.8319986 4.8319986 Ca 4.8319986 2.4159993 4.8319986 Ca 4.8319986 -2.4159993 4.8319986 Ca -2.4159993 0.0000000 0.0000000 Ca -2.5426367 4.8147867 4.8653196 Ca -2.4159993 -4.8319986 4.8319986 Ca -4.8319986 2.4159993 4.8319986 Ca -4.8319986 -2.4159993 4.8319986 Ca 7.2479979 0.0000000 4.8319986 Ca -7.2479979 0.0000000 4.8319986 Ca -0.0040749 0.0064080 2.3859743 Ca 0.0000000 0.0000000 -2.4159993 Ca -0.1608820 2.4159979 4.9844586 Ca -0.0040748 4.8255887 2.3859766 Ca 0.0564612 -2.5309900 4.8610695 Ca 0.0000000 -4.8319986 2.4159993 Ca 2.5019014 -0.0564860 4.8748489 Ca 2.4159993 2.4159993 2.4159993 Ca 2.4159993 -2.4159993 2.4159993 Ca 4.8319986 0.0000000 2.4159993 Ca -2.5426377 0.0172110 4.8653169 Ca -2.4159993 2.4159993 2.4159993 Ca -2.4159993 -2.4159993 2.4159993 Ca -4.8319986 0.0000000 2.4159993 Ca -0.0044282 2.4159995 0.0044542 O 0.0007208 4.8345731 0.0186760 Ca -2.4159993 4.8319986 0.0000000 Ca 2.4159993 4.8319986 0.0000000 Ca 0.0000000 4.8319986 -2.4159993 Ca 0.0000000 7.2479979 0.0000000 O -2.3912177 2.4159993 -0.0223372 O 0.0035738 2.4159993 -2.4055209 Ca 0.0000000 2.4159993 -4.8319986 Ca 2.4159993 2.4159993 -2.4159993 Ca -2.4159993 2.4159993 -2.4159993 Ca -4.8319986 2.4159993 0.0000000 Ca -7.2479984 4.8319996 4.8319976 Ca 7.2479979 4.8319986 4.8319986 Ca 0.0000000 12.0799965 4.8319986 Ca 4.8319986 7.2479979 4.8319986	Ca 2.4159993 9.6639972 4.8319986 Ca -2.4159993 9.6639972 4.8319986 Ca -4.8319986 7.2479979 4.8319986 O 4.7869866 4.8140709 4.8142523 O 2.4327908 7.2550690 4.7133917 O 0.0070045 9.6217947 4.8156955 O -2.3848369 7.2099227 4.7975591 O -4.8053298 4.8170227 4.8109387 O -2.4126109 4.8488679 2.4045233 O 2.4105331 4.8315050 2.4159118 O -0.0019671 7.2430111 2.4257304 Ca 4.8319986 4.8319986 2.4159993 Ca 2.4159993 7.2479979 2.4159993 Ca 0.0000000 9.6639972 2.4159993 Ca -2.4159993 7.2479979 2.4159993 Ca -4.8319986 4.8319986 2.4159993 O 2.3920426 2.4159993 -0.0047302 Ca 4.8319986 2.4159993 0.0000000 C -0.0655201 -0.0963784 6.2206985 O 0.7634657 -0.8673594 6.7592348 O -0.9597338 0.6055441 6.7530030 C -0.0655246 4.9283837 6.2207013 O 0.7634775 5.6993487 6.7592355 O -0.9597553 4.2264873 6.7530098 -20069.90229034 Hartrees
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T4	
O -4.7912700 -4.8384056 4.8284579	Ca 2.4159993 -9.6639973 4.8319986
O -4.7912699 0.0064073 4.8284579	Ca 2.4159993 -4.8330569 4.8046815
O -2.4438996 -7.2758977 4.8072532	Ca 2.4159993 0.0010583 4.8046815
O -2.4399783 -2.4159992 4.7941398	Ca 2.4159993 4.8319986 4.8319986
O -2.4438997 2.4438997 4.8072532	Ca 4.8319986 -12.0799966 4.8319986
O -0.0064073 -9.6232684 4.8284579	Ca 4.8300299 -7.2448839 4.8226518
O 0.0060610 -4.8259374 4.8054068	Ca 4.8330568 -2.4159992 4.8046815
O 0.0060610 -0.0060609 4.8054068	Ca 4.8300299 2.4128852 4.8226518
O -0.0064072 4.7912695 4.8284579	Ca 4.8319986 7.2479960 4.8319986
O 2.4159993 -7.2719768 4.7941398	Ca 7.2479980 -9.6639973 4.8319986
O 2.4159993 -2.4159992 4.7803890	Ca 7.2448836 -4.8300296 4.8226518
O 2.4159993 2.4399784 4.7941398	Ca 7.2448840 -0.0019688 4.8226518
O 4.8384059 -9.6232684 4.8284579	Ca 7.2479980 4.8319986 4.8319986
O 4.8259376 -4.8259375 4.8054068	Ca 9.6639973 -7.2479960 4.8319986
O 4.8259377 -0.0060609 4.8054068	Ca 9.6639973 -2.4159993 4.8319986
O 4.8384058 4.7912695 4.8284579	Ca 9.6639973 2.4159993 4.8319986
O 7.2758982 -7.2758977 4.8072532	Ca 12.0799966 -4.8319986 4.8319986
O 7.2719769 -2.4159992 4.7941398	Ca 12.0799966 0.0000000 4.8319986
O 7.2758983 2.4438997 4.8072532	Ca -4.8319986 -4.8319986 2.4159993
O 9.6232686 -4.8384056 4.8284579	Ca -4.8319986 0.0000000 2.4159993
O 9.6232685 0.0064073 4.8284579	Ca -2.4159993 -7.2479980 2.4159993
O -2.4010610 -4.8311540 2.4463793	Ca -2.4159993 -2.4159993 2.4159993
O -2.4010610 -0.0008446 2.4463794	Ca -2.4159993 2.4159993 2.4159993
O 0.0008446 -7.2330593 2.4463794	Ca 0.0000000 -9.6639973 2.4159993
O -0.0033421 -2.4159993 2.4270417	Ca 0.0000000 -4.8319986 2.4159993
O 0.0008446 2.4010610 2.4463794	Ca 0.0000000 0.0000000 2.4159993
O 2.4159993 -4.8353407 2.4270415	Ca 0.0000000 4.8319986 2.4159993
O 2.4159993 0.0033422 2.4270417	Ca 2.4159993 -7.2479980 2.4159993
O 4.8311540 -7.2330593 2.4463794	Ca 2.4159993 -2.4159993 2.4159993
O 4.8353408 -2.4159993 2.4270417	Ca 2.4159993 2.4159993 2.4159993
O 4.8311540 2.4010610 2.4463794	Ca 4.8319986 -9.6639973 2.4159993
O 7.2330596 -4.8311540 2.4463793	Ca 4.8319986 -4.8319986 2.4159993
O 7.2330596 -0.0008446 2.4463794	Ca 4.8319986 0.0000000 2.4159993
Ca -2.4159993 -4.8319986 0.0000000	Ca 4.8319986 4.8319986 2.4159993
Ca -2.4159993 0.0000000 0.0000000	Ca 7.2479980 -7.2479980 2.4159993
Ca 0.0000000 -7.2479960 0.0000000	Ca 7.2479980 -2.4159993 2.4159993
Ca 0.0000000 -2.4159993 0.0000000	Ca 7.2479980 2.4159993 2.4159993
Ca 0.0000000 2.4159993 0.0000000	Ca 9.6639973 -4.8319986 2.4159993
Ca 2.4159993 -4.8319986 0.0000000	Ca 9.6639973 0.0000000 2.4159993
Ca 2.4159993 0.0000000 0.0000000	-25017.43417311 Hartrees
Ca 4.8319986 -7.2479960 0.0000000	
Ca 4.8319986 -2.4159993 0.0000000	
Ca 4.8319986 2.4159993 0.0000000	
Ca 7.2479980 -4.8319986 0.0000000	
Ca 7.2479980 0.0000000 0.0000000	
Ca -7.2479980 -4.8319986 4.8319986	
Ca -7.2479980 0.0000000 4.8319986	
Ca -4.8319986 -7.2479960 4.8319986	
Ca -4.8319986 -2.4159993 4.8319986	
Ca -4.8319986 2.4159993 4.8319986	
Ca -2.4159993 -9.6639973 4.8319986	
Ca -2.4128850 -4.8300296 4.8226518	
Ca -2.4128854 -0.0019688 4.8226518	
Ca -2.4159993 4.8319986 4.8319986	
Ca 0.0000000 -12.0799966 4.8319986	
Ca 0.0019688 -7.2448839 4.8226518	
Ca -0.0010582 -2.4159992 4.8046815	
Ca 0.0019688 2.4128852 4.8226518	
Ca 0.0000000 7.2479960 4.8319986	

T4-1CO₂ (position 1)	
O -4.7888081 -4.8432954 4.8239069	Ca 2.4159993 -9.6639973 4.8319986
O -4.7888080 0.0112972 4.8239069	Ca 2.4160011 -4.9759465 4.8261788
O -2.4444385 -7.2784877 4.8009073	Ca 2.4160011 0.1439479 4.8261776
O -2.4624178 -2.4159992 4.7947198	Ca 2.4159993 4.8319986 4.8319986
O -2.4444385 2.4464897 4.8009073	Ca 4.8319986 -12.0799966 4.8319986
O -0.0074531 -9.6230476 4.8248748	Ca 4.8549226 -7.2572115 4.8185799
O 0.0088827 -4.8560563 4.7679421	Ca 4.9641855 -2.4159994 4.9297262
O 0.0088827 0.0240577 4.7679433	Ca 4.8549226 2.4252129 4.8185800
O -0.0074531 4.7910488 4.8248748	Ca 4.8319986 7.2479960 4.8319986
O 2.4160075 -7.2818865 4.7891750	Ca 7.2479980 -9.6639973 4.8319986
O 2.4159731 -2.4159947 4.9239640	Ca 7.2538715 -4.8489466 4.8182867
O 2.4160075 2.4498885 4.7891749	Ca 7.2538720 0.0169482 4.8182869
O 4.8394511 -9.6230467 4.8248772	Ca 7.2479980 4.8319986 4.8319986
O 4.8231209 -4.8560266 4.7680215	Ca 9.6639973 -7.2479960 4.8319986
O 4.8231210 0.0240280 4.7680227	Ca 9.6639973 -2.4159993 4.8319986
O 4.8394511 4.7910479 4.8248772	Ca 9.6639973 2.4159993 4.8319986
O 7.2764393 -7.2784890 4.8009184	Ca 12.0799966 -4.8319986 4.8319986
O 7.2943837 -2.4159992 4.7947959	Ca 12.0799966 0.0000000 4.8319986
O 7.2764394 2.4464911 4.8009184	Ca -4.8319986 -4.8319986 2.4159993
O 9.6208045 -4.8432843 4.8239125	Ca -4.8319986 0.0000000 2.4159993
O 9.6208044 0.0112861 4.8239126	Ca -2.4159993 -7.2479980 2.4159993
O -2.4041912 -4.8305647 2.4451713	Ca -2.4159993 -2.4159993 2.4159993
O -2.4041912 -0.0014338 2.4451714	Ca -2.4159993 2.4159993 2.4159993
O 0.0040439 -7.2384856 2.4432988	Ca 0.0000000 -9.6639973 2.4159993
O 0.0230853 -2.4159992 2.4436548	Ca 0.0000000 -4.8319986 2.4159993
O 0.0040439 2.4064872 2.4432989	Ca 0.0000000 0.0000000 2.4159993
O 2.4160072 -4.8189122 2.4532302	Ca 0.0000000 4.8319986 2.4159993
O 2.4160072 -0.0130860 2.4532300	Ca 2.4159993 -7.2479980 2.4159993
O 4.8279646 -7.2384739 2.4433096	Ca 2.4159993 -2.4159993 2.4159993
O 4.8089123 -2.4159992 2.4436770	Ca 2.4159993 2.4159993 2.4159993
O 4.8279646 2.4064755 2.4433097	Ca 4.8319986 -9.6639973 2.4159993
O 7.2361943 -4.8305567 2.4451781	Ca 4.8319986 -4.8319986 2.4159993
O 7.2361942 -0.0014419 2.4451783	Ca 4.8319986 0.0000000 2.4159993
Ca -2.4159993 -4.8319986 0.0000000	Ca 4.8319986 4.8319986 2.4159993
Ca -2.4159993 0.0000000 0.0000000	Ca 7.2479980 -7.2479980 2.4159993
Ca 0.0000000 -7.2479960 0.0000000	Ca 7.2479980 -2.4159993 2.4159993
Ca 0.0000000 -2.4159993 0.0000000	Ca 7.2479980 2.4159993 2.4159993
Ca 0.0000000 2.4159993 0.0000000	Ca 9.6639973 -4.8319986 2.4159993
Ca 2.4159993 -4.8319986 0.0000000	Ca 9.6639973 0.0000000 2.4159993
Ca 2.4159993 0.0000000 0.0000000	C 2.4158215 -2.4160036 6.3154949
Ca 4.8319986 -7.2479960 0.0000000	O 1.2890713 -2.4160093 6.8676038
Ca 4.8319986 -2.4159993 0.0000000	O 3.5424708 -2.4160091 6.8677976
Ca 4.8319986 2.4159993 0.0000000	-25206.07294949 Hartrees
Ca 7.2479980 -4.8319986 0.0000000	
Ca 7.2479980 0.0000000 0.0000000	
Ca -7.2479980 -4.8319986 4.8319986	
Ca -7.2479980 0.0000000 4.8319986	
Ca -4.8319986 -7.2479960 4.8319986	
Ca -4.8319986 -2.4159993 4.8319986	
Ca -4.8319986 2.4159993 4.8319986	
Ca -2.4159993 -9.6639973 4.8319986	
Ca -2.4218721 -4.8489646 4.8182763	
Ca -2.4218726 0.0169662 4.8182765	
Ca -2.4159993 4.8319986 4.8319986	
Ca 0.0000000 -12.0799966 4.8319986	
Ca -0.0229134 -7.2572089 4.8185563	
Ca -0.1322585 -2.4159994 4.9294907	
Ca -0.0229134 2.4252103 4.8185564	
Ca 0.0000000 7.2479960 4.8319986	

T5	
O -4.7885255 -4.8370002 4.8257551	Ca 2.4159993 -9.6639973 4.8319986
O -4.7885254 0.0050019 4.8257552	Ca 2.4159994 -4.8325582 4.7978055
O -2.4418058 -7.2738039 4.8011848	Ca 2.4159993 0.0005596 4.7978056
O -2.4363696 -2.4159992 4.7840858	Ca 2.4159993 4.8319986 4.8319986
O -2.4418058 2.4418059 4.8011848	Ca 4.8319986 -12.0799966 4.8319986
O -0.0050019 -9.6205240 4.8257552	Ca 4.8313729 -7.2437483 4.8161190
O 0.0068646 -4.8251339 4.8077693	Ca 4.8325581 -2.4159992 4.7978055
O 0.0068645 -0.0068645 4.8077693	Ca 4.8313729 2.4117497 4.8161190
O -0.0050018 4.7885251 4.8257551	Ca 4.8319986 7.2479960 4.8319986
O 2.4159993 -7.2683681 4.7840857	Ca 7.2479980 -9.6639973 4.8319986
O 2.4159993 -2.4159993 4.7805303	Ca 7.2437480 -4.8313726 4.8161189
O 2.4159994 2.4363697 4.7840858	Ca 7.2437485 -0.0006257 4.8161190
O 4.8370005 -9.6205239 4.8257552	Ca 7.2479980 4.8319986 4.8319986
O 4.8251341 -4.8251339 4.8077693	Ca 9.6639973 -7.2479960 4.8319986
O 4.8251341 -0.0068645 4.8077694	Ca 9.6639973 -2.4159993 4.8319986
O 4.8370004 4.7885251 4.8257551	Ca 9.6639973 2.4159993 4.8319986
O 7.2738044 -7.2738039 4.8011848	Ca 12.0799966 -4.8319986 4.8319986
O 7.2683682 -2.4159992 4.7840858	Ca 12.0799966 0.0000000 4.8319986
O 7.2738045 2.4418059 4.8011848	Ca -4.8319986 -4.8319986 2.4159993
O 9.6205242 -4.8370002 4.8257551	Ca -4.8319986 0.0000000 2.4159993
O 9.6205241 0.0050019 4.8257552	Ca -2.4159993 -7.2479980 2.4159993
O -2.4024702 -4.8416226 2.4282301	Ca -2.4159993 -2.4159993 2.4159993
O -2.4024702 0.0096241 2.4282302	Ca -2.4159993 2.4159993 2.4159993
O -0.0096241 -7.2344684 2.4282301	Ca 0.0000000 -9.6639973 2.4159993
O -0.0089672 -2.4159993 2.4077528	Ca 0.0000000 -4.8319986 2.4159993
O -0.0096240 2.4024702 2.4282302	Ca 0.0000000 0.0000000 2.4159993
O 2.4159993 -4.8409658 2.4077526	Ca 0.0000000 4.8319986 2.4159993
O 2.4159993 0.0089672 2.4077528	Ca 2.4159993 -7.2479980 2.4159993
O 4.8416227 -7.2344684 2.4282301	Ca 2.4159993 -2.4159993 2.4159993
O 4.8409658 -2.4159993 2.4077528	Ca 2.4159993 2.4159993 2.4159993
O 4.8416227 2.4024702 2.4282302	Ca 4.8319986 -9.6639973 2.4159993
O 7.2344688 -4.8416226 2.4282301	Ca 4.8319986 -4.8319986 2.4159993
O 7.2344688 0.0096241 2.4282302	Ca 4.8319986 0.0000000 2.4159993
Ca -2.4159993 -4.8319986 0.0000000	Ca 4.8319986 4.8319986 2.4159993
Ca -2.4159993 0.0000000 0.0000000	Ca 7.2479980 -7.2479980 2.4159993
Ca 0.0000000 -7.2479960 0.0000000	Ca 7.2479980 -2.4159993 2.4159993
Ca 0.0000000 -2.4159993 0.0000000	Ca 7.2479980 2.4159993 2.4159993
Ca 0.0000000 2.4159993 0.0000000	Ca 9.6639973 -4.8319986 2.4159993
Ca 2.4159993 -4.8319986 0.0000000	Ca 9.6639973 0.0000000 2.4159993
Ca 2.4159993 0.0000000 0.0000000	O 0.0260306 -4.8059678 -0.0097052
Ca 4.8319986 -7.2479960 0.0000000	O 0.0260306 -0.0260306 -0.0097051
Ca 4.8319986 -2.4159993 0.0000000	O 2.4159993 -2.4159993 -0.0062696
Ca 4.8319986 2.4159993 0.0000000	O 4.8059680 -4.8059678 -0.0097052
Ca 7.2479980 -4.8319986 0.0000000	O 4.8059680 -0.0260306 -0.0097051
Ca 7.2479980 0.0000000 0.0000000	Ca 0.0000000 -4.8319986 -2.4159993
Ca -7.2479980 -4.8319986 4.8319986	Ca 0.0000000 0.0000000 -2.4159993
Ca -7.2479980 0.0000000 4.8319986	Ca 2.4159993 -2.4159993 -2.4159993
Ca -4.8319986 -7.2479960 4.8319986	Ca 4.8319986 -4.8319986 -2.4159993
Ca -4.8319986 -2.4159993 4.8319986	Ca 4.8319986 0.0000000 -2.4159993
Ca -4.8319986 2.4159993 4.8319986	-28777.46591821 Hartrees
Ca -2.4159993 -9.6639973 4.8319986	
Ca -2.4117494 -4.8313727 4.8161189	
Ca -2.4117498 -0.0006257 4.8161190	
Ca -2.4159993 4.8319986 4.8319986	
Ca 0.0000000 -12.0799966 4.8319986	
Ca 0.0006257 -7.2437484 4.8161190	
Ca -0.0005595 -2.4159992 4.7978056	
Ca 0.0006257 2.4117496 4.8161190	
Ca 0.0000000 7.2479960 4.8319986	

T5-1CO₂ (position 1)	
O -4.7861167 -4.8419704 4.8210436	Ca 2.4159993 -9.6639973 4.8319986
O -4.7861166 0.0099721 4.8210436	Ca 2.4159983 -4.9747881 4.8164812
O -2.4426295 -7.2764192 4.7950392	Ca 2.4159983 0.1427895 4.8164798
O -2.4594551 -2.4159992 4.7860291	Ca 2.4159993 4.8319986 4.8319986
O -2.4426295 2.4444212 4.7950393	Ca 4.8319986 -12.0799966 4.8319986
O -0.0062759 -9.6204406 4.8220948	Ca 4.8557665 -7.2558975 4.8122561
O 0.0092979 -4.8556122 4.7701573	Ca 4.9624537 -2.4159996 4.9257742
O 0.0092978 0.0236135 4.7701588	Ca 4.8557665 2.4238989 4.8122563
O -0.0062759 4.7884418 4.8220948	Ca 4.8319986 7.2479960 4.8319986
O 2.4159991 -7.2794622 4.7797600	Ca 7.2479980 -9.6639973 4.8319986
O 2.4159962 -2.4159941 4.9246542	Ca 7.2526839 -4.8501217 4.8117893
O 2.4159991 2.4474643 4.7797600	Ca 7.2526843 0.0181232 4.8117895
O 4.8382744 -9.6204405 4.8220948	Ca 7.2479980 4.8319986 4.8319986
O 4.8226993 -4.8556113 4.7701577	Ca 9.6639973 -7.2479960 4.8319986
O 4.8226992 0.0236125 4.7701593	Ca 9.6639973 -2.4159993 4.8319986
O 4.8382744 4.7884416 4.8220948	Ca 9.6639973 2.4159993 4.8319986
O 7.2746278 -7.2764189 4.7950391	Ca 12.0799966 -4.8319986 4.8319986
O 7.2914521 -2.4159992 4.7860293	Ca 12.0799966 0.0000000 4.8319986
O 7.2746278 2.4444209 4.7950392	Ca -4.8319986 -4.8319986 2.4159993
O 9.6181150 -4.8419701 4.8210435	Ca -4.8319986 0.0000000 2.4159993
O 9.6181149 0.0099718 4.8210436	Ca -2.4159993 -7.2479980 2.4159993
O -2.4054894 -4.8415363 2.4258656	Ca -2.4159993 -2.4159993 2.4159993
O -2.4054893 0.0095377 2.4258657	Ca -2.4159993 2.4159993 2.4159993
O -0.0069394 -7.2397032 2.4244301	Ca 0.0000000 -9.6639973 2.4159993
O 0.0126030 -2.4159992 2.4247670	Ca 0.0000000 -4.8319986 2.4159993
O -0.0069394 2.4077048 2.4244303	Ca 0.0000000 0.0000000 2.4159993
O 2.4159992 -4.8288276 2.4370361	Ca 0.0000000 4.8319986 2.4159993
O 2.4159992 -0.0031706 2.4370359	Ca 2.4159993 -7.2479980 2.4159993
O 4.8389381 -7.2397030 2.4244302	Ca 2.4159993 -2.4159993 2.4159993
O 4.8193949 -2.4159992 2.4247674	Ca 2.4159993 2.4159993 2.4159993
O 4.8389381 2.4077047 2.4244304	Ca 4.8319986 -9.6639973 2.4159993
O 7.2374878 -4.8415362 2.4258656	Ca 4.8319986 -4.8319986 2.4159993
O 7.2374877 0.0095376 2.4258658	Ca 4.8319986 0.0000000 2.4159993
Ca -2.4159993 -4.8319986 0.0000000	Ca 4.8319986 4.8319986 2.4159993
Ca -2.4159993 0.0000000 0.0000000	Ca 7.2479980 -7.2479980 2.4159993
Ca 0.0000000 -7.2479960 0.0000000	Ca 7.2479980 -2.4159993 2.4159993
Ca 0.0000000 -2.4159993 0.0000000	Ca 7.2479980 2.4159993 2.4159993
Ca 0.0000000 2.4159993 0.0000000	Ca 9.6639973 -4.8319986 2.4159993
Ca 2.4159993 -4.8319986 0.0000000	Ca 9.6639973 0.0000000 2.4159993
Ca 2.4159993 0.0000000 0.0000000	O 0.0308503 -4.8037690 -0.0127723
Ca 4.8319986 -7.2479960 0.0000000	O 0.0308503 -0.0282293 -0.0127721
Ca 4.8319986 -2.4159993 0.0000000	O 2.4159993 -2.4159993 0.0201480
Ca 4.8319986 2.4159993 0.0000000	O 4.8011484 -4.8037690 -0.0127722
Ca 7.2479980 -4.8319986 0.0000000	O 4.8011484 -0.0282294 -0.0127720
Ca 7.2479980 0.0000000 0.0000000	Ca 0.0000000 -4.8319986 -2.4159993
Ca -7.2479980 -4.8319986 4.8319986	Ca 0.0000000 0.0000000 -2.4159993
Ca -7.2479980 0.0000000 4.8319986	Ca 2.4159993 -2.4159993 -2.4159993
Ca -4.8319986 -7.2479960 4.8319986	Ca 4.8319986 -4.8319986 -2.4159993
Ca -4.8319986 -2.4159993 4.8319986	Ca 4.8319986 0.0000000 -2.4159993
Ca -4.8319986 2.4159993 4.8319986	C 2.4159953 -2.4160053 6.3170331
Ca -2.4159993 -9.6639973 4.8319986	O 1.2889253 -2.4160120 6.8680128
Ca -2.4206859 -4.8501223 4.8117893	O 3.5430653 -2.4160122 6.8680118
Ca -2.4206864 0.0181238 4.8117895	-28966.10453495 Hartrees
Ca -2.4159993 4.8319986 4.8319986	
Ca 0.0000000 -12.0799966 4.8319986	
Ca -0.0237685 -7.2558979 4.8122561	
Ca -0.1304581 -2.4159996 4.9257729	
Ca -0.0237685 2.4238993 4.8122563	
Ca 0.0000000 7.2479960 4.8319986	

MS1

O -0.0115531 -0.0000000 0.1008705
 O 0.1863976 -0.0000000 4.8794167
 O -0.0434978 2.4265819 2.5094264
 O 0.1064928 4.7713780 4.8451269
 O -0.0434978 -2.4265819 2.5094264
 O 0.1064928 -4.7713780 4.8451269
 O 2.4156431 -0.0000000 2.4470425
 O 2.4371686 2.4124392 4.7928821
 O 2.4371686 -2.4124392 4.7928821
 O 4.7846882 -0.0000000 4.8736431
 O -2.4892706 0.0000000 2.3917791
 Ca 0.0000000 2.4159993 0.0000000
 Ca 0.0000000 -2.4159993 0.0000000
 Ca 0.0000000 7.2479980 4.8319986
 Ca 0.0000000 -7.2479980 4.8319986
 Ca 2.4159993 0.0000000 0.0000000
 Ca 2.4159993 4.8319986 4.8319986
 Ca 2.4159993 -4.8319986 4.8319986
 Ca 4.8319986 2.4159993 4.8319986
 Ca 4.8319986 -2.4159993 4.8319986
 Ca -2.4159993 0.0000000 0.0000000
 Ca 7.2479980 0.0000000 4.8319986
 Ca -0.0798322 0.0000000 2.5547113
 Ca 0.0000000 0.0000000 -2.4159993
 Ca 0.2065153 2.4258169 4.8639284
 Ca 0.0000000 4.8319986 2.4159993
 Ca 0.2065154 -2.4258169 4.8639284
 Ca 0.0000000 -4.8319986 2.4159993
 Ca 2.4745299 0.0000000 4.8060415
 Ca 2.4159993 2.4159993 2.4159993
 Ca 2.4159993 -2.4159993 2.4159993
 Ca 4.8319986 0.0000000 2.4159993
 Ca -2.4159993 2.4159993 2.4159993
 Ca -2.4159993 -2.4159993 2.4159993
 Ca -4.8319986 0.0000000 2.4159993
 -8325.722470268 Hartrees

MS1-1CO₂

O 0.0014852 -0.0000000 0.0999772
 O 0.1466228 -0.0000034 4.8856842
 O -0.0278589 2.4215379 2.5014624
 O 0.1306298 4.8285361 4.8195867
 O -0.0278586 -2.4215385 2.5014614
 O 0.1306301 -4.8285374 4.8195864
 O 2.3992423 -0.0000000 2.4588704
 O 2.4074425 2.3952511 4.8048484
 O 2.4074432 -2.3952519 4.8048481
 O 4.7640088 -0.0000001 4.8588887
 O -2.4248910 0.0000003 2.3400736
 Ca 0.0000000 2.4159986 0.0000000
 Ca 0.0000000 -2.4159986 0.0000000
 Ca 0.0000000 7.2479960 4.8319972
 Ca 0.0000000 -7.2479960 4.8319972
 Ca 2.4159986 0.0000000 0.0000000
 Ca 2.4159986 4.8319972 4.8319972
 Ca 2.4159986 -4.8319972 4.8319972
 Ca 4.8319972 2.4159986 4.8319972
 Ca 4.8319972 -2.4159986 4.8319972
 Ca -2.4159986 0.0000000 0.0000000
 Ca 7.2479960 0.0000000 4.8319972
 Ca -0.0769467 -0.0000005 2.4348263
 Ca 0.0000000 0.0000000 -2.4159986
 Ca 0.1053923 2.6071319 4.8786953
 Ca 0.0000000 4.8319972 2.4159986
 Ca 0.1053928 -2.6071341 4.8786939
 Ca 0.0000000 -4.8319972 2.4159986
 Ca 2.5010983 -0.0000006 4.7969918
 Ca 2.4159986 2.4159986 2.4159986
 Ca 2.4159986 -2.4159986 2.4159986
 Ca 4.8319972 0.0000000 2.4159986
 Ca -2.4159986 2.4159986 2.4159986
 Ca -2.4159986 -2.4159986 2.4159986
 Ca -4.8319972 0.0000000 2.4159986
 C -1.0862454 -0.0000034 5.4437597
 O -1.6046381 1.1317980 5.6743830
 O -1.6046413 -1.1318055 5.6743752
 -8514.419149307 Hartrees

MS1-2CO₂ (1,2 T)

O 0.0099029 0.0050521 0.1145950
 O 0.1761168 0.1245594 4.9650812
 O 0.0038580 2.4278578 2.5448794
 O 0.0811227 4.8846973 4.7088988
 O -0.0126451 -2.4147683 2.5182856
 O 0.1296339 -4.8249956 4.8182131
 O 2.3996385 0.0366055 2.5030546
 O 2.4577503 2.4553905 4.8040368
 O 2.4144239 -2.4059432 4.8140340
 O 4.7604885 -0.0335563 4.7501375
 O -2.4139879 0.0036747 2.3330081
 Ca 0.0000000 2.4159986 0.0000000
 Ca 0.0000000 -2.4159986 0.0000000
 Ca 0.0000000 7.2479960 4.8319972
 Ca 0.0000000 -7.2479960 4.8319972
 Ca 2.4159986 0.0000000 0.0000000
 Ca 2.4159986 4.8319972 4.8319972
 Ca 2.4159986 -4.8319972 4.8319972
 Ca 4.8319972 2.4159986 4.8319972
 Ca 4.8319972 -2.4159986 4.8319972
 Ca -2.4159986 0.0000000 0.0000000
 Ca 7.2479960 0.0000000 4.8319972
 Ca -0.0705524 0.0218857 2.4692628
 Ca 0.0000000 0.0000000 -2.4159986
 Ca -0.1128572 2.7628254 5.0035903
 Ca 0.0000000 4.8319972 2.4159986
 Ca 0.0973015 -2.6218145 4.8810581
 Ca 0.0000000 -4.8319972 2.4159986
 Ca 2.5615597 -0.1306289 4.8834901
 Ca 2.4159986 2.4159986 2.4159986
 Ca 2.4159986 -2.4159986 2.4159986
 Ca 4.8319972 0.0000000 2.4159986
 Ca -2.4159986 2.4159986 2.4159986
 Ca -2.4159986 -2.4159986 2.4159986
 Ca -4.8319972 0.0000000 2.4159986
 C -1.1130277 0.0485808 5.3662714
 O -1.7374365 1.1445016 5.5106898
 O -1.5975398 -1.1082993 5.5411546
 C 2.4751667 2.4673117 6.1893258
 O 1.6446957 3.2452479 6.7163933
 O 3.3421730 1.7468131 6.7236198
 -8703.060408617 Hartrees

MS1-2CO₂ (1,3 T)

O 0.0053318 -0.0010840 0.1007274
 O 0.0684571 0.0110115 4.8760345
 O -0.0405490 2.4153157 2.4888627
 O 0.1201845 4.8339977 4.8146658
 O -0.0203927 -2.4162890 2.4994438
 O 0.1325146 -4.8126551 4.8132968
 O 2.4195119 -0.0013710 2.4902676
 O 2.3538435 2.3859674 4.7039569
 O 2.4066782 -2.3194009 4.7888737
 O 4.8086898 0.0433367 4.7491549
 O -2.4162557 -0.0048758 2.3214191
 Ca 0.0000000 2.4159986 0.0000000
 Ca 0.0000000 -2.4159986 0.0000000
 Ca 0.0000000 7.2479960 4.8319972
 Ca 0.0000000 -7.2479960 4.8319972
 Ca 2.4159986 0.0000000 0.0000000
 Ca 2.4159986 4.8319972 4.8319972
 Ca 2.4159986 -4.8319972 4.8319972
 Ca 4.8319972 2.4159986 4.8319972
 Ca 4.8319972 -2.4159986 4.8319972
 Ca -2.4159986 0.0000000 0.0000000
 Ca 7.2479960 0.0000000 4.8319972
 Ca -0.1026853 0.0042564 2.4049151
 Ca 0.0000000 0.0000000 -2.4159986
 Ca 0.0492078 2.6380221 4.8514876
 Ca 0.0000000 4.8319972 2.4159986
 Ca 0.0737444 -2.6046932 4.8666021
 Ca 0.0000000 -4.8319972 2.4159986
 Ca 2.3036233 0.0695421 4.8061916
 Ca 2.4159986 2.4159986 2.4159986
 Ca 2.4159986 -2.4159986 2.4159986
 Ca 4.8319972 0.0000000 2.4159986
 Ca -2.4159986 2.4159986 2.4159986
 Ca -2.4159986 -2.4159986 2.4159986
 Ca -4.8319972 0.0000000 2.4159986
 C -1.2181676 0.0068994 5.3122542
 O -1.7518467 1.1383860 5.4835103
 O -1.7399427 -1.1305045 5.4894747
 C 4.8170716 0.0437530 6.1551747
 O 4.2520294 1.0201699 6.6849072
 O 5.4122922 -0.9200682 6.6685945
 -8703.064410956 Hartrees

MS2	
O -0.0113368 0.0064353 0.0493827	Ca 2.4159986 0.0000000 0.0000000
O 0.2164086 0.0086261 4.8826812	Ca 0.0000000 2.4159986 -4.8319972
O -0.0830658 2.4162357 2.6113138	Ca -2.4159986 2.4159986 -2.4159986
O 0.2165544 4.8240449 4.8824984	Ca 0.0000000 0.0000000 -2.4159986
O -0.0451274 -2.4158284 2.5072864	Ca 2.4159986 2.4159986 -2.4159986
O 0.1137564 -4.7694801 4.8406405	Ca 0.0000000 4.8319972 -2.4159986
O 2.4476037 -0.0162821 2.4259492	-16652.44552943 Hartrees
O 2.4889754 2.4163889 4.8081689	
O 2.4509155 -2.4100090 4.8048089	
O 4.8272201 0.0161877 4.8199888	
O -2.4977985 -0.0185341 2.3636021	
O -0.0111189 4.8260462 0.0491532	
O -2.4191587 2.4160848 0.0559967	
O -0.0064324 2.4162102 -2.3295292	
O 4.8275893 4.8163686 4.8193731	
O 2.4511591 7.2422106 4.8046929	
O 0.1137246 9.6015396 4.8407867	
O -2.4976816 4.8508426 2.3635982	
O 2.4482273 4.8488439 2.4256416	
O -0.0449091 7.2480206 2.5071338	
O 2.3942937 2.4163889 0.0426832	
O -4.8674111 2.4161003 2.3992214	
Ca 0.2112458 7.2587542 4.8601411	
Ca 2.4896667 4.8363311 4.7960068	
Ca -0.1048221 0.0323184 2.5641070	
Ca 0.2464004 2.4159819 4.9251503	
Ca -0.1049771 4.7997221 2.5640925	
Ca 0.2111579 -2.4267904 4.8601864	
Ca 0.0000000 -4.8319972 2.4159986	
Ca 2.4896206 -0.0043097 4.7961502	
Ca 2.4159986 2.4159986 2.4159986	
Ca 2.4159986 -2.4159986 2.4159986	
Ca 4.8319972 0.0000000 2.4159986	
Ca -2.4920505 2.4159109 2.3666161	
Ca -2.4159986 -2.4159986 2.4159986	
Ca -4.8319972 0.0000000 2.4159986	
Ca -0.0053482 2.4159920 0.0078806	
Ca 4.8319972 4.8319972 2.4159986	
Ca 2.4159986 7.2479958 2.4159986	
Ca 0.0000000 9.6639944 2.4159986	
Ca -2.4159986 7.2479958 2.4159986	
Ca -4.8319972 4.8319972 2.4159986	
Ca -7.2459979 2.4159993 2.4159993	
Ca 0.0000000 12.0799930 4.8319972	
Ca 0.0000000 -7.2479938 4.8319972	
Ca 2.4159986 -4.8319972 4.8319972	
Ca 4.8319972 -2.4159986 4.8319972	
Ca 7.2479958 0.0000000 4.8319972	
Ca 4.8319972 2.4159986 4.8319972	
Ca 7.2479958 4.8319972 4.8319972	
Ca 4.8319972 7.2479958 4.8319972	
Ca 2.4159986 9.6639944 4.8319972	
Ca -4.8319972 2.4159986 0.0000000	
Ca -2.4159986 4.8319972 0.0000000	
Ca 0.0000000 7.2479958 0.0000000	
Ca 2.4159986 4.8319972 0.0000000	
Ca -2.4159986 0.0000000 0.0000000	
Ca 0.0000000 -2.4159986 0.0000000	
Ca 4.8319972 2.4159986 0.0000000	

MS2-1CO₂	
O -0.0066051 0.0016062 0.0465065	
O 0.2305841 -0.0698413 4.8494300	
O -0.0637909 2.4110933 2.6041655	
O 0.1718351 4.8200025 4.8817521	
O -0.0387216 -2.4201247 2.4916540	
O 0.1174968 -4.7731043 4.8359829	
O 2.4544894 -0.0123345 2.4224633	
O 2.4624179 2.4343334 4.8260466	
O 2.4604057 -2.4118404 4.8006752	
O 4.8282492 0.0208701 4.8166415	
O -2.4832121 -0.0253143 2.3613964	
O -0.0036517 4.8341353 0.0566639	
O -2.4047740 2.4146314 0.0571928	
O -0.0049712 2.4150801 -2.3260219	
O 4.8084178 4.8190353 4.8069106	
O 2.4219972 7.2239958 4.8148602	
O 0.1341517 9.6597968 4.8158215	
O -2.4469013 4.8444565 2.3218528	
O 2.4259265 4.8481989 2.4416823	
O -0.0315796 7.2441372 2.4950283	
O 2.3943451 2.4223280 0.0469180	
O -4.8616052 2.4151987 2.3866313	
Ca 0.1096292 7.4353234 4.8737498	
Ca 2.5121408 4.8301172 4.7851166	
Ca -0.1025293 0.0061260 2.5232154	
Ca 0.1565456 2.2002426 4.9477423	
Ca -0.1005714 4.7911249 2.4257792	
Ca 0.2108159 -2.4453737 4.8536067	
Ca 0.0000000 -4.8319972 2.4159986	
Ca 2.5023664 -0.0265232 4.7871403	
Ca 2.4159986 2.4159986 2.4159986	
Ca 2.4159986 -2.4159986 2.4159986	
Ca 4.8319972 0.0000000 2.4159986	
Ca -2.5024780 2.4245261 2.4183048	
Ca -2.4159986 -2.4159986 2.4159986	
Ca -4.8319972 0.0000000 2.4159986	
Ca -0.0146979 2.3955774 0.0050049	
Ca 4.8319972 4.8319972 2.4159986	
Ca 2.4159986 7.2479958 2.4159986	
Ca 0.0000000 9.6639944 2.4159986	
Ca -2.4159986 7.2479958 2.4159986	
Ca -4.8319972 4.8319972 2.4159986	
Ca -7.2459979 2.4159993 2.4159993	
Ca 0.0000000 12.0799930 4.8319972	
Ca 0.0000000 -7.2479938 4.8319972	
Ca 2.4159986 -4.8319972 4.8319972	
Ca 4.8319972 -2.4159986 4.8319972	
Ca 7.2479958 0.0000000 4.8319972	
Ca 4.8319972 2.4159986 4.8319972	
Ca 7.2479958 4.8319972 4.8319972	
Ca 4.8319972 7.2479958 4.8319972	
Ca 2.4159986 9.6639944 4.8319972	
Ca -4.8319972 2.4159986 0.0000000	
Ca -2.4159986 4.8319972 0.0000000	
Ca 0.0000000 7.2479958 0.0000000	
Ca 2.4159986 4.8319972 0.0000000	
Ca -2.4159986 0.0000000 0.0000000	
Ca 0.0000000 -2.4159986 0.0000000	
Ca 4.8319972 2.4159986 0.0000000	
Ca 2.4159986 0.0000000 0.0000000	
Ca 0.0000000 2.4159986 -4.8319972	
Ca -2.4159986 2.4159986 -2.4159986	
Ca 0.0000000 0.0000000 -2.4159986	
Ca 2.4159986 2.4159986 -2.4159986	
Ca 0.0000000 4.8319972 -2.4159986	
C -1.0433249 4.8188903 5.4775191	
O -1.5707281 5.9493466 5.6941184	
O -1.5374712 3.6872278 5.7553366	
-16841.13799444 Hartrees	

MS2-2CO₂

O -0.0058854 -0.0037503 0.0610073
O 0.1491529 -0.0496187 4.8774607
O -0.0409936 2.4096955 2.6149701
O 0.1060500 4.8857965 4.9085315
O -0.0410124 -2.4096188 2.5003420
O 0.1412614 -4.8405327 4.8026085
O 2.4310685 -0.0116313 2.4561097
O 2.4503950 2.4363856 4.8273076
O 2.4403364 -2.3918271 4.8012230
O 4.8115920 0.0182285 4.8063722
O -2.4533847 -0.0241397 2.3637044
O 0.0073749 4.8336344 0.0478139
O -2.3912178 2.4160342 0.0566932
O -0.0037028 2.4141814 -2.3227762
O 4.7996058 4.8170209 4.8032595
O 2.4243994 7.2205193 4.8127399
O 0.1368903 9.6668629 4.8134838
O -2.4283892 4.8479941 2.2735664
O 2.4232332 4.8452727 2.4428637
O -0.0074419 7.2467804 2.4731514
O 2.3962881 2.4153080 0.0517884
O -4.8565831 2.4143771 2.3852166
Ca 0.1007071 7.4582116 4.8428607
Ca 2.5045068 4.8554319 4.7827791
Ca -0.1220703 0.0231603 2.4530746
Ca 0.1219608 2.4173866 5.0085303
Ca -0.0962167 4.8054435 2.3810575
Ca 0.1455777 -2.6341059 4.9043327
Ca 0.0000000 -4.8319972 2.4159986
Ca 2.5316415 -0.0164765 4.7928270
Ca 2.4159986 2.4159986 2.4159986
Ca 2.4159986 -2.4159986 2.4159986
Ca 4.8319972 0.0000000 2.4159986
Ca -2.5075394 2.4710068 2.4791872
Ca -2.4159986 -2.4159986 2.4159986
Ca -4.8319972 0.0000000 2.4159986
Ca -0.0239426 2.4085784 0.0015653
Ca 4.8319972 4.8319972 2.4159986
Ca 2.4159986 7.2479958 2.4159986
Ca 0.0000000 9.6639944 2.4159986
Ca -2.4159986 7.2479958 2.4159986
Ca -4.8319972 4.8319972 2.4159986
Ca -7.2459979 2.4159993 2.4159993
Ca 0.0000000 12.0799930 4.8319972
Ca 0.0000000 -7.2479938 4.8319972
Ca 2.4159986 -4.8319972 4.8319972
Ca 4.8319972 -2.4159986 4.8319972
Ca 7.2479958 0.0000000 4.8319972
Ca 4.8319972 2.4159986 4.8319972
Ca 7.2479958 4.8319972 4.8319972
Ca 4.8319972 7.2479958 4.8319972
Ca 2.4159986 9.6639944 4.8319972
Ca -4.8319972 2.4159986 0.0000000
Ca -2.4159986 4.8319972 0.0000000
Ca 0.0000000 7.2479958 0.0000000
Ca 2.4159986 4.8319972 0.0000000
Ca -2.4159986 0.0000000 0.0000000
Ca 0.0000000 -2.4159986 0.0000000
Ca 4.8319972 2.4159986 0.0000000

Ca 2.4159986 0.0000000 0.0000000
Ca 0.0000000 2.4159986 -4.8319972
Ca -2.4159986 2.4159986 -2.4159986
Ca 0.0000000 0.0000000 -2.4159986
Ca 2.4159986 2.4159986 -2.4159986
Ca 0.0000000 4.8319972 -2.4159986
C -1.2407573 4.9171712 5.1417963
O -1.7698117 6.0636487 5.2372902
O -1.8208161 3.8023192 5.2119782
C -0.5114844 -0.1129612 6.0745881
O -0.6012003 0.9663002 6.7144393
O -0.9419310 -1.2447401 6.4289964
-17029.80656433 Hartrees

DS

O -0.0622453 0.0000166 0.1101642
 O 0.1126024 0.0000466 4.7501047
 O 0.1290345 2.4365601 2.4734397
 O 0.0251436 4.7795519 4.7287664
 O 0.1290569 -2.4365060 2.4734517
 O 0.0251415 -4.7795222 4.7287696
 O 2.4430122 0.0000431 2.4248571
 O 2.4106906 2.3985994 4.8382804
 O 2.4106465 -2.3985524 4.8382638
 O 4.7877011 -0.0000061 4.8246954
 Ca 0.0000000 2.4159993 0.0000000
 Ca 0.0000000 -2.4159993 0.0000000
 Ca 0.0000000 7.2479980 4.8319986
 Ca 0.0000000 -7.2479980 4.8319986
 Ca 2.4159993 0.0000000 0.0000000
 Ca 2.4159993 4.8319986 4.8319986
 Ca 2.4159993 -4.8319986 4.8319986
 Ca 4.8319986 2.4159993 4.8319986
 Ca 4.8319986 -2.4159993 4.8319986
 Ca -2.4159993 0.0000000 0.0000000
 Ca 7.2479980 0.0000000 4.8319986
 Ca 0.1012315 0.0000356 2.4768403
 Ca 0.0000000 0.0000000 -2.4159993
 Ca 0.1198993 2.4058078 4.7388317
 Ca 0.0000000 4.8319986 2.4159993
 Ca 0.1198837 -2.4057733 4.7387921
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 Ca 2.4529538 0.0000256 4.8372595
 Ca 2.4159993 2.4159993 2.4159993
 Ca 2.4159993 -2.4159993 2.4159993
 Ca 4.8319986 0.0000000 2.4159993
 -7563.163273284 Hartrees

DS-1CO₂

O -0.0467705 0.0000276 0.1245153
 O 0.0877586 0.0000295 4.7901476
 O 0.1227587 2.4062384 2.4925350
 O 0.0552228 4.8223916 4.7071640
 O 0.1227000 -2.4062235 2.4924877
 O 0.0552015 -4.8224007 4.7071618
 O 2.4220454 0.0000062 2.4445920
 O 2.4026417 2.3807674 4.8423553
 O 2.4026132 -2.3807559 4.8422797
 O 4.7797098 0.0000248 4.8114235
 Ca 0.0000000 2.4159993 0.0000000
 Ca 0.0000000 -2.4159993 0.0000000
 Ca 0.0000000 7.2479980 4.8319986
 Ca 0.0000000 -7.2479980 4.8319986
 Ca 2.4159993 0.0000000 0.0000000
 Ca 2.4159993 4.8319986 4.8319986
 Ca 2.4159993 -4.8319986 4.8319986
 Ca 4.8319986 2.4159993 4.8319986
 Ca 4.8319986 -2.4159993 4.8319986
 Ca -2.4159993 0.0000000 0.0000000
 Ca 7.2479980 0.0000000 4.8319986
 Ca 0.1032214 0.0000202 2.4295506
 Ca 0.0000000 0.0000000 -2.4159993
 Ca 0.0579255 2.5723464 4.8051719
 Ca 0.0000000 4.8319986 2.4159993
 Ca 0.0579191 -2.5723562 4.8050586
 Ca 0.0000000 -4.8319986 2.4159993
 Ca 2.5100918 0.0000268 4.8403931
 Ca 2.4159993 2.4159993 2.4159993
 Ca 2.4159993 -2.4159993 2.4159993
 Ca 4.8319986 0.0000000 2.4159993
 C -0.9131902 -0.0000413 5.7185282
 O -1.3253743 -1.1292067 6.1000889
 O -1.3253712 1.1290572 6.1002696
 -7751.843806340 Hartrees

RC	RC-1CO ₂
O -0.0073887 -0.0079266 0.1169868	O -0.0072214 -0.0091166 0.1233724
O -0.1438113 -0.1448077 4.8865547	O -0.0447044 0.0669331 4.8255850
O -0.0107975 2.4116882 2.4567668	O -0.0183754 2.4090741 2.4587561
O 0.0008063 4.7487478 4.8204085	O 0.0014804 4.7710951 4.8102665
O -0.0395485 -2.4256530 2.4964769	O -0.0634630 -2.4142932 2.5365629
O 0.1190103 -4.7790529 4.8349350	O 0.1347872 -4.8486379 4.8055559
O 2.4132768 -0.0112670 2.4564089	O 2.3979454 -0.0133501 2.4599508
O 2.3739902 2.3730214 4.8068049	O 2.3841148 2.4001699 4.7656845
O 2.4160518 -2.3983310 4.8027964	O 2.3689471 -2.4061746 4.7880220
O 4.7504991 0.0008422 4.8195711	O 4.7655064 0.0046172 4.8193874
O -2.4251959 -0.0400916 2.4964769	O -2.4095499 -0.0552501 2.5267380
O -2.3982743 2.4155391 4.8026337	O -2.3896421 2.3883979 4.8124538
O -4.7786462 0.1188683 4.8347397	O -4.8262451 0.1364202 4.8085717
Ca 0.0000000 2.4159993 0.0000000	Ca 0.0000000 2.4159993 0.0000000
Ca 0.0000000 -2.4159993 0.0000000	Ca 0.0000000 -2.4159993 0.0000000
Ca 0.0000000 7.2479980 4.8319986	Ca 0.0000000 7.2479980 4.8319986
Ca 0.0000000 -7.2479980 4.8319986	Ca 0.0000000 -7.2479980 4.8319986
Ca 2.4159993 0.0000000 0.0000000	Ca 2.4159993 0.0000000 0.0000000
Ca 2.4159993 4.8319986 4.8319986	Ca 2.4159993 4.8319986 4.8319986
Ca 2.4159993 -4.8319986 4.8319986	Ca 2.4159993 -4.8319986 4.8319986
Ca 4.8319986 2.4159993 4.8319986	Ca 4.8319986 2.4159993 4.8319986
Ca 4.8319986 -2.4159993 4.8319986	Ca 4.8319986 -2.4159993 4.8319986
Ca -2.4159993 0.0000000 0.0000000	Ca -2.4159993 0.0000000 0.0000000
Ca -2.4159993 4.8319986 4.8319986	Ca -2.4159993 4.8319986 4.8319986
Ca -4.8319986 2.4159993 4.8319986	Ca -4.8319986 2.4159993 4.8319986
Ca 7.2479980 0.0000000 4.8319986	Ca 7.2479980 0.0000000 4.8319986
Ca -7.2479980 0.0000000 4.8319986	Ca -7.2479980 0.0000000 4.8319986
Ca -0.0124881 -0.0123922 2.4791353	Ca 0.0075938 -0.0006592 2.4298525
Ca 0.0000000 0.0000000 -2.4159993	Ca 0.0000000 0.0000000 -2.4159993
Ca 0.0107572 2.4315948 4.8196402	Ca 0.0373439 2.5295499 4.8321463
Ca 0.0000000 4.8319986 2.4159993	Ca 0.0000000 4.8319986 2.4159993
Ca 0.1985271 -2.5146679 4.8471778	Ca 0.1366083 -2.7026290 4.9015315
Ca 0.0000000 -4.8319986 2.4159993	Ca 0.0000000 -4.8319986 2.4159993
Ca 2.4313640 0.0108808 4.8194030	Ca 2.5086254 0.0397444 4.9186284
Ca 2.4159993 2.4159993 2.4159993	Ca 2.4159993 2.4159993 2.4159993
Ca 2.4159993 -2.4159993 2.4159993	Ca 2.4159993 -2.4159993 2.4159993
Ca 4.8319986 0.0000000 2.4159993	Ca 4.8319986 0.0000000 2.4159993
Ca -2.5146383 0.1983677 4.8471907	Ca -2.6510379 0.1419415 4.9084863
Ca -2.4159993 2.4159993 2.4159993	Ca -2.4159993 2.4159993 2.4159993
Ca -2.4159993 -2.4159993 2.4159993	Ca -2.4159993 -2.4159993 2.4159993
Ca -4.8319986 0.0000000 2.4159993	Ca -4.8319986 0.0000000 2.4159993
-9840.533157313 Hartrees	C -0.1096111 -0.3206115 6.1128399
	O -1.0941102 -1.1148228 6.3751898
	O 0.7860128 0.0524244 6.8922079
	-10029.19635694 Hartrees

E	E-1CO₂
O -0.0038950 0.0000103 0.0332000	O 0.0116891 -0.0000004 0.0422770
O 0.0654522 -0.0000115 4.6940178	O 0.0410322 0.0000010 4.7159095
O 0.0521441 2.4325390 2.3719693	O 0.0440612 2.4095241 2.3835182
O 0.0287124 4.7651151 4.7328875	O 0.0578091 4.8123937 4.7150788
O 0.0521499 -2.4325611 2.3719365	O 0.0440606 -2.4095229 2.3835214
O 0.0287104 -4.7651246 4.7328775	O 0.0578111 -4.8123944 4.7150811
O 2.3926970 0.0000016 2.4266757	O 2.3706514 0.0000000 2.4476250
O 2.3852568 2.3999204 4.7947609	O 2.3766659 2.3854039 4.8009090
O 2.3852454 -2.3999157 4.7947535	O 2.3766707 -2.3854058 4.8009087
O 4.7580144 -0.0000038 4.8697254	O 4.7481953 0.0000004 4.8529836
Ca 0.0000000 2.4159993 0.0000000	Ca 0.0000000 2.4159993 0.0000000
Ca 0.0000000 -2.4159993 0.0000000	Ca 0.0000000 -2.4159993 0.0000000
Ca 0.0000000 7.2479980 4.8319986	Ca 0.0000000 7.2479980 4.8319986
Ca 0.0000000 -7.2479980 4.8319986	Ca 0.0000000 -7.2479980 4.8319986
Ca 2.4159993 0.0000000 0.0000000	Ca 2.4159993 0.0000000 0.0000000
Ca 2.4159993 4.8319986 4.8319986	Ca 2.4159993 4.8319986 4.8319986
Ca 2.4159993 -4.8319986 4.8319986	Ca 2.4159993 -4.8319986 4.8319986
Ca 4.8319986 2.4159993 4.8319986	Ca 4.8319986 2.4159993 4.8319986
Ca 4.8319986 -2.4159993 4.8319986	Ca 4.8319986 -2.4159993 4.8319986
Ca 7.2479980 0.0000000 4.8319986	Ca 7.2479980 0.0000000 4.8319986
Ca 0.0089211 0.0000060 2.3882800	Ca 0.0045085 -0.0000014 2.3293457
Ca 0.0000000 0.0000000 -2.4159993	Ca 0.0000000 0.0000000 -2.4159993
Ca 0.0945672 2.3982997 4.6977316	Ca 0.0352822 2.5706663 4.7725193
Ca 0.0000000 4.8319986 2.4159993	Ca 0.0000000 4.8319986 2.4159993
Ca 0.0945424 -2.3983130 4.6977008	Ca 0.0352969 -2.5706661 4.7725359
Ca 0.0000000 -4.8319986 2.4159993	Ca 0.0000000 -4.8319986 2.4159993
Ca 2.4219236 0.0000099 4.7995743	Ca 2.4793037 -0.0000002 4.8048560
Ca 2.4159993 2.4159993 2.4159993	Ca 2.4159993 2.4159993 2.4159993
Ca 2.4159993 -2.4159993 2.4159993	Ca 2.4159993 -2.4159993 2.4159993
Ca 4.8319986 0.0000000 2.4159993	Ca 4.8319986 0.0000000 2.4159993
-7558.342851235 Hartrees	C -0.9245038 -0.0000027 5.6780105
	O -1.3223085 -1.1290056 6.0776493
	O -1.3224034 1.1290050 6.0775396
	-7747.025144129 Hartrees

E-2CO₂

O 0.0119245 0.0002105 0.0461743
 O -0.0120282 -0.0426552 4.6986961
 O 0.0992878 2.4250313 2.3790751
 O 0.2048724 4.8780692 4.8817485
 O 0.0462204 -2.4076384 2.3783198
 O 0.0603460 -4.8161133 4.7083584
 O 2.3666503 -0.0038409 2.4546750
 O 2.3340336 2.3987204 4.7862477
 O 2.3796234 -2.3816942 4.7935403
 O 4.7389266 0.0015787 4.8484496
 Ca 0.0000000 2.4159993 0.0000000
 Ca 0.0000000 -2.4159993 0.0000000
 Ca 0.0000000 7.2479980 4.8319986
 Ca 0.0000000 -7.2479980 4.8319986
 Ca 2.4159993 0.0000000 0.0000000
 Ca 2.4159993 4.8319986 4.8319986
 Ca 2.4159993 -4.8319986 4.8319986
 Ca 4.8319986 2.4159993 4.8319986
 Ca 4.8319986 -2.4159993 4.8319986
 Ca 7.2479980 0.0000000 4.8319986
 Ca 0.0046197 -0.0350046 2.3119501
 Ca 0.0000000 0.0000000 -2.4159993
 Ca -0.0119915 2.3701090 4.7204895
 Ca 0.0000000 4.8319986 2.4159993
 Ca 0.0447889 -2.5942734 4.7747218
 Ca 0.0000000 -4.8319986 2.4159993
 Ca 2.4858271 -0.0208982 4.8047533
 Ca 2.4159993 2.4159993 2.4159993
 Ca 2.4159993 -2.4159993 2.4159993
 Ca 4.8319986 0.0000000 2.4159993
 C -0.7245740 -0.0691254 5.8764964
 O -1.0656096 -1.2013115 6.3025399
 O -0.9394055 1.0478207 6.4134120
 C -1.1678578 4.9187461 5.0296286
 O -1.7804785 4.0005287 4.4215378
 O -1.6342432 5.8830499 5.6651426
 -7935.680893919 Hartrees

E-2CO₂ (1,2 T)

O 0.0227337 0.0108256 0.0649658
 O 0.1137920 0.1098043 4.8223551
 O 0.0778286 2.4166291 2.4366706
 O -0.0239182 4.8529911 4.6295936
 O 0.0612170 -2.3944480 2.4021250
 O 0.0609536 -4.8089740 4.7118772
 O 2.3735414 0.0320982 2.4868082
 O 2.4359732 2.4539307 4.7708058
 O 2.3903313 -2.4029278 4.8121015
 O 4.7528392 -0.0295869 4.7538517
 Ca 0.0000000 2.4159993 0.0000000
 Ca 0.0000000 -2.4159993 0.0000000
 Ca 0.0000000 7.2479980 4.8319986
 Ca 0.0000000 -7.2479980 4.8319986
 Ca 2.4159993 0.0000000 0.0000000
 Ca 2.4159993 4.8319986 4.8319986
 Ca 2.4159993 -4.8319986 4.8319986
 Ca 4.8319986 2.4159993 4.8319986
 Ca 4.8319986 -2.4159993 4.8319986
 Ca 7.2479980 0.0000000 4.8319986
 Ca 0.0292883 0.0224833 2.3736691
 Ca 0.0000000 0.0000000 -2.4159993
 Ca -0.2198853 2.6987553 4.8430809
 Ca 0.0000000 4.8319986 2.4159993
 Ca 0.0304458 -2.5851263 4.7680348
 Ca 0.0000000 -4.8319986 2.4159993
 Ca 2.5511279 -0.1343049 4.9109199
 Ca 2.4159993 2.4159993 2.4159993
 Ca 2.4159993 -2.4159993 2.4159993
 Ca 4.8319986 0.0000000 2.4159993
 C -1.0618635 0.0242639 5.5071530
 O -1.4607258 -1.1293097 5.8246787
 O -1.6655787 1.1098871 5.7412674
 C 2.4034504 2.4638788 6.1523819
 O 3.1819539 1.6578817 6.7092413
 O 1.6368231 3.3155007 6.6561100
 -7935.667065334 Hartrees

E-2CO₂ (1,3 T) O 0.0172539 -0.0053706 0.0411487 O -0.0241317 0.0082037 4.6969707 O 0.0147695 2.3995535 2.3674071 O 0.0423430 4.8181251 4.7072558 O 0.0413434 -2.4026801 2.3836591 O 0.0612055 -4.7986240 4.7091805 O 2.3817841 0.0010409 2.4776423 O 2.3128216 2.3790241 4.7002376 O 2.3774234 -2.3107508 4.7834255 O 4.7943877 0.0436817 4.7398662 Ca 0.0000000 2.4159993 0.0000000 Ca 0.0000000 -2.4159993 0.0000000 Ca 0.0000000 7.2479980 4.8319986 Ca 0.0000000 -7.2479980 4.8319986 Ca 2.4159993 0.0000000 0.0000000 Ca 2.4159993 4.8319986 4.8319986 Ca 2.4159993 -4.8319986 4.8319986 Ca 4.8319986 2.4159993 4.8319986 Ca 4.8319986 -2.4159993 4.8319986 Ca 7.2479980 0.0000000 4.8319986 Ca -0.0318014 0.0042016 2.3032645 Ca 0.0000000 0.0000000 -2.4159993 Ca -0.0393276 2.6011212 4.7363589 Ca 0.0000000 4.8319986 2.4159993 Ca -0.0049821 -2.5707846 4.7570388 Ca 0.0000000 -4.8319986 2.4159993 Ca 2.2670637 0.0723309 4.8175234 Ca 2.4159993 2.4159993 2.4159993 Ca 2.4159993 -2.4159993 2.4159993 Ca 4.8319986 0.0000000 2.4159993 C -1.0673367 0.0057858 5.5871632 O -1.4819082 -1.1269470 5.9473583 O -1.4934133 1.1341120 5.9432468 C 4.8036307 0.0456154 6.1448340 O 5.4065495 -0.9127321 6.6594666 O 4.2333138 1.0195875 6.6738678 -7935.669217411 Hartrees	C1 O 0.0794441 0.0794489 -0.1096344 O 0.2006528 0.2006823 4.5706969 O 0.0384709 2.4110445 2.3469856 O 0.0127345 4.7690243 4.8098093 O 2.4110233 0.0384865 2.3469772 O 2.4126691 2.4126964 4.7753049 O 4.7689655 0.0127650 4.8097772 Ca 0.0000000 2.4159993 0.0000000 Ca 0.0000000 7.2479980 4.8319986 Ca 2.4159993 0.0000000 0.0000000 Ca 2.4159993 4.8319986 4.8319986 Ca 4.8319986 2.4159993 4.8319986 Ca 7.2479980 0.0000000 4.8319986 Ca 0.0985592 0.0985616 2.3747083 Ca 0.0000000 0.0000000 -2.4159993 Ca 0.0919029 2.4367320 4.7217916 Ca 0.0000000 4.8319986 2.4159993 Ca 2.4367361 0.0918970 4.7218003 Ca 2.4159993 2.4159993 2.4159993 Ca 4.8319986 0.0000000 2.4159993 -5284.560052472 Hartrees C1-1CO₂ O 0.0769692 0.0769767 -0.1004855 O 0.3680625 0.3680903 5.9817495 O 0.0660041 2.3804851 2.3668115 O 0.0170555 4.7735549 4.8061861 O 2.3804569 0.0660161 2.3668012 O 2.3838509 2.3838818 4.7479883 O 4.7735006 0.0170804 4.8061541 Ca 0.0000000 2.4159993 0.0000000 Ca 0.0000000 7.2479980 4.8319986 Ca 2.4159993 0.0000000 0.0000000 Ca 2.4159993 4.8319986 4.8319986 Ca 4.8319986 2.4159993 4.8319986 Ca 7.2479980 0.0000000 4.8319986 Ca 0.0407500 0.0407656 2.2472576 Ca 0.0000000 0.0000000 -2.4159993 Ca 0.0356608 2.5335948 4.7794438 Ca 0.0000000 4.8319986 2.4159993 Ca 2.5335841 0.0356467 4.7794478 Ca 2.4159993 2.4159993 2.4159993 Ca 4.8319986 0.0000000 2.4159993 C -0.1848471 -0.1848037 4.9541282 O -1.1842490 0.3954513 4.3718117 O 0.3953617 -1.1841932 4.3717904 -5473.244242959 Hartrees
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C1-2CO₂ O 0.0867288 0.0781243 -0.1091049 O 0.4617228 0.0627642 5.8704519 O 0.0502101 2.3616498 2.3991524 O 0.0358216 4.7976145 4.7513516 O 2.3890857 0.0678192 2.3618477 O 2.3464896 2.3730446 4.7586285 O 4.7861703 0.0123176 4.7914589 Ca 0.0000000 2.4159993 0.0000000 Ca 0.0000000 7.2479980 4.8319986 Ca 2.4159993 0.0000000 0.0000000 Ca 2.4159993 4.8319986 4.8319986 Ca 4.8319986 2.4159993 4.8319986 Ca 7.2479980 0.0000000 4.8319986 Ca 0.0619962 -0.0418982 2.1807674 Ca 0.0000000 0.0000000 -2.4159993 Ca -0.0074116 2.1860893 4.8108664 Ca 0.0000000 4.8319986 2.4159993 Ca 2.5861938 -0.0508681 4.7433707 Ca 2.4159993 2.4159993 2.4159993 Ca 4.8319986 0.0000000 2.4159993 C -0.0809550 -0.4978767 4.8347028 O -1.0922057 0.0927260 4.2706157 O 0.5102478 -1.4641172 4.2365449 C -0.8897443 4.7687165 5.7783749 O -1.2538629 3.6322646 6.1570944 O -1.2562114 5.8848508 6.2147511 -5661.920881236 Hartrees	C2 Ca 4.8572392 0.0346824 2.3704881 Ca 2.5112446 2.5015996 2.3396473 Ca 2.5163773 0.1793796 4.6717717 Ca 0.0627325 4.8551278 2.3573268 Ca 0.1986676 2.5198099 4.6805763 Ca 0.0000000 0.0000000 -2.4159993 Ca 0.1562524 0.1595339 2.3768593 Ca 7.2298017 0.1257323 4.7240497 Ca 4.8675894 2.5028617 4.7390383 Ca 2.5215029 4.8743873 4.7400998 Ca 2.4159993 0.0000000 0.0000000 Ca 0.1206369 7.2219165 4.7269871 Ca 0.0000000 2.4159993 0.0000000 Ca 7.2479979 0.0000000 0.0000000 Ca 9.6639972 0.0000000 2.4159993 Ca 4.8319986 0.0000000 -2.4159993 Ca 2.4159993 2.4159993 -2.4159993 Ca 0.0000000 4.8319986 -2.4159993 Ca 4.8319986 2.4159993 0.0000000 Ca 12.0799965 0.0000000 4.8319986 Ca 9.6639972 2.4159993 4.8319986 Ca 0.0000000 12.0799965 4.8319986 Ca 2.4159993 9.6639972 4.8319986 Ca 4.8319986 7.2479979 4.8319986 Ca 7.2479979 4.8319986 4.8319986 Ca 0.0000000 9.6639972 2.4159993 Ca 2.4159993 7.2479979 2.4159993 Ca 4.8319986 4.8319986 2.1459994 Ca 7.2479979 2.4159993 2.4159993 Ca 2.4159993 4.8319986 0.0000000 Ca 0.0000000 7.2479979 0.0000000 O 4.8863727 0.1321214 4.7085888 O 2.5029961 2.4920178 4.7378950 O 2.4767036 0.0679504 2.3620006 O 0.1540148 4.8805625 4.7094990 O 0.0796010 2.4718208 2.3674752 O 0.2801778 0.2747823 4.6099958 O 0.0765409 0.0766128 -0.0010477 O 7.2490658 0.0252634 2.4186060 O 4.8752808 -0.0045237 0.0137366 O 2.4233835 2.4117660 0.0298220 O -0.0004572 4.8605775 0.0244114 O 9.6211376 0.0080779 4.8385137 O 7.2509138 2.4097008 4.8130769 O 4.8478555 4.8430513 4.8161128 O 2.4151332 7.2477322 4.8128150 O 0.0080798 9.6191553 4.8419642 O 0.0297044 7.2466040 2.4262269 O 2.4598117 4.8573311 2.3747926 O 4.8553769 2.4455848 2.3833470 -15020.29249130 Hartrees
C1-2CO₂ (1,2 T) O 0.0911626 0.0910699 -0.0772078 O 0.5044353 0.5048778 5.8813768 O 0.0988847 2.3883664 2.4189987 O -0.0721492 4.8033899 4.7030639 O 2.3883258 0.0989531 2.4189688 O 2.4447738 2.4450162 4.7593242 O 4.8034692 -0.0720075 4.7031145 Ca 0.0000000 2.4159993 0.0000000 Ca 0.0000000 7.2479980 4.8319986 Ca 2.4159993 0.0000000 0.0000000 Ca 2.4159993 4.8319986 4.8319986 Ca 4.8319986 2.4159993 4.8319986 Ca 7.2479980 0.0000000 4.8319986 Ca 0.0601082 0.0598677 2.2815929 Ca 0.0000000 0.0000000 -2.4159993 Ca -0.1734338 2.6498883 4.8757871 Ca 0.0000000 4.8319986 2.4159993 Ca 2.6500731 -0.1731163 4.8765065 Ca 2.4159993 2.4159993 2.4159993 Ca 4.8319986 0.0000000 2.4159993 C -0.1263237 -0.1263340 4.9454170 O -1.1733364 0.4085863 4.4108589 O 0.4089998 -1.1733375 4.4112963 C 2.5002358 2.5002679 6.1447683 O 1.7547582 3.3565517 6.6668428 O 3.3558035 1.7536753 6.6665185 -5661.886619113 Hartrees	

C2-1CO₂

Ca 4.8591063 0.0601581 2.3539204
 Ca 2.4745942 2.4665274 2.3469049
 Ca 2.6206254 0.1071648 4.7476154
 Ca 0.0738930 4.8530303 2.3515771
 Ca 0.1270824 2.6181282 4.7541055
 Ca 0.0000000 0.0000000 -2.4159993
 Ca 0.0932687 0.0929626 2.2781498
 Ca 7.2360282 0.1198855 4.7217604
 Ca 4.8523431 2.5004419 4.7504150
 Ca 2.5121609 4.8559099 4.7503456
 Ca 2.4159993 0.0000000 0.0000000
 Ca 0.1191422 7.2315238 4.7208338
 Ca 0.0000000 2.4159993 0.0000000
 Ca 7.2479979 0.0000000 0.0000000
 Ca 9.6639972 0.0000000 2.4159993
 Ca 4.8319986 0.0000000 -2.4159993
 Ca 2.4159993 2.4159993 -2.4159993
 Ca 0.0000000 4.8319986 -2.4159993
 Ca 4.8319986 2.4159993 0.0000000
 Ca 12.0799965 0.0000000 4.8319986
 Ca 9.6639972 2.4159993 4.8319986
 Ca 0.0000000 12.0799965 4.8319986
 Ca 2.4159993 9.6639972 4.8319986
 Ca 4.8319986 7.2479979 4.8319986
 Ca 7.2479979 4.8319986 4.8319986
 Ca 0.0000000 9.6639972 2.4159993
 Ca 2.4159993 7.2479979 2.4159993
 Ca 4.8319986 4.8319986 2.1459994
 Ca 7.2479979 2.4159993 2.4159993
 Ca 2.4159993 4.8319986 0.0000000
 Ca 0.0000000 7.2479979 0.0000000
 O 4.8851007 0.1297983 4.7174308
 O 2.4577130 2.4510542 4.7206845
 O 2.4381488 0.0937608 2.4052525
 O 0.1421987 4.8837471 4.7176910
 O 0.1021197 2.4357134 2.4067881
 O -1.1236151 0.4554541 4.4513470
 O 0.0707612 0.0718282 0.0039437
 O 7.2443522 0.0314226 2.4212002
 O 4.8536748 -0.0011703 0.0305461
 O 2.4026837 2.4017190 0.0333327
 O -0.0027686 4.8547930 0.0311907
 O 9.6145500 0.0116302 4.8367634
 O 7.2443038 2.4105398 4.8112515
 O 4.8410107 4.8407128 4.8202680
 O 2.4126725 7.2454828 4.8097096
 O 0.0112590 9.6146799 4.8354510
 O 0.0340413 7.2448116 2.4202449
 O 2.4484385 4.8644149 2.3875789
 O 4.8620324 2.4429560 2.3909365
 C -0.1082871 -0.1127716 5.0155024
 O 0.4724999 0.4622222 6.0180829
 O 0.4532257 -1.1300972 4.4475863
 -15208.98510236 Hartrees

C2-2CO₂

Ca 4.8752657 0.0596395 2.3353676
 Ca 2.4514534 2.4454044 2.3683552
 Ca 2.6752196 0.0180751 4.7150940
 Ca 0.0576509 4.8331900 2.3178798
 Ca 0.0759205 2.3263214 4.8412315
 Ca 0.0000000 0.0000000 -2.4159993
 Ca 0.1031465 0.0280133 2.2300200
 Ca 7.2514857 0.1091421 4.7156852
 Ca 4.8580268 2.4696587 4.7494796
 Ca 2.5576784 4.8293326 4.7619154
 Ca 2.4159993 0.0000000 0.0000000
 Ca 0.0593365 7.4065307 4.7817428
 Ca 0.0000000 2.4159993 0.0000000
 Ca 7.2479979 0.0000000 0.0000000
 Ca 9.6639972 0.0000000 2.4159993
 Ca 4.8319986 0.0000000 -2.4159993
 Ca 2.4159993 2.4159993 -2.4159993
 Ca 0.0000000 4.8319986 -2.4159993
 Ca 4.8319986 2.4159993 0.0000000
 Ca 12.0799965 0.0000000 4.8319986
 Ca 9.6639972 2.4159993 4.8319986
 Ca 0.0000000 12.0799965 4.8319986
 Ca 2.4159993 9.6639972 4.8319986
 Ca 4.8319986 7.2479979 4.8319986
 Ca 7.2479979 4.8319986 4.8319986
 Ca 0.0000000 9.6639972 2.4159993
 Ca 2.4159993 7.2479979 2.4159993
 Ca 4.8319986 4.8319986 2.1459994
 Ca 7.2479979 2.4159993 2.4159993
 Ca 2.4159993 4.8319986 0.0000000
 Ca 0.0000000 7.2479979 0.0000000
 O 4.9133529 0.1102393 4.6954296
 O 2.4447246 2.4187990 4.7483321
 O 2.4468520 0.0854731 2.3914328
 O 0.0930927 4.8275556 4.7700815
 O 0.0755365 2.4131366 2.4306625
 O -1.0270166 0.1777937 4.3679446
 O 0.0791191 0.0726483 -0.0162916
 O 7.2477158 0.0340074 2.4126928
 O 4.8534195 0.0045792 0.0259021
 O 2.3938976 2.4118511 0.0459967
 O 0.0021580 4.8488023 0.0475494
 O 9.6127145 0.0124438 4.8311472
 O 7.2398318 2.4076316 4.8096704
 O 4.8288511 4.8333582 4.8044949
 O 2.3976986 7.2238755 4.8156426
 O 0.0366409 9.6555526 4.8075736
 O 0.0233120 7.2245310 2.4339468
 O 2.4120151 4.8582794 2.4240881
 O 4.8539801 2.4422958 2.3945312
 C -0.0037551 -0.4070569 4.9106868
 O 0.5775138 0.1659440 5.9197655
 O 0.5568982 -1.4003225 4.3233354
 C -0.8210060 4.8597277 5.7790608
 O -1.2123758 5.9980628 6.1666432
 O -1.1917351 3.7453251 6.2382806
 -15397.66397172 Hartrees

C2-2CO₂ (1,2 T)

Ca 4.8699857 0.0653688 2.3343397
Ca 2.4806191 2.4802774 2.3657595
Ca 2.7136620 -0.0744963 4.8159613
Ca 0.0655832 4.8696803 2.3344565
Ca -0.0737783 2.7133236 4.8164697
Ca 0.0000000 0.0000000 -2.4159993
Ca 0.1108886 0.1107646 2.3007911
Ca 7.2677336 0.0639078 4.6861141
Ca 4.9691132 2.4304929 4.8475386
Ca 2.4307472 4.9689461 4.8474997
Ca 2.4159993 0.0000000 0.0000000
Ca 0.0640065 7.2675261 4.6861010
Ca 0.0000000 2.4159993 0.0000000
Ca 7.2479979 0.0000000 0.0000000
Ca 9.6639972 0.0000000 2.4159993
Ca 4.8319986 0.0000000 -2.4159993
Ca 2.4159993 2.4159993 -2.4159993
Ca 0.0000000 4.8319986 -2.4159993
Ca 4.8319986 2.4159993 0.0000000
Ca 12.0799965 0.0000000 4.8319986
Ca 9.6639972 2.4159993 4.8319986
Ca 0.0000000 12.0799965 4.8319986
Ca 2.4159993 9.6639972 4.8319986
Ca 4.8319986 7.2479979 4.8319986
Ca 7.2479979 4.8319986 4.8319986
Ca 0.0000000 9.6639972 2.4159993
Ca 2.4159993 7.2479979 2.4159993
Ca 4.8319986 4.8319986 2.1459994
Ca 7.2479979 2.4159993 2.4159993
Ca 2.4159993 4.8319986 0.0000000
Ca 0.0000000 7.2479979 0.0000000
O 4.9463351 0.0250406 4.6208407
O 2.4133977 2.4127884 4.8060400
O 2.4468351 0.1130259 2.4605887
O 0.0253137 4.9461214 4.6209985
O 0.1133388 2.4466234 2.4607017
O -1.1377933 0.4465355 4.4455718
O 0.0820845 0.0820826 0.0167639
O 7.2636846 0.0326343 2.3944386
O 4.8420882 0.0018812 0.0166179
O 2.4012751 2.4012390 0.0616273
O 0.0018902 4.8420659 0.0166867
O 9.6202500 0.0001112 4.8218664
O 7.2577968 2.3957840 4.8045815
O 4.8062520 4.8062367 4.8152983
O 2.3958295 7.2577548 4.8045878
O 0.0001090 9.6202926 4.8219486
O 0.0326509 7.2636422 2.3944965
O 2.4382125 4.8516846 2.4150423
O 4.8517826 2.4380786 2.4150556
C -0.0939493 -0.0945641 4.9859549
O 0.5205251 0.5195497 5.9383040
O 0.4467557 -1.1384224 4.4452156
C 2.5105375 2.5101651 6.1730636
O 1.7660904 3.3700140 6.7091933
O 3.3707110 1.7664183 6.7095354
-15397.63154237 Hartrees

S6.2. Periodic models

T1-pbc-OCO2 (-609.05956 eV)

1.000000000000000

9.621999999999999	0.000000000000000	0.000000000000000
0.000000000000000	9.621999999999999	0.000000000000000
0.000000000000000	0.000000000000000	24.432999999999998

Ca O

48 48

Selective dynamics

Direct

0.000000000000000	0.000000000000000	0.000000000000000	F	F	F
-0.0000000119886620	0.0000002199171667	0.1975496196938507	T	T	T
0.0000002850500234	-0.0000006786198641	0.3957866705650152	T	T	T
0.000000000000000	0.250000000000000	0.0984529120451825	F	F	F
0.0000007153031546	0.2500001090775719	0.2966223765621011	T	T	T
0.0000000570071093	0.2499994964793976	0.4935270726047673	T	T	T
0.250000000000000	0.000000000000000	0.0984529120451825	F	F	F
0.249998535618076	-0.0000000825157842	0.2966223525337989	T	T	T
0.2500005822863960	0.9999992536268336	0.4935277355905729	T	T	T
0.250000000000000	0.250000000000000	0.000000000000000	F	F	F
0.2499996154209043	0.2500001906444176	0.1975493813577079	T	T	T
0.2500009723169287	0.2499996880598108	0.3957865729660624	T	T	T
0.000000000000000	0.500000000000000	0.000000000000000	F	F	F
0.9999999134996114	0.5000004498128953	0.1975496387213367	T	T	T
0.0000003422426691	0.4999998747711844	0.3957867765339410	T	T	T
0.000000000000000	0.750000000000000	0.0984529120451825	F	F	F
0.0000003071151207	0.7500002022844121	0.2966224803662690	T	T	T
0.0000001472652140	0.7500003020531522	0.4935274196462595	T	T	T
0.250000000000000	0.500000000000000	0.0984529120451825	F	F	F
0.2500001917855182	0.4999998594848179	0.2966224732254432	T	T	T
0.2500003400990033	0.4999997824037208	0.4935280015651481	T	T	T
0.250000000000000	0.750000000000000	0.000000000000000	F	F	F
0.2499998408465674	0.749999982784056	0.1975494577984933	T	T	T
0.2500004333491271	0.7499991617603006	0.3957867164648768	T	T	T
0.500000000000000	0.000000000000000	0.000000000000000	F	F	F
0.4999998635868271	0.0000004756966527	0.1975494810806754	T	T	T
0.5000003729482595	-0.0000000382829340	0.3957862026298256	T	T	T
0.500000000000000	0.250000000000000	0.0984529120451825	F	F	F
0.4999999404268205	0.2500002115975662	0.2966221477701733	T	T	T
0.5000004092855570	0.2499993060006838	0.4935272693739493	T	T	T
0.750000000000000	0.000000000000000	0.0984529120451825	F	F	F
0.7500000645923616	0.0000000263561727	0.2966221082913947	T	T	T
0.7500003413595495	0.0000000879085289	0.4935280503442743	T	T	T
0.750000000000000	0.250000000000000	0.000000000000000	F	F	F
0.7500001743882649	0.2500004224591821	0.1975492974829397	T	T	T
0.7499996286530271	0.2499990558350445	0.3957863618308324	T	T	T
0.500000000000000	0.500000000000000	0.000000000000000	F	F	F
0.5000004984222600	0.5000002322475320	0.1975495501487853	T	T	T
0.5000005293448783	0.4999995127169967	0.3957865148011909	T	T	T
0.500000000000000	0.750000000000000	0.0984529120451825	F	F	F
0.5000003606187168	0.749999842153879	0.2966221539060066	T	T	T
0.5000002689192179	0.7500001321149344	0.4935271189361188	T	T	T
0.750000000000000	0.500000000000000	0.0984529120451825	F	F	F
0.7500005799091052	0.5000005477332116	0.2966220403591623	T	T	T
0.7500004051498542	0.5000001537074810	0.4935272569073161	T	T	T
0.750000000000000	0.750000000000000	0.000000000000000	F	F	F
0.7500004062779930	0.7500009914304588	0.1975492390163679	T	T	T
0.7500008605939579	0.7500001305604168	0.3957865920470559	T	T	T
0.250000000000000	0.250000000000000	0.0984529120451825	F	F	F

0.2500000014137869	0.2500000729541271	0.2964290499006000	T	T	T
0.2500000743662431	0.2500003110117886	0.4924622783181281	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2500004924543213	0.0000007443257819	0.1976217912493650	T	T	T
0.2499998243404314	0.9999997258921658	0.3961331636129198	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.9999999279904682	0.2500001932921851	0.1976221976392976	T	T	T
-0.0000000220896123	0.2500002679173086	0.3961331305003600	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.0000003350779372	0.0000005180539269	0.2964287279428501	T	T	T
0.0000003278133098	0.9999998236503087	0.4924625310686234	T	T	T
0.2500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.2500000019693797	0.7500008614611505	0.2964291171994036	T	T	T
0.2500003354811092	0.7499997931514030	0.4924623233363145	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2500005663872273	0.5000004413133117	0.1976219956656921	T	T	T
0.2500001792433896	0.4999991589057798	0.3961333051853347	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.9999999345502207	0.7500003454560720	0.1976217826049830	T	T	T
0.0000000559181790	0.7499996490460827	0.3961333735182109	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.9999995836969735	0.5000006965367696	0.2964286994788009	T	T	T
0.0000000488329357	0.4999998148218652	0.4924625595142805	T	T	T
0.7500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.7499997649256976	0.2499999206662443	0.2964288682705798	T	T	T
0.7499998929602963	0.2499999406765176	0.4924627470230577	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7500000876742922	0.0000003572390639	0.1976217125000003	T	T	T
0.7499999475207175	0.0000005651140933	0.3961332152793230	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4999999365265184	0.2499995665040996	0.1976219768862876	T	T	T
0.5000004239370279	0.2500003790659041	0.3961328528706676	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.4999999064519686	0.0000001722575756	0.2964289887334005	T	T	T
0.5000001347192932	0.9999994354188771	0.4924623099796108	T	T	T
0.7500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.7500000171471342	0.7500003492886753	0.2964290329933143	T	T	T
0.7500002181115516	0.7500003905734125	0.4924625727944811	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7500002072162910	0.5000003524281251	0.1976215829201650	T	T	T
0.7499999430891471	0.4999996888724411	0.3961328415290993	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.5000002043475955	0.7500004414972619	0.1976214921173619	T	T	T
0.5000004487059233	0.7499996293849125	0.3961329415188896	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.5000000808868372	0.4999998794502316	0.2964289425003717	T	T	T
0.5000001955988582	0.5000001508068331	0.4924625474234568	T	T	T

Tl-pbc-1CO2 (-633.47883 eV)

1.0000000000000000		
9.621999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.621999999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	24.432999999999998

Ca O C
48 50 1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
-0.0000394939238223	0.9998491913048317	0.1977417939482587	T	T	T

0.0019303912732211	0.0000672592616862	0.3967486086948340	T	T	T
0.0000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
-0.0000894521193276	0.2500028575780537	0.2967043173278353	T	T	T
0.9864908164423486	0.2500060789944249	0.4948995741514817	T	T	T
0.2500000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.2499977302640568	0.9994612117900777	0.2971188758577358	T	T	T
0.2500009383702362	0.9873244529594956	0.5005357883555208	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2499976464922704	0.2500003184873492	0.1976129331854480	T	T	T
0.2499971884834438	0.2500029733837813	0.3951123608026353	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
-0.0000399963223003	0.5001526806901795	0.1977413367800894	T	T	T
0.0019321238213675	0.4999393425373391	0.3967501437598062	T	T	T
0.0000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.0001915971672375	0.7500025287243336	0.2969747562640984	T	T	T
0.9966819756639730	0.7500039224520588	0.4939046819677260	T	T	T
0.2500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.2499974942958275	0.5005400916628396	0.2971178658008218	T	T	T
0.2499932476336269	0.5126696606887929	0.5005427524699483	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2499975586578786	0.7500011868618673	0.1976337505586948	T	T	T
0.2499990722192212	0.7499955401277041	0.3965135523577789	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5000371866522232	0.9998486345665349	0.1977413394546119	T	T	T
0.4980652195681892	0.0000719682369103	0.3967511428155651	T	T	T
0.5000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.5000815341190402	0.2500029033038504	0.2967045159989881	T	T	T
0.5135005540235003	0.2500011472817480	0.4949014096571951	T	T	T
0.7500000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.7499964886502454	0.9996936214443908	0.2970373915150596	T	T	T
0.7499992442748242	0.9962848136306063	0.4936831523292736	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7499987911995060	0.2499996253150110	0.1975957261137073	T	T	T
0.7499947763467910	0.2500042127341849	0.3950460186605047	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000363132783275	0.5001526023339444	0.1977426683044422	T	T	T
0.4980682068961677	0.4999414213759298	0.3967541138740848	T	T	T
0.5000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.4997997930659142	0.7500032530284094	0.2969749553128043	T	T	T
0.5033109570292522	0.7500031602103322	0.4939061912657822	T	T	T
0.7500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.7499976106442007	0.5003100166479836	0.2970374938594936	T	T	T
0.7500007959425038	0.5037230399485613	0.4936837878231662	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7499991376698122	0.7500018495042620	0.1976216541481868	T	T	T
0.7499951125983271	0.7500037536142373	0.3952216213974749	T	T	T
0.2500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.2499981060154930	0.2500036281414713	0.2982483161730155	T	T	T
0.2499927514393775	0.2499946263803632	0.4993033330855813	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2499986230764850	0.0002963118204591	0.1981179118922081	T	T	T
0.2499980466229619	0.0020695065114662	0.3971336091071980	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0002255159724120	0.2499997952097548	0.1982937532664314	T	T	T
0.0015050224780961	0.2500065051444162	0.3984178405043166	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.0002090700464571	0.0004722538977603	0.2966302225633759	T	T	T
0.9974842979233614	0.0001820397279621	0.4916825545944784	T	T	T
0.2500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.2499978245647670	0.7500023573508667	0.2971691313670777	T	T	T

0.2500003703880346	0.7499965707800630	0.4936322929585300	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2499969415313737	0.4997058044523642	0.1981185744651944	T	T	T
0.2499904281442099	0.4979343876987247	0.3971346714511560	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0001312747649661	0.7500005964981377	0.1980547958268807	T	T	T
0.0002885422173246	0.7500011246726696	0.3967429837558319	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.0002063949778268	0.4995342328500054	0.2966323647796794	T	T	T
0.9974788999372063	0.4998253302654526	0.4916888493068275	T	T	T
0.7500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.7499989319649957	0.2500028733487443	0.2971949753070447	T	T	T
0.7499976986655350	0.2500071855596120	0.4929752433406521	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7499980819670162	0.0001828824935693	0.1979668490658395	T	T	T
0.7499947579255070	0.0003775788548842	0.3961950499566651	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4997741300246286	0.2499991942741072	0.1982935263597248	T	T	T
0.4984863903858416	0.2500002971330134	0.3984214857478899	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.4997874936310193	0.0004714563987085	0.2966325713170846	T	T	T
0.5025192393175872	0.0001811417891743	0.4916865579641034	T	T	T
0.7500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.7499978060176854	0.7500057390266234	0.2967128388352226	T	T	T
0.7499964326190699	0.7500026652609219	0.4923925762618700	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7499979083771369	0.4998215578616719	0.1979669622561968	T	T	T
0.7499922702341302	0.4996335760696928	0.3961976316692676	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.4998660094737960	0.7500017500792807	0.1980546622626140	T	T	T
0.4997031872020534	0.7499995056165905	0.3967450987346571	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.4997845847794566	0.4995325699904773	0.2966323971814177	T	T	T
0.5025071165498088	0.4998181133764503	0.4916857497401826	T	T	T
0.2499782087282548	0.3684899132311428	0.5795778117977652	T	T	T
0.2500012738156080	0.1314861060525674	0.5795731842027072	T	T	T
0.2499938152698837	0.2499838354938474	0.5568172094444513	T	T	T

Tl-pbc-2CO2 (1,2) (-657.83526 eV)

1.0000000000000000

9.6219999999999999 0.0000000000000000 0.0000000000000000

0.0000000000000000 9.6219999999999999 0.0000000000000000

0.0000000000000000 0.0000000000000000 24.4329999999999998

Ca O C

48 52 2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0000809541031609	0.0001025155119651	0.1975999493828607	T	T	T
0.0029533621837181	0.0029906463106950	0.3957305582688269	T	T	T
0.0000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.0000857333196840	0.2504313124371169	0.2969396114028237	T	T	T
0.9890142455687645	0.2516754830963628	0.4970970147188057	T	T	T
0.2500000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.2503947551586773	0.0001156189329649	0.2969443124666685	T	T	T
0.2514854923658102	0.9890047397947976	0.4971758563304105	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2500100053902643	0.2500311916309260	0.1975683635697171	T	T	T
0.2527479112732497	0.2527568860241463	0.3954295682607389	T	T	T

0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.9997350941615760	0.5002327922772096	0.1975661074659978	T	T	T
0.0011501614113383	0.5001526107248362	0.3959066705561313	T	T	T
0.0000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.9992837352518832	0.7506667678066644	0.2970379916107411	T	T	T
0.9936851968453946	0.7561625463838357	0.4922194324409103	T	T	T
0.2500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.2492649393938278	0.5006865821338395	0.2967198254230208	T	T	T
0.2283327379233895	0.5215901085586315	0.5055851261223733	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2497415691285957	0.7502336069259522	0.1975686922015311	T	T	T
0.2497923068658614	0.7488020982636814	0.3959348984495721	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5002044066375764	0.9997614267476328	0.1975687812918994	T	T	T
0.5000683172275006	0.0011834478694254	0.3959316826692178	T	T	T
0.5000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.5006308589183840	0.2493056865061057	0.2967217992795921	T	T	T
0.5214714962379643	0.2283921065575335	0.5055894155901511	T	T	T
0.7500000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.7506167328886603	0.9993254940332137	0.2970400975393647	T	T	T
0.7561463687032827	0.9938289442303582	0.4922158239498212	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7502072764317111	0.2497627778992502	0.1975683027343134	T	T	T
0.7487075504360251	0.2498234343695170	0.3959043410955551	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4999386720255478	0.4999673713004228	0.1975689533796242	T	T	T
0.4971189411663833	0.4972381040370555	0.3954215330253592	T	T	T
0.5000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.4995072745621424	0.7498792886902607	0.2969438503419635	T	T	T
0.4983587971696640	0.7609684211219162	0.4971725556049512	T	T	T
0.7500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.7498200321168670	0.4995617282392716	0.2969361644772567	T	T	T
0.7607866074583213	0.4982981237580835	0.4970859399419456	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7498665195937955	0.7498936533762678	0.1975991049693299	T	T	T
0.7469202197223455	0.7470089163819740	0.3957270821037792	T	T	T
0.2500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.2505273257785928	0.2505755418765846	0.2977546159774879	T	T	T
0.2576191098394448	0.2575698560721738	0.4940725348466069	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2502180773314054	0.0003401912946312	0.1982330453932940	T	T	T
0.2516661468248633	0.0030601571658597	0.3978070061652327	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0003150976922547	0.2502422423829347	0.1982353992368716	T	T	T
0.0030234815383354	0.2517344985364117	0.3978192520381058	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.0009650344896012	0.0010141507388940	0.2967438048655598	T	T	T
0.0037783523482748	0.0039162871149629	0.4924402623984968	T	T	T
0.2500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.2497131775367285	0.7504124722359657	0.2968341165970534	T	T	T
0.2415082792683438	0.7551156036180162	0.4908053248243240	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2500217391708030	0.4999437308100533	0.1982746734145053	T	T	T
0.2499007305823648	0.5000083872805822	0.3975657503694121	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.9998343898522362	0.7501379089686167	0.1980821375262093	T	T	T
0.9979166594681723	0.7519894254061736	0.3959902901233969	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.9995229730192824	0.5002188663379282	0.2968316733116030	T	T	T
0.9946857845488458	0.5082783220093552	0.4907780476411698	T	T	T

0.7500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.7503744562236100	0.2497667794927768	0.2968325512510384	T	T	T
0.7551325602094973	0.2417193644225245	0.4907741843360661	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7501125303252052	0.9998599020949239	0.1980821242689072	T	T	T
0.7519497442729355	0.9979987905792037	0.3959959332751007	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4999225822749770	0.2500476832443278	0.1982738692485699	T	T	T
0.4999482845263997	0.2499835967917146	0.3975519457931588	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.5001803016646015	0.9995787725217901	0.2968318813984176	T	T	T
0.5083193555349437	0.9948614401217083	0.4908007644965034	T	T	T
0.7500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.7489388832924281	0.7489786450372246	0.2967421861971786	T	T	T
0.7460691283135630	0.7460736746345973	0.4924355021886608	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7496299990153695	0.4997467063306242	0.1982337861329494	T	T	T
0.7468490151658763	0.4982498143123112	0.3978132286743833	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.4997276415955315	0.7496572492458184	0.1982302402805535	T	T	T
0.4981987854147842	0.7469288267108598	0.3977955849465880	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.4993687761703656	0.4994155943093566	0.2977483799959437	T	T	T
0.4922114766889710	0.4924989023203378	0.4940623835871432	T	T	T
0.1563195778684070	0.3253276875583781	0.5725185400454955	T	T	T
0.3235228024839176	0.1551009253596268	0.5725278604002427	T	T	T
0.4263465152815623	0.5949369062730347	0.5725441545356736	T	T	T
0.5933303213923098	0.4244388583697031	0.5725139872994548	T	T	T
0.2456036590498261	0.2457474404903972	0.5502893495030406	T	T	T
0.5041733580018484	0.5041993670359617	0.5502813169233020	T	T	T

Tl-pbc-2CO2 (1,3) (-657.4356 eV)

1.0000000000000000

9.621999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.621999999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	24.432999999999998

Ca O C

48 52 2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0000007023506346	0.9993280074595592	0.1977542539987096	T	T	T
0.0000011659732961	0.9981860511369239	0.3954104602385810	T	T	T
0.0000000000000000	0.2500000000000000	0.0984529099999989	F	F	F
0.0000009333327061	0.2493994228702635	0.2965238643594534	T	T	T
0.0000029687116622	0.2296480900125787	0.4998646035400977	T	T	T
0.2500000000000000	0.0000000000000000	0.0984529099999989	F	F	F
0.2507270292371050	0.9990852052405523	0.2970232074522755	T	T	T
0.2471821538594367	0.9851683789390444	0.4984545503576841	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2500001110576397	0.2499125513347616	0.1974470219612741	T	T	T
0.2499995470580191	0.2497251170167725	0.3939882385177363	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0000005795629803	0.4998233190683934	0.1976380936084488	T	T	T
0.0000006798614073	0.4948464250911876	0.3986607308910305	T	T	T
0.0000000000000000	0.7500000000000000	0.0984529099999989	F	F	F
0.0000006530092151	0.7480892137023329	0.2970520787309051	T	T	T
0.0000011301528738	0.7466661665512461	0.4931821228474411	T	T	T
0.2500000000000000	0.5000000000000000	0.0984529099999989	F	F	F

0.2492759841756094	0.5005339545181532	0.2970252897241372	T	T	T
0.2528176860094030	0.5140938682260492	0.4984838161711826	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2500005816930849	0.7499106503265358	0.1975082085463888	T	T	T
0.2499988078788051	0.7497060516485274	0.3953116406024864	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5000002692363693	0.0000004212678681	0.1976386970264777	T	T	T
0.5000009888354400	0.0045896551932688	0.3986522640871266	T	T	T
0.5000000000000000	0.2500000000000000	0.0984529099999989	F	F	F
0.5000009150218540	0.2502367681334421	0.2965256018216613	T	T	T
0.5000025536574301	0.2696350048385557	0.4998669808541186	T	T	T
0.7500000000000000	0.0000000000000000	0.0984529099999989	F	F	F
0.7492746982821018	0.9990854932951870	0.2970231474387272	T	T	T
0.7528225410021475	0.9851702334483426	0.4984546072008701	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7500008848942452	0.2499125406344681	0.1974469303671279	T	T	T
0.7500031112188704	0.2497258092588397	0.3939884951447835	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000003606861007	0.5004946652363947	0.1977551411025203	T	T	T
0.5000009829972930	0.5012588072793844	0.3954257603930802	T	T	T
0.5000000000000000	0.7500000000000000	0.0984529099999989	F	F	F
0.5000008217821384	0.7515332057740352	0.2970555934765698	T	T	T
0.5000010442874681	0.7526495571573748	0.4931863001179985	T	T	T
0.7500000000000000	0.5000000000000000	0.0984529099999989	F	F	F
0.7507255631665727	0.5005342241292461	0.2970252936124695	T	T	T
0.7471839832316015	0.5140950645866355	0.4984849296605206	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7500003313140331	0.7499107103202806	0.1975082392235025	T	T	T
0.7500026407793239	0.7497061643978402	0.3953118268533180	T	T	T
0.2500000000000000	0.2500000000000000	0.0984529099999989	F	F	F
0.2500017392932943	0.2498096975460448	0.2979849863586042	T	T	T
0.2499876694640336	0.2496208261419793	0.4935709016193790	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2501376145359291	0.0001832426242869	0.1981941217635131	T	T	T
0.2507471412569225	0.0012285774280820	0.3972373836986113	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0000004252607664	0.2496833688372477	0.1983954686986459	T	T	T
0.0000011766649432	0.2463457388161013	0.3991129838566443	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529099999989	F	F	F
0.0000008128880342	0.9993968507552954	0.2961400349400013	T	T	T
0.0000005472477760	0.9889198525797169	0.4876530732761600	T	T	T
0.2500000000000000	0.7500000000000000	0.0984529099999989	F	F	F
0.2500002218800944	0.7498001264687407	0.2970920831385592	T	T	T
0.2499931257632715	0.7496244640359385	0.4933433837039680	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2498596435884408	0.4996381229392305	0.1981933793786898	T	T	T
0.2492507949167216	0.4981878048945509	0.3972510316098175	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0000005327006378	0.7494053041810737	0.1981100851868374	T	T	T
0.0000006148809231	0.7459087939839361	0.3963510117842186	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529099999989	F	F	F
0.0000007072110822	0.4979284227463119	0.2966926167797645	T	T	T
0.0000001532159775	0.4934304126273916	0.4940352697288313	T	T	T
0.7500000000000000	0.2500000000000000	0.0984529099999989	F	F	F
0.7500002615068416	0.2498098563476886	0.2979852806048816	T	T	T
0.7500157785693295	0.2496226998944154	0.4935733889218842	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7498633539187251	0.0001833766013504	0.1981942872274806	T	T	T
0.7492550782174985	0.0012292088489569	0.3972382673607119	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F

0.5000004561407566	0.2501412343407156	0.1983956594541305	T	T	T
0.5000015936138018	0.2530922495377701	0.3991152433354064	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529099999989	F	F	F
0.5000010223873033	0.0016999664616681	0.2966908689285367	T	T	T
0.5000034487001108	0.0058108194334153	0.4940139811563530	T	T	T
0.7500000000000000	0.7500000000000000	0.0984529099999989	F	F	F
0.7500014500882186	0.7498003945690831	0.2970922657902747	T	T	T
0.7500085644831338	0.7496261928849874	0.4933439562994167	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7501412491857380	0.4996381194911405	0.1981934656368735	T	T	T
0.7507512235503281	0.4981880560615373	0.3972513723155992	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.5000004987653909	0.7504147571469557	0.1981126887805043	T	T	T
0.5000009599582645	0.7535140177358365	0.3963544138866613	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529099999989	F	F	F
0.5000008618359350	0.5002307063327112	0.2961462094022353	T	T	T
0.5000012838056286	0.5103784879598228	0.4876787710977064	T	T	T
0.3209724347094634	0.3455552083520382	0.5727154161184870	T	T	T
0.1791432021275888	0.1534342760091624	0.5726940721137742	T	T	T
0.6790257877904061	0.3455488472647775	0.5727164938237029	T	T	T
0.8208817884235462	0.1534636669455536	0.5726927167432065	T	T	T
0.2500376722665197	0.2495318262525422	0.5508339201465348	T	T	T
0.7499761292180148	0.2495342425762496	0.5508364910419054	T	T	T

Tl-pbc-3CO₂ (B) (-681.5626 eV)

1.0000000000000000

9.621999999999999 0.0000000000000000 0.0000000000000000

0.0000000000000000 9.621999999999999 0.0000000000000000

0.0000000000000000 0.0000000000000000 24.432999999999998

Ca O C

48 54 3

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0004683312813972	0.9997715149552480	0.1975892171035727	T	T	T
0.0053198651977611	0.9997466378377077	0.3962152049115134	T	T	T
0.0000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.0007747342630577	0.2495688044406709	0.2970147786717758	T	T	T
0.9890111036846924	0.2465629284195330	0.4972479629849655	T	T	T
0.2500000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.2511663717025752	0.9999941118926610	0.2968840712174962	T	T	T
0.2612682495665475	0.0063650965111134	0.4967641270374972	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2502763888857360	0.2498159656252095	0.1974417644033720	T	T	T
0.2530935038172457	0.2551525264256548	0.3950378358044681	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
-0.0001882306525560	0.4998196502100933	0.1975895098808516	T	T	T
0.0028202950543938	0.4992542139362709	0.3960925891875784	T	T	T
0.0000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
-0.0004668797528555	0.7496515465785453	0.2972780857585151	T	T	T
0.9808274942256043	0.7518425242813407	0.4967130967707420	T	T	T
0.2500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.2497013813702063	0.5001445994779929	0.2964342314785795	T	T	T
0.2106739603151549	0.5083568701925280	0.5175137624177378	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2499311284887513	0.7500492954183660	0.1974931354424365	T	T	T
0.2506105165679116	0.7464508881777968	0.3953891500713305	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5006941636248884	0.9997941031221567	0.1975829276998024	T	T	T

0.5019349458072242	0.0003141993410802	0.3953434215218547	T	T	T
0.5000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.5011143878968447	0.2497788570029482	0.2967845233634260	T	T	T
0.5254343653541304	0.2325594794701788	0.5045665376204267	T	T	T
0.7500000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.7518755495617763	0.9988248061502439	0.2969062136723641	T	T	T
0.7581642305519234	0.9976151526478820	0.4911989005028909	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7505332225758353	0.2496368198575388	0.1975140454234502	T	T	T
0.7501422014485831	0.2498214100674034	0.3949011931309927	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5003018035822242	0.4997812548777346	0.1975260031439365	T	T	T
0.4958667994027779	0.4988245640197690	0.3962794216107807	T	T	T
0.5000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.5001957092138656	0.7494317802202329	0.2968836825709159	T	T	T
0.5079236875068205	0.7687318274383306	0.5034061031173322	T	T	T
0.7500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.7500572899106781	0.4993205850993528	0.2970254291415093	T	T	T
0.7593667244205623	0.4933476007592477	0.4963634765633018	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7502297302690066	0.7496225634250649	0.1975360491495528	T	T	T
0.7464678096154204	0.7461607177564140	0.3959862143023350	T	T	T
0.2500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.2512237614514677	0.2496096338309320	0.2979215246216289	T	T	T
0.2539378395248222	0.2577469664285009	0.4958051448602249	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2506633580373263	0.9998488296546404	0.1984498037218899	T	T	T
0.2540930286818863	0.0009147991931448	0.3989553098396946	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0007639255166603	0.2497756504152580	0.1982805933520647	T	T	T
0.0045063251432739	0.2492374127332681	0.3972502992196368	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.0022008483170712	0.9994913990516608	0.2967129750003764	T	T	T
0.0075040147771468	0.9996868609800517	0.4919388256289352	T	T	T
0.2500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.2503021391293771	0.7505721086121251	0.2982334356526588	T	T	T
0.2465274065893179	0.7522459921905550	0.4960754752774522	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2503010045617000	0.5000364262042999	0.1981942139339019	T	T	T
0.2497600044265821	0.5009427952742956	0.3949628312968555	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0003303909245911	0.7498172378656065	0.1984377663567060	T	T	T
0.0005465228824014	0.7497440661881458	0.3978872223565846	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
-0.0004460413560760	0.4997349377807898	0.2964918349022442	T	T	T
0.9915096273228533	0.4998033019708598	0.4896665647850423	T	T	T
0.7500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.7507798670664805	0.2492011300378539	0.2967100312215862	T	T	T
0.7570867490803735	0.2408580107585678	0.4897025041264895	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7505773029342167	0.9994399796103571	0.1981093319445874	T	T	T
0.7540667416893311	0.9970296724347663	0.3956364504673207	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.5000658788113659	0.2499986795951847	0.1983734115075960	T	T	T
0.5000654078393683	0.2508277879565440	0.3977237214313464	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.5010260761674087	0.9993021309690249	0.2966697135258352	T	T	T
0.5129835132026915	0.9996972415091271	0.4889186016637380	T	T	T
0.7500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.7493936534225200	0.7487949822974007	0.2973280727979777	T	T	T

0.7441347327840045	0.7467354340422112	0.4936602025757550	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7497674057621415	0.4997726437806189	0.1982112190176797	T	T	T
0.7466689300974104	0.4982949528236836	0.3972917422671434	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.4997709934199809	0.7495687549107987	0.1985728686868420	T	T	T
0.4968713244498893	0.7478786672164262	0.3995122664099319	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.4999315154352995	0.4998729312970354	0.2976274475665377	T	T	T
0.4923599587511736	0.4935366187116273	0.4937167864739060	T	T	T
0.1475407745414851	0.3098613432939762	0.5751994629394369	T	T	T
0.3483933527048694	0.1810467472458213	0.5746285479865449	T	T	T
0.4197988858479199	0.5807344591190884	0.5739011283702710	T	T	T
0.6020682477846604	0.4281585963880292	0.5706823584452377	T	T	T
0.3082148998145823	0.8623780827660863	0.5738422947849482	T	T	T
0.1317930441770840	0.7019487326573042	0.5739400454572519	T	T	T
0.2504738453535426	0.2482492015518664	0.5529661035671170	T	T	T
0.5049669518122040	0.5007735145870852	0.5496722612573025	T	T	T
0.2293518328523418	0.7731801085412935	0.5525981867076389	T	T	T

Tl-pbc-3CO₂ (A) (-681.73767 eV)

1.0000000000000000		
9.621999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.621999999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	24.432999999999998

Ca O C
48 54 3

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0000868110641268	0.0000888522545654	0.1975271903978638	T	T	T
0.0002579938572903	0.0002556283474043	0.3959948484380510	T	T	T
0.0000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.0003413840910866	0.2499223133910643	0.2969135031337113	T	T	T
0.9939896302633957	0.2492556406215757	0.4954420609971754	T	T	T
0.2500000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.2499246753435840	0.0003382669850499	0.2969271859650952	T	T	T
0.2491491862976061	0.9938579554592002	0.4955258889915097	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2501385573661907	0.2501358648646932	0.1974727622774286	T	T	T
0.2533878383692218	0.2533603754346740	0.3945141218788475	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0000839820590404	0.5000919042284340	0.1975652334301738	T	T	T
0.0002649229632638	0.5002597286699537	0.3954348504241632	T	T	T
0.0000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
-0.0000054637467216	0.7504360975297626	0.2969158509485476	T	T	T
0.0066754688417413	0.7513822367547786	0.4954352588112041	T	T	T
0.2500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.2502424416268847	0.5008594554859755	0.2967768779294536	T	T	T
0.2306315583986455	0.5163792648689415	0.5040804944637459	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2498499511287197	0.7503285115805551	0.1974555915837574	T	T	T
0.2516258680634828	0.7488493652728272	0.3957098462365324	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5000908158109876	0.0000862082044152	0.1975681072346987	T	T	T
0.5002685104687916	0.0002874886384701	0.3954566559921515	T	T	T
0.5000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.5008687718446724	0.2502421682866204	0.2967726077376922	T	T	T
0.5163552179860711	0.2306260635123576	0.5039695860545371	T	T	T

0.7500000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.7504302483760076	0.0000117357347777	0.2969312985601912	T	T	T
0.7515287802342300	0.0067880328968875	0.4955177430484595	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7503264625778205	0.2498527993655828	0.1974557516909570	T	T	T
0.7488817428616896	0.2516733342764483	0.3957156860254880	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000865910522180	0.5000885671594679	0.1975177955854536	T	T	T
0.5002335203812641	0.5002197742150092	0.3964976548160401	T	T	T
0.5000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.4994953134297374	0.7501121781643623	0.2967778654001934	T	T	T
0.4843376128003870	0.7700494123163848	0.5038826762222595	T	T	T
0.7500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.7501015933467852	0.4995075873407301	0.2967816866582172	T	T	T
0.7700820982267370	0.4842826310384359	0.5040711148732764	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7500316412909178	0.7500402990875358	0.1974724989314574	T	T	T
0.7471108773899715	0.7471267700508011	0.3945272794341901	T	T	T
0.2500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.2509672762476849	0.2509567416881835	0.2976570882781294	T	T	T
0.2586274924328540	0.2584881567647448	0.4939445835680069	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2500997173321188	0.0003229383940261	0.1982940359925686	T	T	T
0.2496539420479492	0.0032897059373370	0.3971933842728405	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0003252585116506	0.2500968672885869	0.1982986507488344	T	T	T
0.0033249320557385	0.2496517965659826	0.3972292164959714	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.0001805860289643	0.0001783180062822	0.2964996987607096	T	T	T
0.0003192786215363	0.0002938937719100	0.4920416733500123	T	T	T
0.2500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.2499055157126421	0.7504692505895678	0.2971758480290643	T	T	T
0.2440629668646130	0.7564065907962221	0.4914529783368146	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2504071214388073	0.5001597402041527	0.1983838276405382	T	T	T
0.2519471972122702	0.5005293591632624	0.3979597586952074	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.9998313528257710	0.7500778268408824	0.1982996831371707	T	T	T
0.9971668966183279	0.7508578148649530	0.3972308680838200	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.0001716285496511	0.5001910679415073	0.2963449894723576	T	T	T
0.0003389325098566	0.5003047431254591	0.4879168555319609	T	T	T
0.7500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.7504711654211970	0.2499135062924087	0.2971744793396749	T	T	T
0.7565575170487195	0.2442018865849328	0.4914663241874781	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7500732379708158	0.9998369001837587	0.1982943524538340	T	T	T
0.7508695543725283	0.9972040306429457	0.3971906281520605	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.5001600998664990	0.2504054957713486	0.1983947258359096	T	T	T
0.5005619134748810	0.2519310461565388	0.3980299402840303	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.5001872473475834	0.0001696673840489	0.2963573970311813	T	T	T
0.5003113761739434	0.0003326727529639	0.4879546644514991	T	T	T
0.7500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.7493749280407898	0.7493975475648715	0.2976687620281838	T	T	T
0.7418257729349452	0.7419696743779653	0.4939748244100048	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7497572519701687	0.5000269026757824	0.1983803800543075	T	T	T
0.7485570082138736	0.4999895586028992	0.3979856943007105	T	T	T

0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.5000219446278859	0.7497611687933444	0.1983928421232550	T	T	T
0.4999648124297799	0.7485664020507666	0.3980825571813204	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.5001815437711327	0.5001916040242100	0.2977300047390551	T	T	T
0.5001131015311494	0.5000707229775812	0.4940216668652776	T	T	T
0.1535727159496789	0.3227120307771461	0.5722770768186508	T	T	T
0.3209169098838583	0.1524183464930140	0.5723244047637395	T	T	T
0.4168829185841919	0.5856508222227480	0.5729522800923038	T	T	T
0.5843221881734443	0.4156214337770039	0.5729836605699471	T	T	T
0.6802008421012513	0.8486221713784319	0.5723214309895164	T	T	T
0.8472728977604080	0.6780664710815733	0.5722670475251638	T	T	T
0.2440586423499972	0.2441927792535525	0.5507091151732014	T	T	T
0.5004037341480980	0.5004384443406678	0.5505624722078239	T	T	T
0.7567934118143845	0.7566105805293237	0.5507150490202789	T	T	T

Tl-pbc-4CO2 (-705.35558 eV)

1.0000000000000000

9.621999999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.621999999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	24.432999999999998

Ca O C

48 56 4

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0000632566460289	0.0000698124742320	0.1973117466237528	T	T	T
0.0002157732497152	0.0001994698786459	0.3947637747357168	T	T	T
0.0000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.0000961792946518	0.2501969559908569	0.2965987532653009	T	T	T
0.9872833869898765	0.2635218254567595	0.5006186419817809	T	T	T
0.2500000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.2501930002185544	0.0000995326983081	0.2966013780648158	T	T	T
0.2633730946038018	0.9869914463892071	0.5006503273653726	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2500632742711466	0.2500670019502439	0.1973137750572610	T	T	T
0.2502342107019367	0.2502220800075157	0.3947888536142561	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0000647974628615	0.5000710037506841	0.1973140085305743	T	T	T
0.0002355739174881	0.5002169870534917	0.3949926758691139	T	T	T
0.0000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.0001881545247941	0.7500979912687478	0.2966006470633122	T	T	T
0.0134035536263903	0.7370270937870952	0.5006350910981227	T	T	T
0.2500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.2501156500711706	0.5001899273770584	0.2966024520037377	T	T	T
0.2372878580832243	0.5135376263897951	0.5007292008321359	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2500703285439373	0.7500667360411324	0.1973162027796616	T	T	T
0.2502778346529402	0.7501879331801533	0.3950065064574467	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5000630523375177	0.0000686419844543	0.1973172541470243	T	T	T
0.5002316595338022	0.0002096984404285	0.3950027504047802	T	T	T
0.5000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.5001788152667912	0.2501158595794500	0.2966025831658996	T	T	T
0.5133562593607844	0.2369931346810873	0.5007242696035291	T	T	T
0.7500000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.7500920391385134	0.0001917179752606	0.2965996047346315	T	T	T
0.7373116231116504	0.0135654174063244	0.5006404300719203	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F

0.7500583141193777	0.2500737405392385	0.1973153940320633	T	T	T
0.7501836362992302	0.2502443385431349	0.3949949882442408	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000646183237839	0.5000710794514823	0.1973128717622065	T	T	T
0.5002144437462734	0.5002092064151920	0.3948186022173387	T	T	T
0.5000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.5001051285613152	0.7501799093477908	0.2966052268288846	T	T	T
0.4873340496980400	0.7635639094225627	0.5007464831048601	T	T	T
0.7500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.7501735845462149	0.5001092198380132	0.2966013516888355	T	T	T
0.7634117788934067	0.4870170871950711	0.5007186518779805	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7500636643191996	0.7500747341875476	0.1973139421387012	T	T	T
0.7501949928376458	0.7501839983501692	0.3947925576783672	T	T	T
0.2500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.2501438256692411	0.2501504167354993	0.2973063559957395	T	T	T
0.2501640891972245	0.2501463898588815	0.4925320918467852	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2499038029566031	0.0002207696579972	0.1983402030106027	T	T	T
0.2485855075294257	0.0018286245241636	0.3976425911929138	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0002159336691343	0.2499106732990265	0.1983358931063989	T	T	T
0.0018647485747601	0.248588202632973	0.3976269131177854	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.0001492131490778	0.0001542520755375	0.2973000755924404	T	T	T
0.0001275042161281	0.0000869112423886	0.4924900329987645	T	T	T
0.2500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.2501564609763732	0.7501483852560313	0.2964619380168729	T	T	T
0.2503611694374109	0.7502067982751256	0.4881668868268805	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2502230158375505	0.4999058637683381	0.1983388234328352	T	T	T
0.2518790575209712	0.4985896359269689	0.3976371192118117	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.9999095226187729	0.7502284308505982	0.1983375577584598	T	T	T
0.9985891282779659	0.7518278516412582	0.3976291816032107	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.0001511076332872	0.5001554380432935	0.2964526887083731	T	T	T
0.0003195393617658	0.5002432703738150	0.4881455129799169	T	T	T
0.7500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.7501436953899384	0.2501604376139404	0.2964562145626419	T	T	T
0.7502765871790756	0.2502891181466058	0.4881495249612600	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7502198968393832	0.9999147329005663	0.1983386076068021	T	T	T
0.7518635372865029	0.9985896579586594	0.3976392428929033	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4998974131576891	0.2502263482990322	0.1983376063913631	T	T	T
0.4985796945730076	0.2518408012499582	0.3976288068643667	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.5001476221691731	0.0001539680908416	0.2964599378364812	T	T	T
0.5003215568609806	0.0002473320908842	0.4881634056016745	T	T	T
0.7500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.7501539385313659	0.7501625459028353	0.2973080049037429	T	T	T
0.7501104615808803	0.7500485456490147	0.4925378363248533	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7499021550428193	0.5002342468712352	0.1983383115453161	T	T	T
0.7485768588967143	0.5018332605503392	0.3976369677816818	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.5002256818915123	0.7499101309859987	0.1983388047391475	T	T	T
0.5018769116779748	0.7485835274387344	0.3976289621942314	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120451825	F	F	F

0.5001501813443106	0.5001558452034012	0.2973152203655449	T	T	T
0.5001406654632288	0.5001025704978287	0.4925889648584530	T	T	T
0.1672203563991420	0.3361203874699152	0.5716781607986224	T	T	T
0.3335851293873519	0.1645882495488091	0.5716674985877185	T	T	T
0.4175396047381002	0.5863273305800528	0.5717518882589973	T	T	T
0.5836802983436438	0.4145840910986703	0.5717191009586453	T	T	T
0.6675401806706026	0.8363075081015229	0.5716957868693731	T	T	T
0.8340257053704532	0.6648922776397063	0.5716614456098260	T	T	T
0.9173639650256157	0.0862668365685718	0.5716215081545297	T	T	T
0.0837363758565642	0.9147247703500770	0.5716223862504984	T	T	T
0.2503281698007955	0.2502830321896725	0.5500455629669865	T	T	T
0.5004504663382439	0.5003497337719228	0.5501083882352140	T	T	T
0.7505781935358418	0.7504268311309341	0.5500528896685959	T	T	T
0.0004248566893839	0.0003740275751904	0.5500015581416362	T	T	T

T2-pbc-0CO2 (-1376.2724 eV)

1.0000000000000000		
14.432999999999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.432999999999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	24.432999999999998

Ca O

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Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0000063620970502	0.0000000203760022	0.1977006655063929	T	T	T
0.0000122171054131	0.0000000860517238	0.3960331473203902	T	T	T
0.0000000000000000	0.1666666667013104	0.0984529120410897	F	F	F
0.0000138023097029	0.1666665166671125	0.2968394823437287	T	T	T
-0.0000695550953648	0.1666665765851865	0.4938749773317160	T	T	T
0.1666666667013104	0.0000000000000000	0.0984529120410897	F	F	F
0.1666526676246514	0.0000001321585270	0.2968395627112378	T	T	T
0.1667361468075494	0.0000000626154174	0.4938750449058987	T	T	T
0.1666666667013104	0.1666666667013104	0.0000000000000000	F	F	F
0.1666601666699251	0.1666666531665760	0.1977006414883673	T	T	T
0.1666543472630613	0.1666665432895673	0.3960330221051300	T	T	T
0.0000000000000000	0.333333332986896	0.0000000000000000	F	F	F
0.0000062819072663	0.3333331928737264	0.1977006419014397	T	T	T
0.0000123283024108	0.3333332075858076	0.3960328792264948	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529120410897	F	F	F
0.0000139152909901	0.4999999722332790	0.2968395084933861	T	T	T
-0.0000695923471952	0.4999999879078424	0.4938749553740719	T	T	T
0.1666666667013104	0.333333332986896	0.0984529120410897	F	F	F
0.1666528008737900	0.3333333308534775	0.2968394835237499	T	T	T
0.1667361608882630	0.3333333979449338	0.4938747020226070	T	T	T
0.1666666667013104	0.5000000000000000	0.0000000000000000	F	F	F
0.1666603568029638	0.4999999654213884	0.1977005273190721	T	T	T
0.1666545457649834	0.4999998974216965	0.3960330214305494	T	T	T
0.333333332986896	0.0000000000000000	0.0000000000000000	F	F	F
0.3333139832415631	0.999999985673267	0.1976836817372608	T	T	T
0.3333144409922132	-0.0000001031103656	0.3959813226653301	T	T	T
0.333333332986896	0.1666666667013104	0.0984529120410897	F	F	F
0.3333099142932655	0.1666666573910428	0.2968055056113211	T	T	T
0.3333988752211459	0.1666666996673276	0.4937931111412766	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120410897	F	F	F
0.4999625761017179	0.0000001023551350	0.2967661114233778	T	T	T
0.5000251775845500	0.000000003619802	0.4936925152139775	T	T	T
0.5000000000000000	0.1666666667013104	0.0000000000000000	F	F	F
0.5000165374904241	0.1666666848275207	0.1976719299381255	T	T	T

0.4999718529809749	0.1666666211138242	0.3958721572473921	T	T	T
0.333333332986896	0.333333332986896	0.0000000000000000	F	F	F
0.3333141532678769	0.3333332934997607	0.1976836969266225	T	T	T
0.3333145018936692	0.3333333203921379	0.3959813055588920	T	T	T
0.333333332986896	0.5000000000000000	0.0984529120410897	F	F	F
0.3333098959947871	0.4999998796851880	0.2968055047836174	T	T	T
0.3333990618860284	0.4999998601767126	0.4937930914693136	T	T	T
0.5000000000000000	0.333333332986896	0.0984529120410897	F	F	F
0.4999626495974793	0.3333332591492570	0.2967660692900073	T	T	T
0.5000252644116765	0.3333334466588997	0.4936922116459383	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000165263416803	0.5000000958371003	0.1976719861831415	T	T	T
0.4999718877836117	0.4999997440706829	0.3958721747364817	T	T	T
0.666666667013104	0.0000000000000000	0.0000000000000000	F	F	F
0.6666502618641672	0.0000000834471396	0.1976719983507999	T	T	T
0.6666948604917950	0.0000000770915558	0.3958721758080729	T	T	T
0.666666667013104	0.166666667013104	0.0984529120410897	F	F	F
0.6667040739322018	0.1666667169319175	0.2967660781114425	T	T	T
0.6666417988727215	0.1666664921877159	0.4936926568884025	T	T	T
0.666666667013104	0.333333332986896	0.0000000000000000	F	F	F
0.6666502054376273	0.3333333504052088	0.1976718853295139	T	T	T
0.6666949618552701	0.3333333572234653	0.3958720998224649	T	T	T
0.666666667013104	0.5000000000000000	0.0984529120410897	F	F	F
0.6667038687126069	0.4999998483376273	0.2967660400365229	T	T	T
0.6666417488399675	0.5000001140305783	0.4936926411567045	T	T	T
0.833333332986896	0.0000000000000000	0.0984529120410897	F	F	F
0.8333566969544847	0.9999998523661845	0.2968055913527832	T	T	T
0.8332678118480574	0.9999998178993034	0.4937931524177445	T	T	T
0.833333332986896	0.166666667013104	0.0000000000000000	F	F	F
0.8333525283103056	0.1666666619476712	0.1976837421475434	T	T	T
0.8333522794980632	0.1666664928517358	0.3959814007921375	T	T	T
0.833333332986896	0.333333332986896	0.0984529120410897	F	F	F
0.8333567738676567	0.3333331643203293	0.2968055747350676	T	T	T
0.8332677547419619	0.3333332556576596	0.4937930689711533	T	T	T
0.833333332986896	0.5000000000000000	0.0000000000000000	F	F	F
0.8333524639314057	0.4999999677972856	0.1976837425476428	T	T	T
0.8333523530225614	0.4999999981940688	0.3959812463346871	T	T	T
0.0000000000000000	0.666666667013104	0.0000000000000000	F	F	F
0.0000062818103088	0.6666665150246451	0.1977005643618535	T	T	T
0.0000121830150378	0.6666667089902722	0.3960329597953688	T	T	T
0.166666667013104	0.666666667013104	0.0984529120410897	F	F	F
0.1666527932044289	0.6666666836228528	0.2968394881957405	T	T	T
0.1667363106169603	0.6666666701228166	0.4938749348420330	T	T	T
0.333333332986896	0.666666667013104	0.0000000000000000	F	F	F
0.3333140229252943	0.6666667053987823	0.1976836305696136	T	T	T
0.3333144867928408	0.6666665943601072	0.3959812370494164	T	T	T
0.5000000000000000	0.666666667013104	0.0984529120410897	F	F	F
0.4999626631116853	0.6666665792375899	0.2967660168210247	T	T	T
0.5000247951737635	0.6666666726973671	0.4936926682427109	T	T	T
0.666666667013104	0.666666667013104	0.0000000000000000	F	F	F
0.6666502504824723	0.6666666825633302	0.1976719404485112	T	T	T
0.6666948152183074	0.6666667341459152	0.3958720612818888	T	T	T
0.833333332986896	0.666666667013104	0.0984529120410897	F	F	F
0.8333566366119836	0.6666667360925230	0.2968055375621121	T	T	T
0.8332678434734005	0.6666665747072169	0.4937930974570051	T	T	T
0.0000000000000000	0.833333332986896	0.0984529120410897	F	F	F
0.0000138159919514	0.8333333483857551	0.2968395863778983	T	T	T
-0.0000693833766951	0.8333331769126131	0.4938749320109430	T	T	T
0.166666667013104	0.833333332986896	0.0000000000000000	F	F	F
0.1666601405651212	0.8333333302302768	0.1977005341863723	T	T	T

0.1666544823669053	0.8333333919911832	0.3960330462041264	T	T	T
0.3333333332986896	0.8333333332986896	0.0984529120410897	F	F	F
0.3333098381974348	0.8333333348606189	0.2968055788183336	T	T	T
0.3333988682287463	0.8333331612314872	0.4937931126287686	T	T	T
0.5000000000000000	0.8333333332986896	0.0000000000000000	F	F	F
0.5000165293277167	0.8333334818210372	0.1976718998382122	T	T	T
0.4999719972789849	0.8333333805016996	0.3958721076242055	T	T	T
0.6666666667013104	0.8333333332986896	0.0984529120410897	F	F	F
0.6667038671233193	0.8333333154758124	0.2967661236323004	T	T	T
0.6666418332765418	0.8333331431989658	0.4936925414097192	T	T	T
0.8333333332986896	0.8333333332986896	0.0000000000000000	F	F	F
0.8333524744660485	0.8333334036298783	0.1976837451369233	T	T	T
0.8333523394521721	0.8333333937405577	0.3959814344736092	T	T	T
0.1666666667013104	0.1666666667013104	0.0984529120410897	F	F	F
0.1666634825787944	0.1666666488149946	0.2966930469151051	T	T	T
0.1666739979921645	0.1666666755178825	0.4930640057272515	T	T	T
0.1666666667013104	0.0000000000000000	0.0000000000000000	F	F	F
0.1666469781423472	-0.0000000166716497	0.1977650539957085	T	T	T
0.1666503783379192	-0.0000000272599761	0.3963568518261252	T	T	T
0.0000000000000000	0.1666666667013104	0.0000000000000000	F	F	F
0.0000196554771474	0.1666667442161893	0.1977650460954560	T	T	T
0.0000164757198552	0.1666666794436964	0.3963568512423352	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529120410897	F	F	F
0.0000032552008039	-0.0000000042568475	0.2966931192664640	T	T	T
-0.0000072014832298	0.9999999383276124	0.4930642197754625	T	T	T
0.1666666667013104	0.5000000000000000	0.0984529120410897	F	F	F
0.1666634156372710	0.5000000088341141	0.2966930376511936	T	T	T
0.1666739376876610	0.4999998842148186	0.4930640417919475	T	T	T
0.1666666667013104	0.3333333332986896	0.0000000000000000	F	F	F
0.1666469453832884	0.3333333312656326	0.1977649846494424	T	T	T
0.1666502409888849	0.3333332956287140	0.3963566896502956	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0000196023707457	0.4999999724637704	0.1977650166087880	T	T	T
0.0000164090090159	0.4999999265641678	0.3963567219511790	T	T	T
0.0000000000000000	0.3333333332986896	0.0984529120410897	F	F	F
0.0000031800941991	0.3333333401273616	0.2966930890880970	T	T	T
-0.0000072242098704	0.3333333758886515	0.4930639480932858	T	T	T
0.5000000000000000	0.1666666667013104	0.0984529120410897	F	F	F
0.4999514545458007	0.1666667031926432	0.2965964624985719	T	T	T
0.5000351733916626	0.1666666869633850	0.4928536206148083	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.4999830155497605	-0.0000000151073161	0.1977302378363483	T	T	T
0.4999910194585859	-0.0000001340865849	0.3962504451639738	T	T	T
0.3333333332986896	0.1666666667013104	0.0000000000000000	F	F	F
0.3332980898934115	0.1666666256420992	0.1977659066082129	T	T	T
0.3332969094394073	0.1666666526372425	0.3963106906138672	T	T	T
0.3333333332986896	0.0000000000000000	0.0984529120410897	F	F	F
0.3332525246188414	-0.0000000409634583	0.2966538284349881	T	T	T
0.3333968238754459	-0.0000000904775043	0.4929796269137023	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120410897	F	F	F
0.4999515152261806	0.50000000547215042	0.2965964726184846	T	T	T
0.5000353007191072	0.4999999008218896	0.4928536505767315	T	T	T
0.5000000000000000	0.3333333332986896	0.0000000000000000	F	F	F
0.4999831854359081	0.3333333144573578	0.1977301662030007	T	T	T
0.4999910853275848	0.3333333822014253	0.3962503064885317	T	T	T
0.3333333332986896	0.5000000000000000	0.0000000000000000	F	F	F
0.3332980784116835	0.4999999837492648	0.1977659180943383	T	T	T
0.3332970347206093	0.4999999313467690	0.3963106368901418	T	T	T
0.3333333332986896	0.3333333332986896	0.0984529120410897	F	F	F
0.3332525835071911	0.3333332884434140	0.2966537148533673	T	T	T

0.3333968165623562	0.3333332399001154	0.4929795797041256	T	T	T
0.666666667013104	0.166666667013104	0.0000000000000000	F	F	F
0.6666835228213027	0.1666667293164697	0.1977302314221706	T	T	T
0.6666755409807302	0.1666666722784263	0.3962505210136553	T	T	T
0.666666667013104	0.0000000000000000	0.0984529120410897	F	F	F
0.6667150629289982	-0.0000000326612472	0.2965965046907404	T	T	T
0.6666313228709498	0.9999998994535896	0.4928536551990526	T	T	T
0.666666667013104	0.5000000000000000	0.0000000000000000	F	F	F
0.6666835921647007	0.5000000180674682	0.1977301368438612	T	T	T
0.6666756311674805	0.5000000469593608	0.3962504397685332	T	T	T
0.666666667013104	0.333333332986896	0.0984529120410897	F	F	F
0.6667152460157199	0.3333333494622561	0.2965964847062757	T	T	T
0.6666313361232700	0.3333334136988555	0.4928535814326258	T	T	T
0.833333332986896	0.166666667013104	0.0984529120410897	F	F	F
0.8334140620645968	0.1666667291430721	0.2966538417042849	T	T	T
0.8332698547310976	0.1666667383703996	0.4929797400553321	T	T	T
0.833333332986896	0.0000000000000000	0.0000000000000000	F	F	F
0.8333686368318534	0.0000000889823680	0.1977659646259528	T	T	T
0.8333696676000388	-0.0000000641145882	0.3963108085371422	T	T	T
0.833333332986896	0.5000000000000000	0.0984529120410897	F	F	F
0.8334140347697760	0.4999999609316048	0.2966537866049350	T	T	T
0.8332698649274183	0.4999999554250277	0.4929796239399260	T	T	T
0.833333332986896	0.333333332986896	0.0000000000000000	F	F	F
0.8333685414195551	0.3333333956333665	0.1977659958317912	T	T	T
0.8333698608391275	0.3333334246396346	0.3963107018187187	T	T	T
0.0000000000000000	0.666666667013104	0.0984529120410897	F	F	F
0.0000032927668280	0.6666665909415337	0.2966930221428434	T	T	T
-0.0000070567695510	0.6666665111650358	0.4930640402235281	T	T	T
0.166666667013104	0.666666667013104	0.0000000000000000	F	F	F
0.1666469780153934	0.6666666472984014	0.1977650526686877	T	T	T
0.1666503216225955	0.6666665908190565	0.3963567314202654	T	T	T
0.333333332986896	0.666666667013104	0.0984529120410897	F	F	F
0.3332525521530965	0.6666667144552281	0.2966537076113010	T	T	T
0.3333967817598288	0.6666665681083978	0.4929794869246920	T	T	T
0.5000000000000000	0.666666667013104	0.0000000000000000	F	F	F
0.4999830825214331	0.6666667133687288	0.1977302125767698	T	T	T
0.4999910830538122	0.6666666498001059	0.3962504030242001	T	T	T
0.666666667013104	0.666666667013104	0.0984529120410897	F	F	F
0.6667151471626063	0.6666666340905288	0.2965965041096774	T	T	T
0.6666312346365822	0.6666666733225463	0.4928535020066739	T	T	T
0.833333332986896	0.666666667013104	0.0000000000000000	F	F	F
0.8333685732270119	0.6666666079833524	0.1977660068991496	T	T	T
0.8333698545427021	0.6666665715794008	0.3963107011485363	T	T	T
0.0000000000000000	0.833333332986896	0.0000000000000000	F	F	F
0.0000197007433433	0.8333333019481024	0.1977650367309742	T	T	T
0.0000165057415292	0.8333332469188166	0.3963568146231353	T	T	T
0.166666667013104	0.833333332986896	0.0984529120410897	F	F	F
0.1666635845863870	0.8333333317631594	0.2966930286095736	T	T	T
0.1666740668155136	0.8333331596359489	0.4930640333256584	T	T	T
0.333333332986896	0.833333332986896	0.0000000000000000	F	F	F
0.3332980805896628	0.8333333493725811	0.1977660267942628	T	T	T
0.3332970627443083	0.8333333178655534	0.3963107126183415	T	T	T
0.5000000000000000	0.833333332986896	0.0984529120410897	F	F	F
0.4999513944039922	0.8333333071327572	0.2965965476188698	T	T	T
0.5000352024610282	0.8333333386922613	0.4928535388572686	T	T	T
0.666666667013104	0.833333332986896	0.0000000000000000	F	F	F
0.6666834704447731	0.8333333349452677	0.1977302380398784	T	T	T
0.6666754631656818	0.8333333181676151	0.3962505052685595	T	T	T
0.8333330000000032	0.833333332986896	0.0984529120410897	F	F	F
0.8334140191937953	0.8333332663933244	0.2966538351285678	T	T	T

0.8332698244987233 0.8333333396408291 0.4929797178490448 T T T

T2-pbc-1CO2 (-1400.6745 eV)

1.0000000000000000

14.432999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.432999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 24.432999999999998

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108 110 1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0000675903678228	-0.0000256405823556	0.1979516059487144	T	T	T
0.0008718006807221	0.9999570303662680	0.3974777473780410	T	T	T
0.0000000000000000	0.1666666667013104	0.0984529120410897	F	F	F
0.9998497481711873	0.1666642836065214	0.2973734208637177	T	T	T
0.9902756079611963	0.1666311915429858	0.4956906634906003	T	T	T
0.1666666667013104	0.0000000000000000	0.0984529120410897	F	F	F
0.1666642537822060	0.9997660343364783	0.2975874663904906	T	T	T
0.1666359914468543	0.9910691901852576	0.5006252698131067	T	T	T
0.1666666667013104	0.1666666667013104	0.0000000000000000	F	F	F
0.1666663211646656	0.1666661447038605	0.1979654004899698	T	T	T
0.1666656773262677	0.1666644937636148	0.3960779938868271	T	T	T
0.0000000000000000	0.333333332986896	0.0000000000000000	F	F	F
0.0000697280647660	0.3333565218245593	0.1979514273581252	T	T	T
0.0008865869927871	0.3333588464069763	0.3974885129775996	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529120410897	F	F	F
0.0001184063765522	0.4998816753672863	0.2973227427187796	T	T	T
0.9983886235876102	0.5009564290593924	0.4945886223812510	T	T	T
0.1666666667013104	0.333333332986896	0.0984529120410897	F	F	F
0.1666676170455972	0.3335664543168947	0.2975865345441600	T	T	T
0.1666967474885042	0.3422600853927893	0.5006167473582646	T	T	T
0.1666666667013104	0.5000000000000000	0.0000000000000000	F	F	F
0.1666671191686222	0.4999907027314640	0.1979222343560782	T	T	T
0.1666703342218020	0.4997899383173618	0.3969866018790805	T	T	T
0.333333332986896	0.0000000000000000	0.0000000000000000	F	F	F
0.3332627010684438	-0.0000231538627846	0.1979519416760571	T	T	T
0.3324446001252948	0.9999733160248854	0.3974905026106884	T	T	T
0.333333332986896	0.1666666667013104	0.0984529120410897	F	F	F
0.3334816802020824	0.1666680454690544	0.2973736430069387	T	T	T
0.3430578797926238	0.1667012377262187	0.4956883469174313	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120410897	F	F	F
0.4997485509411730	0.9998768685649815	0.2972588733255056	T	T	T
0.5011018984654980	0.9982288788286258	0.4943032482668072	T	T	T
0.5000000000000000	0.1666666667013104	0.0000000000000000	F	F	F
0.4999315831072834	0.1666676788692597	0.1978392454583567	T	T	T
0.5007440125143923	0.1666719529915121	0.3961411106019716	T	T	T
0.333333332986896	0.333333332986896	0.0000000000000000	F	F	F
0.3332646853945159	0.3333587956198494	0.1979512311659819	T	T	T
0.3324610914298806	0.3333756650654018	0.3974732446672010	T	T	T
0.333333332986896	0.5000000000000000	0.0984529120410897	F	F	F
0.3332184682370535	0.4998908318250556	0.2973203450928126	T	T	T
0.3349623603090027	0.5009721448704417	0.4945805533326797	T	T	T
0.5000000000000000	0.333333332986896	0.0984529120410897	F	F	F
0.4997576744170121	0.3334631787613968	0.2972549083962747	T	T	T
0.5011185981047199	0.3351271881801648	0.4942950431674082	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4999113871426987	0.4999758544348338	0.1978180498463598	T	T	T
0.4999964161165470	0.5001000891863767	0.3962150727952540	T	T	T

0.666666667013104	0.0000000000000000	0.0000000000000000	F	F	F
0.6666641737587296	0.9999663220319200	0.1978492709416489	T	T	T
0.6666601138236790	0.9997862635044062	0.3963288485152119	T	T	T
0.666666667013104	0.166666667013104	0.0984529120410897	F	F	F
0.666664717929317	0.1666675431427025	0.2969637248085902	T	T	T
0.6666662597991753	0.1666695248765017	0.4944624865659302	T	T	T
0.666666667013104	0.3333333332986896	0.0000000000000000	F	F	F
0.6666685568829919	0.3333675231864469	0.1978486515811235	T	T	T
0.6666730657558235	0.3335510096416299	0.3963276839649991	T	T	T
0.666666667013104	0.5000000000000000	0.0984529120410897	F	F	F
0.6666702343245916	0.4999858708044290	0.2970010494573185	T	T	T
0.6666727798745384	0.5006695668094394	0.4942296776336768	T	T	T
0.8333333332986896	0.0000000000000000	0.0984529120410897	F	F	F
0.8335744936529088	0.9998724769483750	0.2972563279609742	T	T	T
0.8322131684337963	0.9982086418455248	0.4942975297130502	T	T	T
0.8333333332986896	0.166666667013104	0.0000000000000000	F	F	F
0.8334007754075525	0.1666658289657082	0.1978390087868274	T	T	T
0.8325895359319327	0.1666627546719630	0.3961426824568783	T	T	T
0.8333333332986896	0.3333333332986896	0.0984529120410897	F	F	F
0.8335831865671102	0.3334577196781697	0.2972577301582540	T	T	T
0.8322322204408736	0.3351067182654701	0.4943031774136959	T	T	T
0.8333333332986896	0.5000000000000000	0.0000000000000000	F	F	F
0.8334239892299655	0.4999725265373524	0.1978183040895833	T	T	T
0.8333474083013985	0.5000880244485582	0.3962197666250207	T	T	T
0.0000000000000000	0.666666667013104	0.0000000000000000	F	F	F
0.0000759031971795	0.6666651770284842	0.1978964035783108	T	T	T
0.0001366690030323	0.6666613439884915	0.3965509949147493	T	T	T
0.166666667013104	0.666666667013104	0.0984529120410897	F	F	F
0.1666653469643705	0.6666679709727704	0.2973801776292277	T	T	T
0.1666664374783830	0.6666664155596436	0.4948823134664526	T	T	T
0.3333333332986896	0.666666667013104	0.0000000000000000	F	F	F
0.3332564859323711	0.6666693612779530	0.1978967552332561	T	T	T
0.3331958448219857	0.6666741307182409	0.3965502496894180	T	T	T
0.5000000000000000	0.666666667013104	0.0984529120410897	F	F	F
0.4998883151317462	0.6666716112639588	0.2970427378724254	T	T	T
0.5005619267210965	0.6666719490102493	0.4942446284564860	T	T	T
0.666666667013104	0.666666667013104	0.0000000000000000	F	F	F
0.6666665680248497	0.6666670303738396	0.1977851722388198	T	T	T
0.6666664766047741	0.6666679197138388	0.3961955254302366	T	T	T
0.8333333332986896	0.666666667013104	0.0984529120410897	F	F	F
0.8334441892209662	0.6666640502910312	0.2970428317644560	T	T	T
0.8327714399297511	0.6666614655566787	0.4942450020323973	T	T	T
0.0000000000000000	0.8333333332986896	0.0984529120410897	F	F	F
0.0001133851739537	0.8334442965641500	0.2973213989934996	T	T	T
0.9983680801950893	0.8323615216908612	0.4945837680904854	T	T	T
0.166666667013104	0.8333333332986896	0.0000000000000000	F	F	F
0.1666657970328253	0.8333433426844894	0.1979225462525550	T	T	T
0.1666608109933545	0.8335447795899387	0.3969900441714013	T	T	T
0.3333333332986896	0.8333333332986896	0.0984529120410897	F	F	F
0.3332134451878465	0.8334535658403612	0.2973237540613088	T	T	T
0.3349467263511003	0.8323758170872478	0.4945901351018792	T	T	T
0.5000000000000000	0.8333333332986896	0.0000000000000000	F	F	F
0.4999085632918768	0.8333614822976501	0.1978188151498806	T	T	T
0.4999861450739382	0.8332479078203715	0.3962202182671869	T	T	T
0.666666667013104	0.8333333332986896	0.0984529120410897	F	F	F
0.6666622729195658	0.8333498767803850	0.2970014876849718	T	T	T
0.6666607345533148	0.8326650498429615	0.4942302344372241	T	T	T
0.8333333332986896	0.8333333332986896	0.0000000000000000	F	F	F
0.8334210331057532	0.8333586113597634	0.1978182720648102	T	T	T
0.8333372939889312	0.8332369666682327	0.3962164763296196	T	T	T

0.166666667013104	0.166666667013104	0.0984529120410897	F	F	F
0.1666654059160695	0.1666660098838039	0.2986083242807638	T	T	T
0.1666683623435706	0.1666574091815422	0.4996237532293674	T	T	T
0.166666667013104	0.0000000000000000	0.0000000000000000	F	F	F
0.1666656408451672	0.0002300783528888	0.1982491446338426	T	T	T
0.1666587142110555	0.0012866258450850	0.3979896648301121	T	T	T
0.0000000000000000	0.166666667013104	0.0000000000000000	F	F	F
0.0002247966157535	0.1666655704451683	0.1983472482950099	T	T	T
0.0009345602659363	0.1666584531895694	0.3988602450028823	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529120410897	F	F	F
0.0001526263067776	0.0002852091663296	0.2971789640425673	T	T	T
0.9978450684648961	0.9997477144128416	0.4929203219623738	T	T	T
0.166666667013104	0.5000000000000000	0.0984529120410897	F	F	F
0.1666676316316545	0.4998122491815353	0.2973758327788478	T	T	T
0.1666750317056789	0.5020356081486770	0.4941741324314572	T	T	T
0.166666667013104	0.333333332986896	0.0000000000000000	F	F	F
0.1666668362696250	0.3331027196802196	0.1982484025620426	T	T	T
0.1666737206416873	0.3320438899815789	0.3979867198737955	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0000991379375565	0.4999428085503871	0.1980900096800698	T	T	T
0.0000613779080727	0.5002456944521652	0.3971026426756051	T	T	T
0.0000000000000000	0.333333332986896	0.0984529120410897	F	F	F
0.0001586546704115	0.3330420706895237	0.2971823703903722	T	T	T
0.9978900904583249	0.3335398305956487	0.4929434411993221	T	T	T
0.5000000000000000	0.166666667013104	0.0984529120410897	F	F	F
0.4997246492107121	0.1666699239847968	0.2972899121648923	T	T	T
0.5012875567542396	0.1666793160685411	0.4935771300375586	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.4999282165853429	0.0000893980917882	0.1980299677109419	T	T	T
0.5003505448213129	0.0000499440664884	0.3968011181672441	T	T	T
0.333333332986896	0.166666667013104	0.0000000000000000	F	F	F
0.3331072817283536	0.1666671699299504	0.1983470682207039	T	T	T
0.3323978789211141	0.1666726818275871	0.3988581771665423	T	T	T
0.333333332986896	0.0000000000000000	0.0984529120410897	F	F	F
0.3331727004391130	0.0002913195414349	0.2971837234765053	T	T	T
0.3354431195683428	0.9997912008069219	0.4929476018384877	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120410897	F	F	F
0.4999223086509828	0.4999943479129205	0.2969979866345259	T	T	T
0.5005405274420173	0.5005113846600088	0.4933821435870473	T	T	T
0.5000000000000000	0.333333332986896	0.0000000000000000	F	F	F
0.4999318899168547	0.3332468010783323	0.1980283172065331	T	T	T
0.5003673587521466	0.3332970890169972	0.3967922707320540	T	T	T
0.333333332986896	0.5000000000000000	0.0000000000000000	F	F	F
0.3332353375415808	0.4999466750908729	0.1980892175626828	T	T	T
0.3332817131972136	0.5002634472303137	0.3970948135627759	T	T	T
0.333333332986896	0.333333332986896	0.0984529120410897	F	F	F
0.3331796681543746	0.3330489324833298	0.2971780281050817	T	T	T
0.3354876968588190	0.3335829022717943	0.4929157762083303	T	T	T
0.666666667013104	0.166666667013104	0.0000000000000000	F	F	F
0.6666665899742896	0.1666667330362871	0.1980796638221701	T	T	T
0.6666673350004325	0.1666685136790831	0.3968847938603005	T	T	T
0.666666667013104	0.0000000000000000	0.0984529120410897	F	F	F
0.6666607785694113	0.0000827219213810	0.2969558366448132	T	T	T
0.6666566921821038	0.9996046496273379	0.4934630211480874	T	T	T
0.666666667013104	0.5000000000000000	0.0000000000000000	F	F	F
0.6666682073740282	0.4999789700052567	0.1979870410017200	T	T	T
0.6666729651106023	0.5001277461647095	0.3967311653802317	T	T	T
0.666666667013104	0.333333332986896	0.0984529120410897	F	F	F
0.6666710008365085	0.3332529923796495	0.2969549520412388	T	T	T
0.6666756567467981	0.3337330207428434	0.4934614920454600	T	T	T

0.8333333332986896	0.1666666667013104	0.0984529120410897	F	F	F
0.8336077561118559	0.1666650584709657	0.2972911528697046	T	T	T
0.8320456689399217	0.1666578964890150	0.4935800616900499	T	T	T
0.8333333332986896	0.0000000000000000	0.0000000000000000	F	F	F
0.8334004286382487	0.0000870009797056	0.1980292735787776	T	T	T
0.8329655868173761	0.0000396841558492	0.3967945649249044	T	T	T
0.8333333332986896	0.5000000000000000	0.0984529120410897	F	F	F
0.8334170321898796	0.4999863938377093	0.2970002277236337	T	T	T
0.8328089773453637	0.5004947820330115	0.4933869080559125	T	T	T
0.8333333332986896	0.3333333332986896	0.0000000000000000	F	F	F
0.8334043081611955	0.3332441075291680	0.1980295591101234	T	T	T
0.8329823603266078	0.3332856104748138	0.3968001633702039	T	T	T
0.0000000000000000	0.6666666667013104	0.0984529120410897	F	F	F
0.0000680956676779	0.6666627058576838	0.2970625645961398	T	T	T
0.9992062475772757	0.6666584833380724	0.4935821688145349	T	T	T
0.1666666667013104	0.6666666667013104	0.0000000000000000	F	F	F
0.1666661625605734	0.6666672786621273	0.1981123900084125	T	T	T
0.1666657930662254	0.6666673980380787	0.3970694507952254	T	T	T
0.3333333332986896	0.6666666667013104	0.0984529120410897	F	F	F
0.3332634055768319	0.6666730016232670	0.2970625222735389	T	T	T
0.3341274630614319	0.6666736351530896	0.4935809749460364	T	T	T
0.5000000000000000	0.6666666667013104	0.0000000000000000	F	F	F
0.4999521695060073	0.6666690276007073	0.1979820088221723	T	T	T
0.5001027740925695	0.6666744411406755	0.3967194575704328	T	T	T
0.6666666667013104	0.6666666667013104	0.0984529120410897	F	F	F
0.6666661662069029	0.6666678252574965	0.2969030739339240	T	T	T
0.6666668717440151	0.6666670440505003	0.4934025740216074	T	T	T
0.8333333332986896	0.6666666667013104	0.0000000000000000	F	F	F
0.8333805349430705	0.6666654234132831	0.1979819592564837	T	T	T
0.8332305447503240	0.6666618165939683	0.3967199603617156	T	T	T
0.0000000000000000	0.8333333332986896	0.0000000000000000	F	F	F
0.0000970635837799	0.8333873269269001	0.1980896886693732	T	T	T
0.0000505284714313	0.8330702683816413	0.3970972226019019	T	T	T
0.1666666667013104	0.8333333332986896	0.0984529120410897	F	F	F
0.1666635660137580	0.8335222394620507	0.2973773040006525	T	T	T
0.1666585976677817	0.8312959200481767	0.4941786435495637	T	T	T
0.3333333332986896	0.8333333332986896	0.0000000000000000	F	F	F
0.3332334660160640	0.8333913366299073	0.1980907188944709	T	T	T
0.3332710360836318	0.8330882995371572	0.3971036822364954	T	T	T
0.5000000000000000	0.8333333332986896	0.0984529120410897	F	F	F
0.4999153716364472	0.8333490257164786	0.2970007138532565	T	T	T
0.5005260303399808	0.8328394423188290	0.4933873031408854	T	T	T
0.6666666667013104	0.8333333332986896	0.0000000000000000	F	F	F
0.6666649221389522	0.8333550486122162	0.1979875230656147	T	T	T
0.6666609490560864	0.8332092571780499	0.3967314590306100	T	T	T
0.8333330000000032	0.8333333332986896	0.0984529120410897	F	F	F
0.8334096203803871	0.8333418343610488	0.2969987921448688	T	T	T
0.8327908693824382	0.8328230250145464	0.4933833127500840	T	T	T
0.1669552399442362	0.2456433599597682	0.5799888597825528	T	T	T
0.1663724478478939	0.0876857649502887	0.5799965468898739	T	T	T
0.1666666055459533	0.1666690418412121	0.5572149822097017	T	T	T

T2-pbc-2CO2 (-1425.1568 eV)

1.0000000000000000

14.4329999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4329999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 24.4329999999999998

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Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0003246505620271	0.0003257197708936	0.1977852278940178	T	T	T
0.0022302168606016	0.0022283927142959	0.3979176046800574	T	T	T
0.0000000000000000	0.1666666667013104	0.0984529120410897	F	F	F
0.0003786813416127	0.1671136702619733	0.2974293666204553	T	T	T
0.9906201917036408	0.1711092564256990	0.4984005967477826	T	T	T
0.1666666667013104	0.0000000000000000	0.0984529120410897	F	F	F
0.1671133093179971	0.0003788400554032	0.2974302954674737	T	T	T
0.1711076992517690	0.9906175451375490	0.4984084422649904	T	T	T
0.1666666667013104	0.1666666667013104	0.0000000000000000	F	F	F
0.1667909290071697	0.1667915022237346	0.1979130304623957	T	T	T
0.1682739960002392	0.1682717950562084	0.3966734524149412	T	T	T
0.0000000000000000	0.333333332986896	0.0000000000000000	F	F	F
0.9999559454362068	0.3334635873705329	0.1977830754875204	T	T	T
0.0000057419554916	0.3344361839776043	0.3965963191813738	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529120410897	F	F	F
0.9995401518562770	0.5004604564613461	0.2968464142094851	T	T	T
0.9941246372392842	0.5058767621656891	0.4926943226832380	T	T	T
0.1666666667013104	0.333333332986896	0.0984529120410897	F	F	F
0.1661982010246622	0.3338025310479011	0.2974000750394138	T	T	T
0.1513000597516500	0.3486965390304118	0.5048202425068310	T	T	T
0.1666666667013104	0.5000000000000000	0.0000000000000000	F	F	F
0.1665369576146756	0.5000436139888073	0.1977831732022295	T	T	T
0.1655661076305666	0.4999945683374280	0.3965985420174423	T	T	T
0.333333332986896	0.0000000000000000	0.0000000000000000	F	F	F
0.3334625978342889	0.9999565091166049	0.1977829925003994	T	T	T
0.3344354308541725	0.0000065952687641	0.3966017929595640	T	T	T
0.333333332986896	0.1666666667013104	0.0984529120410897	F	F	F
0.3338029126701333	0.1661988129409969	0.2974013882297565	T	T	T
0.3486965951371859	0.1513067214117950	0.5048267174563781	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120410897	F	F	F
0.5004588392314938	0.9995411747492392	0.2968482030664824	T	T	T
0.5058776092186863	0.9941234539753345	0.4926976444773479	T	T	T
0.5000000000000000	0.1666666667013104	0.0000000000000000	F	F	F
0.5000433879322224	0.1665375576367296	0.1977831979829427	T	T	T
0.4999945351472918	0.1655656058007905	0.3966014308939533	T	T	T
0.333333332986896	0.333333332986896	0.0000000000000000	F	F	F
0.3332088457191090	0.3332097614728842	0.1979134349245125	T	T	T
0.3317262081544845	0.3317308212535893	0.3966749935522242	T	T	T
0.333333332986896	0.5000000000000000	0.0984529120410897	F	F	F
0.3328868277924255	0.4996216987314513	0.2974308332924506	T	T	T
0.3288879696092903	0.5093827203245043	0.4984073960939844	T	T	T
0.5000000000000000	0.333333332986896	0.0984529120410897	F	F	F
0.4996201793641342	0.3328874487074963	0.2974314321039339	T	T	T
0.5093781495742924	0.3288941780037823	0.4984062772747125	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4996736156593291	0.4996749407180001	0.1977858962049422	T	T	T
0.4977687063956688	0.4977710586932341	0.3979191600861173	T	T	T
0.6666666667013104	0.0000000000000000	0.0000000000000000	F	F	F
0.6669146454955837	-0.0000197031844149	0.1976482191618738	T	T	T
0.6681158589763991	0.9994260161490512	0.3953802306664354	T	T	T
0.6666666667013104	0.1666666667013104	0.0984529120410897	F	F	F
0.6668314785493479	0.1664607193493164	0.2969348703061621	T	T	T
0.6689353409114870	0.1634413729792758	0.4938505669090459	T	T	T
0.6666666667013104	0.333333332986896	0.0000000000000000	F	F	F
0.6664693997711221	0.3332407812355051	0.1977407517963560	T	T	T
0.6660670817893326	0.3327422411548849	0.3960967013317989	T	T	T
0.6666666667013104	0.5000000000000000	0.0984529120410897	F	F	F

0.6656084125519809	0.4996676281668277	0.2969903521297549	T	T	T
0.6658075794112126	0.5011457123702209	0.4941511573413118	T	T	T
0.8333333332986896	0.0000000000000000	0.0984529120410897	F	F	F
0.8343891611861178	0.0003335106027317	0.2969895510256734	T	T	T
0.8341926041962874	0.9988534049608060	0.4941493467207678	T	T	T
0.8333333332986896	0.1666666667013104	0.0000000000000000	F	F	F
0.8335293218734264	0.1667603760844998	0.1977408482783272	T	T	T
0.8339301672223122	0.1672581055301641	0.3960943287911114	T	T	T
0.8333333332986896	0.3333333332986896	0.0984529120410897	F	F	F
0.8331668247025996	0.3335402958523990	0.2969336167943777	T	T	T
0.8310653465167218	0.3365600038971833	0.4938492586486207	T	T	T
0.8333333332986896	0.5000000000000000	0.0000000000000000	F	F	F
0.8330834317618675	0.5000203798943930	0.1976483304657928	T	T	T
0.8318831836866666	0.5005754069568195	0.3953800686272819	T	T	T
0.0000000000000000	0.6666666667013104	0.0000000000000000	F	F	F
-0.0000206001206917	0.6669158799926566	0.1976483272918978	T	T	T
0.9994252480963323	0.6681158436255754	0.3953798551729426	T	T	T
0.1666666667013104	0.6666666667013104	0.0984529120410897	F	F	F
0.1664602903848581	0.6668315453317114	0.2969342939246158	T	T	T
0.1634410260301065	0.6689338674996856	0.4938491402314776	T	T	T
0.3333333332986896	0.6666666667013104	0.0000000000000000	F	F	F
0.3332397880557343	0.6664703881009901	0.1977412982885139	T	T	T
0.3327420656120811	0.6660671179526858	0.3960961759760835	T	T	T
0.5000000000000000	0.6666666667013104	0.0984529120410897	F	F	F
0.4996660723580323	0.6656096913288693	0.2969905676115498	T	T	T
0.5011446440361660	0.6658070175842106	0.4941506084307064	T	T	T
0.6666666667013104	0.6666666667013104	0.0000000000000000	F	F	F
0.6664782319185976	0.6664797705322444	0.1975961456699652	T	T	T
0.6660801321827583	0.6660812178440357	0.3956423072977590	T	T	T
0.8333333332986896	0.6666666667013104	0.0984529120410897	F	F	F
0.8330733200451542	0.6669252202522338	0.2965608257093409	T	T	T
0.8318308461710573	0.6681693375465226	0.4935538003564931	T	T	T
0.0000000000000000	0.8333333332986896	0.0984529120410897	F	F	F
0.0003316513985286	0.834390001007919	0.2969895864371277	T	T	T
0.9988544149920185	0.8341909884864493	0.4941498781928961	T	T	T
0.1666666667013104	0.8333333332986896	0.0000000000000000	F	F	F
0.1667594215778619	0.8335298202351547	0.1977406709648765	T	T	T
0.1672578597714818	0.8339305393930646	0.3960964562418343	T	T	T
0.3333333332986896	0.8333333332986896	0.0984529120410897	F	F	F
0.3335395752262536	0.8331677157018240	0.2969348994248980	T	T	T
0.3365585337488896	0.8310634532437761	0.4938511347432736	T	T	T
0.5000000000000000	0.8333333332986896	0.0000000000000000	F	F	F
0.5000188838118061	0.8330843825696308	0.1976484405469022	T	T	T
0.5005745589241697	0.8318830561438658	0.3953805031123495	T	T	T
0.6666666667013104	0.8333333332986896	0.0984529120410897	F	F	F
0.6669232561425651	0.8330752569454625	0.2965608561933290	T	T	T
0.6681698953436240	0.8318306501380087	0.4935527061375216	T	T	T
0.8333333332986896	0.8333333332986896	0.0000000000000000	F	F	F
0.8335192723522816	0.8335209143527240	0.1975959688352773	T	T	T
0.8339178171868803	0.8339183242542798	0.3956417261382287	T	T	T
0.1666666667013104	0.1666666667013104	0.0984529120410897	F	F	F
0.1671099075218883	0.1671074517748594	0.2983909276263021	T	T	T
0.1716753430865041	0.1716419711294782	0.4948955484943249	T	T	T
0.1666666667013104	0.0000000000000000	0.0000000000000000	F	F	F
0.1668812889409639	0.0003975507877183	0.1982436590242611	T	T	T
0.1682880225391061	0.0014379475510364	0.3986379974615671	T	T	T
0.0000000000000000	0.1666666667013104	0.0000000000000000	F	F	F
0.0003971232017695	0.1668814895553548	0.1982431722646393	T	T	T
0.0014401304931308	0.1682854969919798	0.3986374121543667	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529120410897	F	F	F

0.0009352371448345	0.0009350409139823	0.2972672959697051	T	T	T
0.0026258751702658	0.0026251885006265	0.4943547853046816	T	T	T
0.1666666667013104	0.5000000000000000	0.0984529120410897	F	F	F
0.1663719875185264	0.4999976307202433	0.2969054569367652	T	T	T
0.1596172137973720	0.5058416922630896	0.4914977200872961	T	T	T
0.1666666667013104	0.333333332986896	0.0000000000000000	F	F	F
0.1667961896818424	0.3332036349444062	0.1983374989720482	T	T	T
0.1664566842525761	0.3335405809519982	0.3988124414330962	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.9998729046854588	0.5001269536872623	0.1978580825594047	T	T	T
0.9979023345696680	0.5020978210898929	0.3956288479184222	T	T	T
0.0000000000000000	0.333333332986896	0.0984529120410897	F	F	F
0.0000014392424491	0.3336273802425608	0.2969049590255444	T	T	T
0.9941549401542340	0.3403829671251574	0.4914926647914045	T	T	T
0.5000000000000000	0.1666666667013104	0.0984529120410897	F	F	F
0.4999970229250533	0.1663723564575508	0.2969070740295933	T	T	T
0.5058395917304549	0.1596186617513786	0.4914997462127165	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5001248602976678	0.9998745940674774	0.1978593068536090	T	T	T
0.5020954002099747	0.9979031464207562	0.3956323450608908	T	T	T
0.333333332986896	0.1666666667013104	0.0000000000000000	F	F	F
0.3332038948051066	0.1667959638730245	0.1983386880091475	T	T	T
0.3335442533162224	0.1664582053783095	0.3988176060985802	T	T	T
0.333333332986896	0.0000000000000000	0.0984529120410897	F	F	F
0.3336272713976084	0.0000033970052980	0.2969077051863235	T	T	T
0.3403823225891041	0.9941618848025893	0.4915021796324985	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120410897	F	F	F
0.4990654006800724	0.4990645919797239	0.2972678934446278	T	T	T
0.4973759256823979	0.4973753472840438	0.4943572815637158	T	T	T
0.5000000000000000	0.333333332986896	0.0000000000000000	F	F	F
0.4996025714996372	0.3331187130386729	0.1982439346614883	T	T	T
0.4985596658514883	0.3317127603941802	0.3986408125864465	T	T	T
0.333333332986896	0.5000000000000000	0.0000000000000000	F	F	F
0.3331186397396870	0.4996030347780753	0.1982429284801222	T	T	T
0.3317130666341388	0.4985620956639783	0.3986366217042857	T	T	T
0.333333332986896	0.333333332986896	0.0984529120410897	F	F	F
0.3328916693035251	0.3328902702672372	0.2983914905310757	T	T	T
0.3283226288420225	0.3283714198437935	0.4949003750919123	T	T	T
0.6666666667013104	0.1666666667013104	0.0000000000000000	F	F	F
0.6667889604406724	0.1666740763544114	0.1979631485249159	T	T	T
0.6679634569361708	0.1661403782710140	0.3963568141761405	T	T	T
0.6666666667013104	0.0000000000000000	0.0984529120410897	F	F	F
0.6674831440839842	0.9998040028939259	0.2965814109120581	T	T	T
0.6698351495204400	0.9976434024243264	0.4926637511542196	T	T	T
0.6666666667013104	0.5000000000000000	0.0000000000000000	F	F	F
0.6662715069734828	0.4997956760300174	0.1979574018123933	T	T	T
0.6652746044726912	0.4994836609395873	0.3968487538742185	T	T	T
0.6666666667013104	0.333333332986896	0.0984529120410897	F	F	F
0.6660052342591883	0.3331046728029679	0.2970431813945675	T	T	T
0.6671507593962733	0.3326395582313561	0.4935751802070267	T	T	T
0.833333332986896	0.1666666667013104	0.0984529120410897	F	F	F
0.8339931888643446	0.1668963378521761	0.2970429778212308	T	T	T
0.8328479551434378	0.1673610777914497	0.4935724428827186	T	T	T
0.833333332986896	0.0000000000000000	0.0000000000000000	F	F	F
0.8337265828014671	0.0002049955669728	0.1979570410368129	T	T	T
0.8347256352894756	0.0005168267507244	0.3968476280058910	T	T	T
0.833333332986896	0.5000000000000000	0.0984529120410897	F	F	F
0.8325139529857601	0.5001976869356332	0.2965814436745423	T	T	T
0.8301646375075170	0.5023573245805458	0.4926637871151799	T	T	T
0.833333332986896	0.333333332986896	0.0000000000000000	F	F	F

0.8332088417610028	0.3333274731350602	0.1979628624741683	T	T	T
0.8320351471722719	0.3338603023648747	0.3963552734442523	T	T	T
0.0000000000000000	0.6666666667013104	0.0984529120410897	F	F	F
0.9998017544217909	0.6674854272038657	0.2965810004792470	T	T	T
0.9976429978215496	0.6698346645211604	0.4926632359550536	T	T	T
0.1666666667013104	0.6666666667013104	0.0000000000000000	F	F	F
0.1666724770589821	0.6667906017502930	0.1979627024420966	T	T	T
0.1661391709899320	0.6679639375223327	0.3963555807866634	T	T	T
0.3333333332986896	0.6666666667013104	0.0984529120410897	F	F	F
0.3331036936256237	0.6660080122942070	0.2970426860885728	T	T	T
0.3326393132337756	0.6671541376557830	0.4935742714926440	T	T	T
0.5000000000000000	0.6666666667013104	0.0000000000000000	F	F	F
0.4997947490266920	0.6662726282552219	0.1979572012098490	T	T	T
0.4994839372133917	0.6652752024294537	0.3968487911550976	T	T	T
0.6666666667013104	0.6666666667013104	0.0984529120410897	F	F	F
0.6663078835478142	0.6663086825042464	0.2966985258063636	T	T	T
0.6661305071588317	0.6661305562315487	0.4929917904907916	T	T	T
0.8333333332986896	0.6666666667013104	0.0000000000000000	F	F	F
0.8332227412508407	0.6667763041291886	0.1978273546829090	T	T	T
0.8326093371230996	0.6673892929446562	0.3961794304508655	T	T	T
0.0000000000000000	0.8333333332986896	0.0000000000000000	F	F	F
0.0002040120234234	0.8337279980628866	0.1979571463671740	T	T	T
0.0005162263753893	0.8347256452877687	0.3968474410573617	T	T	T
0.1666666667013104	0.8333333332986896	0.0984529120410897	F	F	F
0.1668950758138073	0.8339942983741496	0.2970430702365192	T	T	T
0.1673609286966198	0.8328480638955025	0.4935740747934284	T	T	T
0.3333333332986896	0.8333333332986896	0.0000000000000000	F	F	F
0.3333259933470682	0.8332110074162715	0.1979633683748326	T	T	T
0.3338595718730280	0.8320393822443282	0.3963572414782810	T	T	T
0.5000000000000000	0.8333333332986896	0.0984529120410897	F	F	F
0.5001953373364383	0.8325166938679512	0.2965817800893151	T	T	T
0.5023570949858702	0.8301658799566038	0.4926645054782373	T	T	T
0.6666666667013104	0.8333333332986896	0.0000000000000000	F	F	F
0.6667745805913969	0.8332243826720266	0.1978271041294288	T	T	T
0.6673886319444469	0.8326105496798456	0.3961793150620748	T	T	T
0.8333330000000032	0.8333333332986896	0.0984529120410897	F	F	F
0.8336902612920946	0.8336914486228421	0.2966980754345228	T	T	T
0.8338697906676246	0.8338698471436997	0.4929907354814793	T	T	T
0.1030123423766975	0.2155089226080847	0.5732523211570012	T	T	T
0.2154571066581771	0.1029896596893489	0.5732731703791693	T	T	T
0.2845203836702925	0.3970122312172544	0.5732802045008445	T	T	T
0.3969760611524776	0.2844953164588269	0.5732568895070510	T	T	T
0.1631695396352040	0.1631853525066418	0.5509066890901445	T	T	T
0.3368103206918425	0.336828886756795	0.5509071153339591	T	T	T

T2-pbc-3CO2 (-1449.4828 eV)

1.0000000000000000

14.4329999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4329999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 24.4329999999999998

Ca O C

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Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0003302261359061	0.0003277891851065	0.1977150977671540	T	T	T
0.0022241606596458	0.0022230643924731	0.3972980163719277	T	T	T
0.0000000000000000	0.1666666667013104	0.0984529120410897	F	F	F
0.0007787430845962	0.1672163514051379	0.2972726420591825	T	T	T

0.9914761234129137	0.1698924320452178	0.4980196723171759	T	T	T
0.166666667013104	0.0000000000000000	0.0984529120410897	F	F	F
0.1672177638118253	0.0007777918605729	0.2972740323242077	T	T	T
0.1698849989866227	0.9914847123558684	0.4980307981500679	T	T	T
0.166666667013104	0.166666667013104	0.0000000000000000	F	F	F
0.1669823839535913	0.1669816344017632	0.1979003252901753	T	T	T
0.1689166196617607	0.1689207208555647	0.3966947754167964	T	T	T
0.0000000000000000	0.333333332986896	0.0000000000000000	F	F	F
0.0001235781148910	0.3335023739750280	0.1978285832394455	T	T	T
0.0006402032888785	0.3344712554999679	0.3963761671305054	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529120410897	F	F	F
0.9997017141871224	0.5004261525093596	0.2969517798779156	T	T	T
0.9943820806978322	0.5059039981214001	0.4929257831231695	T	T	T
0.166666667013104	0.333333332986896	0.0984529120410897	F	F	F
0.1668437219593547	0.3340594779222444	0.2976837008142260	T	T	T
0.1508467755787142	0.3478967285223148	0.5048103461214470	T	T	T
0.166666667013104	0.5000000000000000	0.0000000000000000	F	F	F
0.1665647281040097	0.5001032844445187	0.1978314358181705	T	T	T
0.1662029009041795	0.5004687038531935	0.3969577779011534	T	T	T
0.333333332986896	0.0000000000000000	0.0000000000000000	F	F	F
0.3335035022871215	0.0001221606405252	0.1978294207167771	T	T	T
0.3344654037827684	0.0006430936267428	0.3963819508743236	T	T	T
0.333333332986896	0.166666667013104	0.0984529120410897	F	F	F
0.3340580036774842	0.1668430784429845	0.2976835610999968	T	T	T
0.3478836175789131	0.1508542938960942	0.5048144205728113	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120410897	F	F	F
0.5004238368198860	0.9996993787012041	0.2969533291228561	T	T	T
0.5058972091512676	0.9943832706715673	0.4929290580915722	T	T	T
0.5000000000000000	0.166666667013104	0.0000000000000000	F	F	F
0.5001032357996879	0.1665630032257442	0.1978312344084895	T	T	T
0.5004645637458689	0.1661988570409655	0.3969571908199710	T	T	T
0.333333332986896	0.333333332986896	0.0000000000000000	F	F	F
0.3333336938241198	0.3333332349825521	0.1980159604895281	T	T	T
0.3333343823097271	0.3333326694439511	0.3981236480663604	T	T	T
0.333333332986896	0.5000000000000000	0.0984529120410897	F	F	F
0.3326097483116529	0.4998240640418457	0.2976842614177788	T	T	T
0.3187865536808133	0.5158124740330209	0.5048085137490691	T	T	T
0.5000000000000000	0.333333332986896	0.0984529120410897	F	F	F
0.4998238183691686	0.3326074621861726	0.2976829023395845	T	T	T
0.5158210730233724	0.3187707475365051	0.5048123686598671	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4996853689141384	0.4996848995532431	0.1979003498309693	T	T	T
0.4977520489020291	0.4977458323550972	0.3966942262408138	T	T	T
0.666666667013104	0.0000000000000000	0.0000000000000000	F	F	F
0.6668696628134643	0.9997968709904146	0.1976868485303016	T	T	T
0.6679823739653991	0.9986816456837169	0.3950366436026682	T	T	T
0.666666667013104	0.166666667013104	0.0984529120410897	F	F	F
0.6669664632323252	0.1662405231252585	0.2969510003435789	T	T	T
0.6722848349333574	0.1607633682968448	0.4929248270552373	T	T	T
0.666666667013104	0.333333332986896	0.0000000000000000	F	F	F
0.6665443831019217	0.3331636109054676	0.1978282265644600	T	T	T
0.6660257280757461	0.3321959730921821	0.3963761755427065	T	T	T
0.666666667013104	0.5000000000000000	0.0984529120410897	F	F	F
0.6658900418491286	0.4994498019192145	0.2972720784211516	T	T	T
0.6751902732920356	0.4967771649421518	0.4980198840808568	T	T	T
0.833333332986896	0.0000000000000000	0.0984529120410897	F	F	F
0.8342923004326003	0.0000283132653538	0.2967862224602181	T	T	T
0.8348481199717974	0.9980683367880582	0.4936958568131376	T	T	T
0.833333332986896	0.166666667013104	0.0000000000000000	F	F	F
0.8335801750740651	0.1667160201978696	0.1977026569694076	T	T	T

0.8345799551946427	0.1667278362165697	0.3953830133988767	T	T	T
0.8333333332986896	0.3333333332986896	0.0984529120410897	F	F	F
0.8333336362586145	0.3333330390479634	0.2969445746611687	T	T	T
0.8333319990747875	0.3333340521079111	0.4933465668999948	T	T	T
0.8333333332986896	0.5000000000000000	0.0000000000000000	F	F	F
0.8330886444445309	0.4999494248609022	0.1977026092582888	T	T	T
0.8320868170029423	0.4999395352340978	0.3953830653436048	T	T	T
0.0000000000000000	0.6666666667013104	0.0000000000000000	F	F	F
0.9997992139808363	0.6668688371507151	0.1976870317355907	T	T	T
0.9986857582523956	0.6679859537846721	0.3950384104687252	T	T	T
0.1666666667013104	0.6666666667013104	0.0984529120410897	F	F	F
0.1662445387574448	0.6669676379675846	0.2969544671108765	T	T	T
0.1607722272547009	0.6722839088860709	0.4929303126054106	T	T	T
0.3333333332986896	0.6666666667013104	0.0000000000000000	F	F	F
0.3331648100208791	0.6665443648241418	0.1978298216031348	T	T	T
0.3322033079228618	0.6660266428512542	0.3963811454889387	T	T	T
0.5000000000000000	0.6666666667013104	0.0984529120410897	F	F	F
0.4994513904173552	0.6658882806169623	0.2972737731454789	T	T	T
0.4967830930717827	0.6751825261539063	0.4980291741291181	T	T	T
0.6666666667013104	0.6666666667013104	0.0000000000000000	F	F	F
0.6663389263317774	0.6663380413368981	0.1977148627781678	T	T	T
0.6644447252765647	0.6644438264277679	0.3972966958103659	T	T	T
0.8333333332986896	0.6666666667013104	0.0984529120410897	F	F	F
0.8323774665747024	0.6666372780744164	0.2967863517312274	T	T	T
0.8318191225562679	0.6685994489955285	0.4936966537334676	T	T	T
0.0000000000000000	0.8333333332986896	0.0984529120410897	F	F	F
0.0000322368895979	0.8342903024582543	0.2967874327426114	T	T	T
0.9980710303615696	0.8348475852608930	0.4936980341210891	T	T	T
0.1666666667013104	0.8333333332986896	0.0000000000000000	F	F	F
0.1667186741642039	0.8335784795621207	0.1977036176421978	T	T	T
0.1667306483676812	0.8345830623285355	0.3953886413430727	T	T	T
0.3333333332986896	0.8333333332986896	0.0984529120410897	F	F	F
0.3333343271709509	0.8333338967595032	0.2969482984816894	T	T	T
0.3333353798350546	0.8333344011437311	0.4933531221396396	T	T	T
0.5000000000000000	0.8333333332986896	0.0000000000000000	F	F	F
0.4999501039015447	0.8330875267704789	0.1977033836041633	T	T	T
0.4999382208206286	0.8320844246959138	0.3953873238929806	T	T	T
0.6666666667013104	0.8333333332986896	0.0984529120410897	F	F	F
0.6666375952551171	0.8323756703981304	0.2967865081422311	T	T	T
0.6685964086940478	0.8318194594511913	0.4936964086666413	T	T	T
0.8333333332986896	0.8333333332986896	0.0000000000000000	F	F	F
0.8333348731838807	0.8333328656595477	0.1975867198265288	T	T	T
0.8333343073499979	0.8333334258601388	0.3953172213732626	T	T	T
0.1666666667013104	0.1666666667013104	0.0984529120410897	F	F	F
0.1674987607074700	0.1674994084172707	0.2985517664656921	T	T	T
0.1735532363547546	0.1735738756367759	0.4954949949806225	T	T	T
0.1666666667013104	0.0000000000000000	0.0000000000000000	F	F	F
0.1669134030227826	0.0005615099368872	0.1982990094612097	T	T	T
0.1681608492469094	0.0021811997959971	0.3984203795342702	T	T	T
0.0000000000000000	0.1666666667013104	0.0000000000000000	F	F	F
0.0005630092341686	0.1669117323361539	0.1982982975549429	T	T	T
0.0021777055580399	0.1681627463979765	0.3984164512575861	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529120410897	F	F	F
0.0009549375279652	0.0009526858972768	0.2971302815189944	T	T	T
0.0025637627766881	0.0025671299576201	0.4938468545328312	T	T	T
0.1666666667013104	0.5000000000000000	0.0984529120410897	F	F	F
0.1665764395211629	0.5000939743982444	0.2972722743328337	T	T	T
0.1592004239418482	0.5074727818766961	0.4925785694901883	T	T	T
0.1666666667013104	0.3333333332986896	0.0000000000000000	F	F	F
0.1670107046864456	0.3333608526699735	0.1985269550388228	T	T	T

0.1670953078667608	0.3341689564499474	0.3994819950164902	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.9998950467235590	0.5001174332709458	0.1980390542520289	T	T	T
0.9982129147204564	0.5020525656018141	0.3958243494842620	T	T	T
0.0000000000000000	0.333333332986896	0.0984529120410897	F	F	F
0.0005051276320193	0.3336646130564621	0.2969041032101478	T	T	T
0.9951127597944048	0.3399356352736517	0.4912472562422481	T	T	T
0.5000000000000000	0.166666667013104	0.0984529120410897	F	F	F
0.5000921169316020	0.1665726458161502	0.2972711823867483	T	T	T
0.5074665236855032	0.1591950553137773	0.4925794036230373	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5001179199831416	0.9998926608711591	0.1980399995568437	T	T	T
0.5020465433092008	0.9982098984283680	0.3958275714172614	T	T	T
0.333333332986896	0.166666667013104	0.0000000000000000	F	F	F
0.3333609090079960	0.1670098609991031	0.1985271816759806	T	T	T
0.3341632021393758	0.1670963076677666	0.3994831898455309	T	T	T
0.333333332986896	0.0000000000000000	0.0984529120410897	F	F	F
0.3336638977051389	0.0005044977351895	0.2969068598322254	T	T	T
0.3399210971731713	0.9951200031814099	0.4912576655911239	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120410897	F	F	F
0.4991684587151080	0.4991676570237818	0.2985516332843167	T	T	T
0.4931187181076019	0.4930896147457171	0.4954954167480350	T	T	T
0.5000000000000000	0.333333332986896	0.0000000000000000	F	F	F
0.4996569302090098	0.3333059680270711	0.1985264814858634	T	T	T
0.4995721134375610	0.3324981581946211	0.3994801651487688	T	T	T
0.333333332986896	0.5000000000000000	0.0000000000000000	F	F	F
0.3333067330441886	0.4996570871039629	0.1985277521275724	T	T	T
0.3325052659338394	0.4995721136957433	0.3994870755797679	T	T	T
0.333333332986896	0.333333332986896	0.0984529120410897	F	F	F
0.3333334167772757	0.3333339123735602	0.2987463298117454	T	T	T
0.3333387026878203	0.3333294120469793	0.4947964261892746	T	T	T
0.666666667013104	0.166666667013104	0.0000000000000000	F	F	F
0.6667739529530587	0.1665486507744583	0.1980386210906617	T	T	T
0.6684542316632895	0.1646149082620294	0.3958238607275585	T	T	T
0.666666667013104	0.0000000000000000	0.0984529120410897	F	F	F
0.6673777177485370	0.9992881676226260	0.2965254669495597	T	T	T
0.6703364040144312	0.9963269279601193	0.4923479551903397	T	T	T
0.666666667013104	0.5000000000000000	0.0000000000000000	F	F	F
0.6661049057518516	0.4997542456838089	0.1982979551969104	T	T	T
0.6644898896775455	0.4985049148105533	0.3984155083143635	T	T	T
0.666666667013104	0.333333332986896	0.0984529120410897	F	F	F
0.6661625173281924	0.33330018989642393	0.2969032681704615	T	T	T
0.6715522147556002	0.3267319659208044	0.4912479638484152	T	T	T
0.833333332986896	0.166666667013104	0.0984529120410897	F	F	F
0.8342998795401585	0.1666342936023932	0.2968942971618897	T	T	T
0.8346086249233005	0.1654744612349221	0.4929199511125265	T	T	T
0.833333332986896	0.0000000000000000	0.0000000000000000	F	F	F
0.8337036286529466	0.0000624885576228	0.1979914278419190	T	T	T
0.8348077821209160	0.9999291922896257	0.3965194514094389	T	T	T
0.833333332986896	0.5000000000000000	0.0984529120410897	F	F	F
0.8323690438394211	0.5000310462773997	0.2968941807472988	T	T	T
0.8320576170201051	0.5011935701834024	0.4929198510714026	T	T	T
0.833333332986896	0.333333332986896	0.0000000000000000	F	F	F
0.8333341314129712	0.3333325327390327	0.1980325511159106	T	T	T
0.8333326590071490	0.3333337887856267	0.3959277670975710	T	T	T
0.0000000000000000	0.666666667013104	0.0984529120410897	F	F	F
0.9992914928183165	0.6673777551593914	0.2965264305521435	T	T	T
0.9963314934476415	0.6703402434507094	0.4923498862108987	T	T	T
0.166666667013104	0.666666667013104	0.0000000000000000	F	F	F
0.1665507295532606	0.6667730762546399	0.1980403942302160	T	T	T

0.1646220137887823	0.6684578660695143	0.3958286757791517	T	T	T
0.3333333332986896	0.6666666667013104	0.0984529120410897	F	F	F
0.3330046806643072	0.6661622416407221	0.2969073698576353	T	T	T
0.3267489286852217	0.6715492573451308	0.4912558254140679	T	T	T
0.5000000000000000	0.6666666667013104	0.0000000000000000	F	F	F
0.4997547573373099	0.6661045342141229	0.1982989494471809	T	T	T
0.4985082094445187	0.6644853492949145	0.3984200974674739	T	T	T
0.6666666667013104	0.6666666667013104	0.0984529120410897	F	F	F
0.6657145634037757	0.6657133184943331	0.2971294224388288	T	T	T
0.6641038666547874	0.6641005593043253	0.4938460862141521	T	T	T
0.8333333332986896	0.6666666667013104	0.0000000000000000	F	F	F
0.8329655144510094	0.6666025121837281	0.1979911371874729	T	T	T
0.8318604983861670	0.6667382522812396	0.3965199199290143	T	T	T
0.0000000000000000	0.8333333332986896	0.0000000000000000	F	F	F
0.0000653095989116	0.8337015783725362	0.1979916936233806	T	T	T
0.9999320213093067	0.8348086137271307	0.3965216375588059	T	T	T
0.1666666667013104	0.8333333332986896	0.0984529120410897	F	F	F
0.1666379839150530	0.8342989275260621	0.2968976555959061	T	T	T
0.1654773488244680	0.8346115876570769	0.4929274294263765	T	T	T
0.3333333332986896	0.8333333332986896	0.0000000000000000	F	F	F
0.3333345128923644	0.8333328283586108	0.1980347306530846	T	T	T
0.3333347971263499	0.8333350631879461	0.3959341845609624	T	T	T
0.5000000000000000	0.8333333332986896	0.0984529120410897	F	F	F
0.5000313226526178	0.8323668980963992	0.2968972002912840	T	T	T
0.5011914411505309	0.8320542435434269	0.4929261606448941	T	T	T
0.6666666667013104	0.8333333332986896	0.0000000000000000	F	F	F
0.6666040692848700	0.8329638682904086	0.1979914342549969	T	T	T
0.6667359375856085	0.8318585528807531	0.3965200326317221	T	T	T
0.8333330000000032	0.8333333332986896	0.0984529120410897	F	F	F
0.8333351262529667	0.8333326456336320	0.2967168542016561	T	T	T
0.8333333270340574	0.8333339744666646	0.4927230026105288	T	T	T
0.1006634783207548	0.2131802049230146	0.5733920661881168	T	T	T
0.2131106160356558	0.1006936023136984	0.5734031725798994	T	T	T
0.2770950615203962	0.3896170118845080	0.5736263848703208	T	T	T
0.3895780370876620	0.2770593516246386	0.5736342789906106	T	T	T
0.4535462207932547	0.5659693378207877	0.5733998772543728	T	T	T
0.5660099772887243	0.4535064857590547	0.5733936263905760	T	T	T
0.1621835172708000	0.1622221938778683	0.5514060735190330	T	T	T
0.3333325383205062	0.3333395070954221	0.5509168986678727	T	T	T
0.5044849547094216	0.5044472168562903	0.5514094430428575	T	T	T

T2-pbc-4CO2 (-1473.6809 eV)

1.0000000000000000

14.432999999999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.432999999999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	24.432999999999998

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Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0001373342914735	0.0001449204252724	0.1976263858193906	T	T	T
0.0016304591242427	0.0016526343664172	0.3969133123706173	T	T	T
0.0000000000000000	0.1666666667013104	0.0984529120410897	F	F	F
0.0007256471808966	0.1669127522643731	0.2969951675777943	T	T	T
0.9922342963753235	0.1688225900352887	0.4976614348531209	T	T	T
0.1666666667013104	0.0000000000000000	0.0984529120410897	F	F	F
0.1668964698680204	0.0007424056961260	0.2969945802354201	T	T	T
0.1688090781476999	0.9922484333584476	0.4976461578969568	T	T	T

0.1666666667013104	0.1666666667013104	0.0000000000000000	F	F	F
0.1669779609138505	0.1669870403604671	0.1977499277483659	T	T	T
0.1689320341752349	0.1689535833304758	0.3963267272516120	T	T	T
0.0000000000000000	0.333333332986896	0.0000000000000000	F	F	F
0.0001652433031688	0.3334536634417441	0.1976972766790752	T	T	T
0.0013384778902534	0.3338420126562121	0.3956229501928739	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529120410897	F	F	F
0.9998549198177549	0.5002160394702523	0.2968448837726047	T	T	T
0.9966265579724976	0.5027902647620506	0.4923135812223960	T	T	T
0.1666666667013104	0.333333332986896	0.0984529120410897	F	F	F
0.1672354515810321	0.3341214047989206	0.2974119948933648	T	T	T
0.1518907954235131	0.3467050341210847	0.5043151537487865	T	T	T
0.1666666667013104	0.5000000000000000	0.0000000000000000	F	F	F
0.1667338431544509	0.5001308431859384	0.1977810791794969	T	T	T
0.1668289929016903	0.5005437708394317	0.3966452762672492	T	T	T
0.333333332986896	0.0000000000000000	0.0000000000000000	F	F	F
0.3334442051188158	0.0001724989927763	0.1976959771319863	T	T	T
0.3338279974212255	0.0013542492820980	0.3956185305998924	T	T	T
0.333333332986896	0.1666666667013104	0.0984529120410897	F	F	F
0.3341029454532217	0.1672509884101498	0.2974123981927573	T	T	T
0.3466892958186649	0.1518894409654301	0.5043252553354929	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120410897	F	F	F
0.5002011845861203	0.9998643854545392	0.2968436164591529	T	T	T
0.5027839079495549	0.9966261863493554	0.4923076181777869	T	T	T
0.5000000000000000	0.1666666667013104	0.0000000000000000	F	F	F
0.5001206095033425	0.1667396630346139	0.1977806522386502	T	T	T
0.5005174868762996	0.1668389845327643	0.3966433384984900	T	T	T
0.333333332986896	0.333333332986896	0.0000000000000000	F	F	F
0.3335200269570745	0.3335286438798408	0.1979216091167637	T	T	T
0.3340131862496087	0.3340328923224644	0.3979493961022823	T	T	T
0.333333332986896	0.5000000000000000	0.0984529120410897	F	F	F
0.3332299117811390	0.5001017069671293	0.2978352068356701	T	T	T
0.3184270867407763	0.5149020684067013	0.5047309935418993	T	T	T
0.5000000000000000	0.333333332986896	0.0984529120410897	F	F	F
0.5000848122772390	0.3332409939383339	0.2978328558806843	T	T	T
0.5148834136138590	0.3184417811850485	0.5047167717563024	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4998031491793744	0.4998111920305945	0.1979208269981714	T	T	T
0.4992988605750542	0.4993115967838289	0.3979418748986641	T	T	T
0.6666666667013104	0.0000000000000000	0.0000000000000000	F	F	F
0.6667907425746917	0.9998085261671336	0.1976579127219385	T	T	T
0.6674200875655791	0.9988274071490563	0.3950231144055790	T	T	T
0.6666666667013104	0.1666666667013104	0.0984529120410897	F	F	F
0.6669265490297177	0.1664031224010012	0.2969493945204910	T	T	T
0.6722782009658268	0.1610441014214661	0.4931591633281845	T	T	T
0.6666666667013104	0.333333332986896	0.0000000000000000	F	F	F
0.6665928261063326	0.3332092351273344	0.1977798858405055	T	T	T
0.6664859494194961	0.3327994564878555	0.3966389649812770	T	T	T
0.6666666667013104	0.5000000000000000	0.0984529120410897	F	F	F
0.6660852087307960	0.4992230558115560	0.2974071863217487	T	T	T
0.6814324305612861	0.4866377882648105	0.5043002912496218	T	T	T
0.833333332986896	0.0000000000000000	0.0984529120410897	F	F	F
0.8340018835055799	0.9993340716636713	0.2969274577438442	T	T	T
0.8352699262226205	0.9980630753078276	0.4938812154889320	T	T	T
0.833333332986896	0.1666666667013104	0.0000000000000000	F	F	F
0.8335247628538459	0.1665429344441816	0.1976597332954423	T	T	T
0.8345012712266806	0.1659146240718818	0.3950279038086794	T	T	T
0.833333332986896	0.333333332986896	0.0984529120410897	F	F	F
0.8334679859353785	0.3331290479569634	0.2968439522015037	T	T	T
0.8366912487040552	0.3305519003005528	0.4923114947187782	T	T	T

0.8333333332986896	0.5000000000000000	0.0000000000000000	F	F	F
0.8331633782552583	0.4998872138805600	0.1976954994073409	T	T	T
0.8319829264405061	0.4995013477002645	0.3956139651616639	T	T	T
0.0000000000000000	0.6666666667013104	0.0000000000000000	F	F	F
0.9998047329702328	0.6667977202667384	0.1976598366920407	T	T	T
0.9988203664747275	0.6674356910032850	0.3950270028184384	T	T	T
0.1666666667013104	0.6666666667013104	0.0984529120410897	F	F	F
0.1663940299719742	0.6669424563399317	0.2969517780329779	T	T	T
0.1610391645949192	0.6723006599322736	0.4931633078972767	T	T	T
0.3333333332986896	0.6666666667013104	0.0000000000000000	F	F	F
0.3332036205586897	0.6665994800273206	0.1977811038539029	T	T	T
0.3327950921663537	0.6665034361411852	0.3966436392402856	T	T	T
0.5000000000000000	0.6666666667013104	0.0984529120410897	F	F	F
0.4992156502973123	0.6660952409674474	0.2974080420308182	T	T	T
0.4866402950601993	0.6814297075385979	0.5043078728757360	T	T	T
0.6666666667013104	0.6666666667013104	0.0000000000000000	F	F	F
0.6663494782454373	0.6663542890696895	0.1977481083546219	T	T	T
0.6643922379227593	0.6643904982578029	0.3963191268424036	T	T	T
0.8333333332986896	0.6666666667013104	0.0984529120410897	F	F	F
0.8325982401115124	0.6664362555273625	0.2969913244091174	T	T	T
0.8410956414040401	0.6645183482710851	0.4976475942689820	T	T	T
0.0000000000000000	0.8333333332986896	0.0984529120410897	F	F	F
0.9993210670112295	0.8340173535982760	0.2969293120435584	T	T	T
0.9980467476682057	0.8352871732726624	0.4938838641414133	T	T	T
0.1666666667013104	0.8333333332986896	0.0000000000000000	F	F	F
0.1665378636237664	0.8335336583961537	0.1976596085618996	T	T	T
0.1658998575670235	0.8345186609726291	0.3950276146302300	T	T	T
0.3333333332986896	0.8333333332986896	0.0984529120410897	F	F	F
0.3331180232851628	0.8334802534870762	0.2968449460191236	T	T	T
0.3305465988336999	0.8367042150469939	0.4923100604801498	T	T	T
0.5000000000000000	0.8333333332986896	0.0000000000000000	F	F	F
0.4998807244193942	0.8331688433609689	0.1976950165963553	T	T	T
0.4994951460654004	0.8319866967982483	0.3956162434971174	T	T	T
0.6666666667013104	0.8333333332986896	0.0984529120410897	F	F	F
0.6664242439903353	0.8326054150062032	0.2969903352180182	T	T	T
0.6645216202748400	0.8410854237134221	0.4976459764546918	T	T	T
0.8333333332986896	0.8333333332986896	0.0000000000000000	F	F	F
0.8331922989224158	0.8331973439751521	0.1976255148128471	T	T	T
0.8316903577447108	0.8317007206369192	0.3969086952947069	T	T	T
0.1666666667013104	0.1666666667013104	0.0984529120410897	F	F	F
0.1675098065330587	0.1675301177081918	0.2983446870872596	T	T	T
0.1739514906286526	0.1739868343068790	0.4957752351755935	T	T	T
0.1666666667013104	0.0000000000000000	0.0000000000000000	F	F	F
0.1667656198733633	0.0005340664750996	0.1982458743906080	T	T	T
0.1674952824481759	0.0023813820660587	0.3980874318598919	T	T	T
0.0000000000000000	0.1666666667013104	0.0000000000000000	F	F	F
0.0005244017766190	0.1667737079379634	0.1982461489053604	T	T	T
0.0023618721707381	0.1675120388106979	0.3980883367168296	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529120410897	F	F	F
0.0005809363831580	0.0005970955374952	0.2970918931691326	T	T	T
0.0019359136277554	0.0019499953931903	0.4936143611941158	T	T	T
0.1666666667013104	0.5000000000000000	0.0984529120410897	F	F	F
0.1669986227497353	0.5001443024657695	0.2971557964745549	T	T	T
0.1602095314357680	0.5069453134308147	0.4922598052953245	T	T	T
0.1666666667013104	0.3333333332986896	0.0000000000000000	F	F	F
0.1671553563394422	0.3333787707729844	0.1984835778066358	T	T	T
0.1678948612677373	0.3340193979917840	0.3993273941398772	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0000133223091701	0.5001232351790329	0.1979962313710610	T	T	T
0.9994451400014414	0.5015392367610473	0.3953729642031000	T	T	T

0.0000000000000000	0.3333333332986896	0.0984529120410897	F	F	F
0.0008062462299510	0.3333908367245294	0.2966585840807235	T	T	T
0.9970708039523768	0.3378189428877765	0.4904936415095055	T	T	T
0.5000000000000000	0.1666666667013104	0.0984529120410897	F	F	F
0.5001259417617391	0.1670128847938152	0.2971559210250823	T	T	T
0.5069229314199433	0.1602193119464251	0.4922570865387686	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5001152035549973	0.0000186293520843	0.1979951464318316	T	T	T
0.5015251477582092	0.9994508977078783	0.3953708648017510	T	T	T
0.3333333332986896	0.1666666667013104	0.0000000000000000	F	F	F
0.3333694781309481	0.1671635145105399	0.1984827837240282	T	T	T
0.3339960499308951	0.1679092775450818	0.3993205138528426	T	T	T
0.3333333332986896	0.0000000000000000	0.0984529120410897	F	F	F
0.3333757436732307	0.0008204372600236	0.2966559328914033	T	T	T
0.3378208663818976	0.9970770424226337	0.4904829548036117	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120410897	F	F	F
0.4996464467377127	0.4996567325839331	0.2987398607061457	T	T	T
0.4969190893657444	0.4969306762170185	0.4949412277006889	T	T	T
0.5000000000000000	0.3333333332986896	0.0000000000000000	F	F	F
0.4998142582445059	0.3335154561751339	0.1985808128891591	T	T	T
0.5002826761975299	0.3330418112653759	0.3997865796136724	T	T	T
0.3333333332986896	0.5000000000000000	0.0000000000000000	F	F	F
0.3335098418316230	0.4998238565449686	0.1985809136411335	T	T	T
0.3330312413353301	0.5003004347657568	0.3997741014611161	T	T	T
0.3333333332986896	0.3333333332986896	0.0984529120410897	F	F	F
0.3336716440840018	0.3336869711060702	0.2987439360813899	T	T	T
0.3364151289787740	0.3364301587892771	0.4949572625996054	T	T	T
0.6666666667013104	0.1666666667013104	0.0000000000000000	F	F	F
0.6667535799979074	0.1665783759669979	0.1981148063689720	T	T	T
0.6684537627748630	0.1648716201073679	0.3959788914265651	T	T	T
0.6666666667013104	0.0000000000000000	0.0984529120410897	F	F	F
0.6672057086545944	0.9991256568218011	0.2967589495553476	T	T	T
0.6691927396435441	0.9981962056227673	0.4926172878692746	T	T	T
0.6666666667013104	0.5000000000000000	0.0000000000000000	F	F	F
0.6661714809155903	0.4999609040320303	0.1984794283034594	T	T	T
0.6654267655603043	0.4993245020085053	0.3993108555064980	T	T	T
0.6666666667013104	0.3333333332986896	0.0984529120410897	F	F	F
0.6663171760283216	0.3332002818064529	0.2971529599091500	T	T	T
0.6730978315642678	0.3263937495948334	0.4922521831231053	T	T	T
0.8333333332986896	0.1666666667013104	0.0984529120410897	F	F	F
0.8342048521670495	0.1661280681583205	0.2967623641248162	T	T	T
0.8351238436244962	0.1641390330716256	0.4926229032605230	T	T	T
0.8333333332986896	0.0000000000000000	0.0000000000000000	F	F	F
0.8335176311485915	0.9998174456261086	0.1980727909505231	T	T	T
0.8341782599385026	0.9991569161959064	0.3968366024555497	T	T	T
0.8333333332986896	0.5000000000000000	0.0984529120410897	F	F	F
0.8325155530312979	0.4999555871071421	0.2966538773013754	T	T	T
0.8362574132215059	0.4955113330077963	0.4904806111937864	T	T	T
0.8333333332986896	0.3333333332986896	0.0000000000000000	F	F	F
0.8333145656892712	0.3332170406411679	0.1979954057501467	T	T	T
0.8338750551789528	0.3318057230219381	0.3953714550689028	T	T	T
0.0000000000000000	0.6666666667013104	0.0984529120410897	F	F	F
0.9991174441741978	0.6672215453522001	0.2967624247647023	T	T	T
0.9981997893803275	0.6692072712963156	0.4926207794486254	T	T	T
0.1666666667013104	0.6666666667013104	0.0000000000000000	F	F	F
0.1665744072203869	0.6667626607483633	0.1981167014969287	T	T	T
0.1648635743504114	0.6684759010317008	0.3959825396436615	T	T	T
0.3333333332986896	0.6666666667013104	0.0984529120410897	F	F	F
0.3331942522868795	0.6663340023540303	0.2971564227662271	T	T	T
0.3264012478651975	0.6731238267105385	0.4922553884545821	T	T	T

0.5000000000000000	0.6666666667013104	0.0000000000000000	F	F	F
0.4999563005346394	0.6661774855497259	0.1984818880890024	T	T	T
0.4993241519042861	0.6654323343835887	0.3993264450574804	T	T	T
0.6666666667013104	0.6666666667013104	0.0984529120410897	F	F	F
0.6658095696000730	0.6658174176864836	0.2983391730654817	T	T	T
0.6593978382759698	0.6593367785641501	0.4957723543054691	T	T	T
0.8333333332986896	0.6666666667013104	0.0000000000000000	F	F	F
0.8328044943360358	0.6665682176602878	0.1982436786858492	T	T	T
0.8309607523695430	0.6658368119403257	0.3980797819688146	T	T	T
0.0000000000000000	0.8333333332986896	0.0000000000000000	F	F	F
0.9998120241363583	0.8335251763315661	0.1980736163927921	T	T	T
0.9991403777615925	0.8341969350293187	0.3968391372114835	T	T	T
0.1666666667013104	0.8333333332986896	0.0984529120410897	F	F	F
0.1661139059162694	0.8342215727760055	0.2967618601500510	T	T	T
0.1641291612756436	0.8351430603948358	0.4926205082898129	T	T	T
0.3333333332986896	0.8333333332986896	0.0000000000000000	F	F	F
0.3332105750822936	0.8333223378374797	0.1979956290456683	T	T	T
0.3317945376690008	0.8338895493995030	0.3953713669711807	T	T	T
0.5000000000000000	0.8333333332986896	0.0984529120410897	F	F	F
0.4999449565322884	0.8325232336141216	0.2966556930989311	T	T	T
0.4955181858765043	0.8362433822756801	0.4904837232022072	T	T	T
0.6666666667013104	0.8333333332986896	0.0000000000000000	F	F	F
0.6665616061354398	0.8328076991717057	0.1982427614437506	T	T	T
0.6658273479227939	0.8309631200571753	0.3980808205915923	T	T	T
0.8333330000000032	0.8333333332986896	0.0984529120410897	F	F	F
0.8327415871118967	0.8327538334938904	0.2970884960433673	T	T	T
0.8313889350775047	0.8313962476281049	0.4936075083454670	T	T	T
0.0994766324688624	0.2118838865130615	0.5735574613264339	T	T	T
0.2119751688351042	0.0994964549629803	0.5735277919807997	T	T	T
0.2742637909513327	0.3867785408142060	0.5736694708952143	T	T	T
0.3868659751426284	0.2743443686230941	0.5736742567612411	T	T	T
0.4463479980743321	0.5589186997924587	0.5736590255401194	T	T	T
0.5591146113275244	0.4466302352331666	0.5736657612853300	T	T	T
0.6214113615525074	0.7338182734335710	0.5735308067351856	T	T	T
0.7339029090822908	0.6214474124321584	0.5735416595893036	T	T	T
0.1615258730421958	0.1615043738110656	0.5517737402711993	T	T	T
0.3323834850624723	0.3324028989889760	0.5511679763644199	T	T	T
0.5009174129427070	0.5009497845324303	0.5511450637358940	T	T	T
0.6718494580812896	0.6718203919850750	0.5517753209049965	T	T	T

T2-pbc-5CO2 (-1497.7527 eV)

1.0000000000000000

14.432999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.432999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 24.432999999999998

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Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0000018589850797	0.0000011272544000	0.1976655343101470	T	T	T
0.0000022296010442	0.0000039687313205	0.3984706773323552	T	T	T
0.0000000000000000	0.1666666667013104	0.0984529120410897	F	F	F
0.0004913147907217	0.1662042644023316	0.2971159781798889	T	T	T
0.9926468013816390	0.1691299400028399	0.4976523232152914	T	T	T
0.1666666667013104	0.0000000000000000	0.0984529120410897	F	F	F
0.1662017653047769	0.0004928546440226	0.2971161171347347	T	T	T
0.1691259385777144	0.9926530569092975	0.4976486367998163	T	T	T
0.1666666667013104	0.1666666667013104	0.0000000000000000	F	F	F

0.1668157064188875	0.1668174167996455	0.1976718411022915	T	T	T
0.1683460078886512	0.1683530267823627	0.3959968148741382	T	T	T
0.0000000000000000	0.333333332986896	0.0000000000000000	F	F	F
0.0001481007147817	0.3332549344287727	0.1976587318436103	T	T	T
0.0012335507771795	0.3330420318748324	0.3951465732535908	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529120410897	F	F	F
0.0000026886229563	0.5000037340920329	0.2966764212665041	T	T	T
0.0000010414201128	0.5000082160368748	0.4910737489836805	T	T	T
0.1666666667013104	0.333333332986896	0.0984529120410897	F	F	F
0.1672155360544849	0.3337989439527220	0.2971356283417279	T	T	T
0.1529766892716395	0.3453092991664448	0.5035832252393320	T	T	T
0.1666666667013104	0.5000000000000000	0.0000000000000000	F	F	F
0.1667999174871539	0.5000823349116743	0.1976689131722651	T	T	T
0.1675447276054740	0.4999937340184033	0.3957972426091274	T	T	T
0.333333332986896	0.0000000000000000	0.0000000000000000	F	F	F
0.3332535579105240	0.0001488346035927	0.1976583545577810	T	T	T
0.3330348454148080	0.0012346527441807	0.3951437295280655	T	T	T
0.333333332986896	0.1666666667013104	0.0984529120410897	F	F	F
0.3337938530770970	0.1672179462861862	0.2971352654284090	T	T	T
0.3452955365526478	0.1529782171991982	0.5035900018319808	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120410897	F	F	F
0.5000000585028417	0.0000016017225661	0.2966735876593916	T	T	T
0.4999961799829507	0.0000036095331808	0.4910674148633731	T	T	T
0.5000000000000000	0.1666666667013104	0.0000000000000000	F	F	F
0.5000802896071903	0.1667989149525511	0.1976676426648396	T	T	T
0.4999840446567205	0.1675429739115586	0.3957949644708734	T	T	T
0.333333332986896	0.333333332986896	0.0000000000000000	F	F	F
0.3335344795024540	0.3335356402961054	0.1977841122815605	T	T	T
0.3340928503489096	0.3340943598272688	0.3974817777235629	T	T	T
0.333333332986896	0.5000000000000000	0.0984529120410897	F	F	F
0.3336131956500736	0.5001775798043369	0.2975340177300367	T	T	T
0.3194751855194085	0.5136861131901327	0.5040045389358667	T	T	T
0.5000000000000000	0.333333332986896	0.0984529120410897	F	F	F
0.5001760950363661	0.3336110461872721	0.2975330435249290	T	T	T
0.5136857747335242	0.3194663878580499	0.5040023188647780	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000015313679498	0.5000007271838172	0.1978427024551408	T	T	T
0.500004228261106	0.4999992437492438	0.3975998507116216	T	T	T
0.6666666667013104	0.0000000000000000	0.0000000000000000	F	F	F
0.6667478793060155	0.9998530143093163	0.1976579378593826	T	T	T
0.6669645156552875	0.9987717376144687	0.3951423077388654	T	T	T
0.6666666667013104	0.1666666667013104	0.0984529120410897	F	F	F
0.6667614500360202	0.1665322272373828	0.2968100859658520	T	T	T
0.6692983667090715	0.1633141071036377	0.4924297868117549	T	T	T
0.6666666667013104	0.333333332986896	0.0000000000000000	F	F	F
0.6666353857951179	0.3333658541777140	0.1977538159860401	T	T	T
0.6666013890308733	0.3334002453171507	0.3962300534384084	T	T	T
0.6666666667013104	0.5000000000000000	0.0984529120410897	F	F	F
0.6663931586866809	0.4998252095190523	0.2975334814608388	T	T	T
0.6805329002626763	0.4863179199244669	0.5039968944213484	T	T	T
0.833333332986896	0.0000000000000000	0.0984529120410897	F	F	F
0.8338018678988348	0.9995120762221035	0.2971149868552274	T	T	T
0.8308757408682510	0.0073562270301508	0.4976470184844644	T	T	T
0.833333332986896	0.1666666667013104	0.0000000000000000	F	F	F
0.8334826940920976	0.1665192605615857	0.1976452774315547	T	T	T
0.8339695164213623	0.1660370006994825	0.3949263773228324	T	T	T
0.833333332986896	0.333333332986896	0.0984529120410897	F	F	F
0.8334709742261950	0.3332419025082629	0.2968114556277470	T	T	T
0.8366878136873979	0.3307053800442858	0.4924322741614731	T	T	T
0.833333332986896	0.5000000000000000	0.0000000000000000	F	F	F

0.8332036606088664	0.4999204896506413	0.1976686029970551	T	T	T
0.8324625632912515	0.5000187622541290	0.3957970331234293	T	T	T
0.0000000000000000	0.6666666667013104	0.0000000000000000	F	F	F
0.9998553355491495	0.6667476390340923	0.1976591797383307	T	T	T
0.9987716627699470	0.6669696601754325	0.3951478963624950	T	T	T
0.1666666667013104	0.6666666667013104	0.0984529120410897	F	F	F
0.1665345891611310	0.6667638431888250	0.2968129472565266	T	T	T
0.1633169022783747	0.6693033451215769	0.4924358465345193	T	T	T
0.333333332986896	0.6666666667013104	0.0000000000000000	F	F	F
0.3333670590892055	0.6666361177796389	0.1977542614770940	T	T	T
0.3334048439239723	0.6666008584265271	0.3962334021295106	T	T	T
0.5000000000000000	0.6666666667013104	0.0984529120410897	F	F	F
0.4998276637972197	0.6663898495677429	0.2975338212854055	T	T	T
0.4863177868411768	0.6805337396082081	0.5040079587049249	T	T	T
0.6666666667013104	0.6666666667013104	0.0000000000000000	F	F	F
0.6664682245292539	0.6664657446648121	0.1977840792673717	T	T	T
0.6659104169872094	0.6659099829232460	0.3974809752773680	T	T	T
0.833333332986896	0.6666666667013104	0.0984529120410897	F	F	F
0.8327894034975358	0.6662072305777187	0.2971362311092562	T	T	T
0.8470252595512591	0.6547102301210970	0.5035905705868799	T	T	T
0.0000000000000000	0.833333332986896	0.0984529120410897	F	F	F
0.9995136638110722	0.8338018901592861	0.2971167238633257	T	T	T
0.0073537855329420	0.8308801222431086	0.4976537707965392	T	T	T
0.1666666667013104	0.833333332986896	0.0000000000000000	F	F	F
0.1665202220134319	0.8334830382844203	0.1976465460950152	T	T	T
0.1660346685852190	0.8339696269727312	0.3949287960711558	T	T	T
0.333333332986896	0.833333332986896	0.0984529120410897	F	F	F
0.3332407211437598	0.8334704330343783	0.2968116801748977	T	T	T
0.3307030699744189	0.8366905398107249	0.4924322119301223	T	T	T
0.5000000000000000	0.833333332986896	0.0000000000000000	F	F	F
0.4999206434564698	0.8332021023524163	0.1976683512367146	T	T	T
0.5000121181448094	0.8324588798066799	0.3957939129101717	T	T	T
0.6666666667013104	0.833333332986896	0.0984529120410897	F	F	F
0.6662073581313805	0.8327857942270782	0.2971342495630225	T	T	T
0.6546942242972307	0.8470296765170175	0.5035793689879569	T	T	T
0.833333332986896	0.833333332986896	0.0000000000000000	F	F	F
0.8331871380145586	0.8331844248890761	0.1976718769303147	T	T	T
0.8316553309926036	0.8316556250230676	0.3959967079520936	T	T	T
0.1666666667013104	0.1666666667013104	0.0984529120410897	F	F	F
0.1672188518993991	0.1672226282060976	0.2982483334367956	T	T	T
0.1729204834445781	0.1729407366467512	0.4953838947025204	T	T	T
0.1666666667013104	0.0000000000000000	0.0000000000000000	F	F	F
0.1665214485147573	0.0003692345161284	0.1983261288749745	T	T	T
0.1667604986754228	0.0017252371725505	0.3982814995683128	T	T	T
0.0000000000000000	0.1666666667013104	0.0000000000000000	F	F	F
0.0003682291803173	0.1665217410850346	0.1983257852093843	T	T	T
0.0017222800429622	0.1667671828373827	0.3982802603506954	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529120410897	F	F	F
0.0000026962277673	0.0000021802772707	0.2973688654757467	T	T	T
0.0000001970466030	0.0000060019615873	0.4943497865401980	T	T	T
0.1666666667013104	0.5000000000000000	0.0984529120410897	F	F	F
0.1673257243632094	0.4998639212708369	0.2968734381265463	T	T	T
0.1621574153754466	0.5050319962046643	0.4913261539102223	T	T	T
0.1666666667013104	0.333333332986896	0.0000000000000000	F	F	F
0.1671555982351194	0.3332505735993649	0.1984543717105041	T	T	T
0.1680758971117484	0.3333972712799280	0.3990551061083352	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0000024512219383	0.5000015027830855	0.1979850424249250	T	T	T
0.0000021030174224	0.5000067518875184	0.3947338933547258	T	T	T
0.0000000000000000	0.333333332986896	0.0984529120410897	F	F	F

0.0007748372726297	0.3328917933458158	0.2964941192422543	T	T	T
0.9976314286729959	0.3362482344548496	0.4900272624328537	T	T	T
0.5000000000000000	0.1666666667013104	0.0984529120410897	F	F	F
0.4998606227484359	0.1673238922688469	0.2968712671304203	T	T	T
0.5050239888252079	0.1621571376870961	0.4913240994128145	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5000008615888021	0.0000001604058824	0.1979829328221498	T	T	T
0.4999985618377139	0.0000022129240804	0.3947294492345392	T	T	T
0.3333333332986896	0.1666666667013104	0.0000000000000000	F	F	F
0.3332474590579153	0.1671573080996396	0.1984533272250033	T	T	T
0.3333887159918731	0.1680783812550715	0.3990521419901825	T	T	T
0.3333333332986896	0.0000000000000000	0.0984529120410897	F	F	F
0.3328895288593401	0.0007756143776163	0.2964929783168202	T	T	T
0.3362360299574476	0.9976322291410042	0.4900215685225575	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120410897	F	F	F
0.5000035696467080	0.4999999135665121	0.2986680347333390	T	T	T
0.5000122895112682	0.4999846852275951	0.4945850388716124	T	T	T
0.5000000000000000	0.3333333332986896	0.0000000000000000	F	F	F
0.4998447353123083	0.3336643744679861	0.1985546599614452	T	T	T
0.5001909112677083	0.3337723212397492	0.3994970481921598	T	T	T
0.3333333332986896	0.5000000000000000	0.0000000000000000	F	F	F
0.3336654579091061	0.4998465180278728	0.1985556105624866	T	T	T
0.3337766893484186	0.5001917737100641	0.3994996787319920	T	T	T
0.3333333332986896	0.3333333332986896	0.0984529120410897	F	F	F
0.3337063812696144	0.3337096192394000	0.2985290701823970	T	T	T
0.3371450883859026	0.3371437852781867	0.4948435135983047	T	T	T
0.6666666667013104	0.1666666667013104	0.0000000000000000	F	F	F
0.6667781825871302	0.1666753965147549	0.1981064835246329	T	T	T
0.6679970171997383	0.1661073454368562	0.3954254963229715	T	T	T
0.6666666667013104	0.0000000000000000	0.0984529120410897	F	F	F
0.6671132537902622	0.9992274968338393	0.2964917594735326	T	T	T
0.6637580314189151	0.0023722430047997	0.4900198775780495	T	T	T
0.6666666667013104	0.5000000000000000	0.0000000000000000	F	F	F
0.6663382787958767	0.5001560356352286	0.1985556090232876	T	T	T
0.6662321117068259	0.4998112634602805	0.3994998313897824	T	T	T
0.6666666667013104	0.3333333332986896	0.0984529120410897	F	F	F
0.6663877717724915	0.3336148162228412	0.2970005284100381	T	T	T
0.6726034090180093	0.3273987123400275	0.4917868276662603	T	T	T
0.8333333332986896	0.1666666667013104	0.0984529120410897	F	F	F
0.8340790495563652	0.1659245167015584	0.2969508948449899	T	T	T
0.8341399824887645	0.1658616493306511	0.4928201241563031	T	T	T
0.8333333332986896	0.0000000000000000	0.0000000000000000	F	F	F
0.8334816826082303	0.9996320887369095	0.1983254352670230	T	T	T
0.8332409774639444	0.9982824872904743	0.3982789053052329	T	T	T
0.8333333332986896	0.5000000000000000	0.0984529120410897	F	F	F
0.8326800186191861	0.5001418427291497	0.2968734666865487	T	T	T
0.8378428606437538	0.4949806122616707	0.4913281663214235	T	T	T
0.8333333332986896	0.3333333332986896	0.0000000000000000	F	F	F
0.8333259298066906	0.3332231146414983	0.1981073524960308	T	T	T
0.8338967382103846	0.3320077071046441	0.3954277239473711	T	T	T
0.0000000000000000	0.6666666667013104	0.0984529120410897	F	F	F
0.9992308916967687	0.6671146907889351	0.2964954769066708	T	T	T
0.0023742604335482	0.6637684563782003	0.4900277607152717	T	T	T
0.1666666667013104	0.6666666667013104	0.0000000000000000	F	F	F
0.1666770778676891	0.6667798582015720	0.1981079751680710	T	T	T
0.1661090010780129	0.6679997806237097	0.3954300690089099	T	T	T
0.3333333332986896	0.6666666667013104	0.0984529120410897	F	F	F
0.3336165562256994	0.6663880927507364	0.2970023184052692	T	T	T
0.3274021126187492	0.6726031205702654	0.4917944392491691	T	T	T
0.5000000000000000	0.6666666667013104	0.0000000000000000	F	F	F

0.5001573170087141	0.6663361333920719	0.1985551741904459	T	T	T
0.4998136989545827	0.6662255527047591	0.3994955334423125	T	T	T
0.666666667013104	0.666666667013104	0.0984529120410897	F	F	F
0.6662972133442793	0.6662947798950896	0.2985289400853830	T	T	T
0.6628612710886870	0.6628460092800879	0.4948388861259332	T	T	T
0.8333333332986896	0.666666667013104	0.0000000000000000	F	F	F
0.8328477098501992	0.6667523966682580	0.1984543838867694	T	T	T
0.8319288366022661	0.6666135607785648	0.3990525384313486	T	T	T
0.0000000000000000	0.8333333332986896	0.0000000000000000	F	F	F
0.9996343662295644	0.8334796766489845	0.1983266363595746	T	T	T
0.9982805490003912	0.8332432730368851	0.3982821823880514	T	T	T
0.166666667013104	0.8333333332986896	0.0984529120410897	F	F	F
0.1659242096759996	0.8340802367868250	0.2969526912322067	T	T	T
0.1658604142316875	0.8341473928964760	0.4928233620577842	T	T	T
0.3333333332986896	0.8333333332986896	0.0000000000000000	F	F	F
0.3332236705148262	0.8333261771106422	0.1981077416231898	T	T	T
0.3320029501175199	0.8338938521717125	0.3954269443467311	T	T	T
0.5000000000000000	0.8333333332986896	0.0984529120410897	F	F	F
0.5001414382069953	0.8326786437879932	0.2968715159047051	T	T	T
0.4949720987337187	0.8378507923095526	0.4913199483962742	T	T	T
0.666666667013104	0.8333333332986896	0.0000000000000000	F	F	F
0.6667543351202667	0.8328443048210303	0.1984536420823346	T	T	T
0.6666098573799886	0.8319272061794436	0.3990549696295318	T	T	T
0.8333330000000032	0.8333333332986896	0.0984529120410897	F	F	F
0.8327834036685786	0.8327822479815978	0.2982483159574940	T	T	T
0.8270630585662033	0.8270781775498435	0.4953847427217823	T	T	T
0.0998140871221125	0.2122843994258261	0.5734137015558431	T	T	T
0.2123662773119506	0.0998705538081737	0.5734056568596344	T	T	T
0.2732706398672775	0.3858216212397636	0.5735526287984243	T	T	T
0.3858114675679829	0.2732837659169718	0.5735558534577763	T	T	T
0.4437072557741999	0.5562595379435038	0.5734736570071917	T	T	T
0.5563274255310375	0.4437169260265250	0.5734738268156363	T	T	T
0.6141007320770413	0.7266934595384811	0.5735383493438633	T	T	T
0.7267662460786397	0.6142729961597979	0.5735656934532187	T	T	T
0.7876602125195546	0.9001617472898715	0.5734104806736866	T	T	T
0.9001658861810924	0.7877014912718678	0.5734084173990226	T	T	T
0.1614202074162492	0.1614187058499041	0.5517526997942213	T	T	T
0.3319335352409780	0.3319277171732367	0.5512565689340434	T	T	T
0.5000135036963087	0.4999901985031201	0.5511097216431438	T	T	T
0.6680581666585823	0.6680910736480214	0.5512544528003218	T	T	T
0.8385790429122082	0.8385934542452418	0.5517518568722579	T	T	T

T2-pbc-6CO2 (-1521.7317 eV)

1.0000000000000000

14.4329999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4329999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 24.4329999999999998

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Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
-0.0000014402027414	0.0000025964130420	0.1976032761317445	T	T	T
-0.0000032364271667	0.0000046474900847	0.3968357503496794	T	T	T
0.0000000000000000	0.166666667013104	0.0984529120410897	F	F	F
0.0001870404983612	0.1664842111065631	0.2970630802810286	T	T	T
0.9873829429466816	0.1793015067293325	0.5030723143594821	T	T	T
0.166666667013104	0.0000000000000000	0.0984529120410897	F	F	F
0.1664760015372837	0.0001879793069469	0.2970611528487515	T	T	T

0.1792820026019673	0.9873772817726573	0.5030699018667425	T	T	T
0.1666666667013104	0.1666666667013104	0.0000000000000000	F	F	F
0.1666656353885979	0.1666679758103982	0.1976038448374525	T	T	T
0.1666646037269942	0.1666709649266567	0.3968350996538407	T	T	T
0.0000000000000000	0.3333333332986896	0.0000000000000000	F	F	F
0.0000836039475444	0.3332507304728979	0.1975212909870843	T	T	T
0.0006842178184605	0.3326561333535163	0.3951378334202868	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529120410897	F	F	F
-0.0000006974725626	0.5000025348566307	0.2965121998428523	T	T	T
0.9999979157212043	0.5000057607031013	0.4911816331252619	T	T	T
0.1666666667013104	0.3333333332986896	0.0984529120410897	F	F	F
0.1668500909322092	0.3331496108172906	0.2970618105301208	T	T	T
0.1540516641126129	0.3459645250232272	0.5030696088404731	T	T	T
0.1666666667013104	0.5000000000000000	0.0000000000000000	F	F	F
0.1667464092904618	0.4999191464982165	0.1975215118660382	T	T	T
0.1673448253809298	0.4993222289272085	0.3951332078232289	T	T	T
0.3333333332986896	0.0000000000000000	0.0000000000000000	F	F	F
0.3332491045658671	0.0000836553544818	0.1975207866357894	T	T	T
0.3326440963115133	0.0006830830311393	0.3951285255132249	T	T	T
0.3333333332986896	0.1666666667013104	0.0984529120410897	F	F	F
0.3331464054705458	0.1668533627247446	0.2970593611135084	T	T	T
0.3459507939430235	0.1540419966313298	0.5030550999390488	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120410897	F	F	F
0.4999973320384185	0.0000052643432972	0.2965059100063044	T	T	T
0.4999954901018508	0.0000079575656973	0.4911677241978231	T	T	T
0.5000000000000000	0.1666666667013104	0.0000000000000000	F	F	F
0.4999168799538231	0.1667505922359785	0.1975193165655587	T	T	T
0.4993147182820840	0.1673490668706560	0.3951247280696229	T	T	T
0.3333333332986896	0.3333333332986896	0.0000000000000000	F	F	F
0.3333324096574459	0.3333333502234931	0.1976019899493736	T	T	T
0.3333302497997958	0.3333368971110749	0.3968243460235990	T	T	T
0.3333333332986896	0.5000000000000000	0.0984529120410897	F	F	F
0.3335130497763500	0.4998173640720268	0.2970574528206968	T	T	T
0.3207132832010767	0.5126337646373209	0.5030526429601728	T	T	T
0.5000000000000000	0.3333333332986896	0.0984529120410897	F	F	F
0.4998141626468821	0.3335187137175809	0.2970549208860024	T	T	T
0.5126175865170295	0.3207160265558125	0.5030434549119901	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000002303454281	0.4999999791141086	0.1976009206483004	T	T	T
0.4999964374034268	0.5000040678911246	0.3968146397087808	T	T	T
0.6666666667013104	0.0000000000000000	0.0000000000000000	F	F	F
0.6667508044702353	0.9999198572049286	0.1975194105111109	T	T	T
0.6673457143334228	0.9993309637640510	0.3951229117615728	T	T	T
0.6666666667013104	0.1666666667013104	0.0984529120410897	F	F	F
0.6666700156748232	0.1666705176074493	0.2965058541793164	T	T	T
0.6666640449628125	0.1666773765441722	0.4911700433749940	T	T	T
0.6666666667013104	0.3333333332986896	0.0000000000000000	F	F	F
0.6665856207954995	0.3334169580392071	0.1975190118258295	T	T	T
0.6659869493840389	0.3340172027785699	0.3951221864629342	T	T	T
0.6666666667013104	0.5000000000000000	0.0984529120410897	F	F	F
0.6664859084500794	0.5001852778452934	0.2970555796427912	T	T	T
0.6792817591994147	0.4873826281750991	0.5030405717480613	T	T	T
0.8333333332986896	0.0000000000000000	0.0984529120410897	F	F	F
0.8335209389505662	0.9998193099882233	0.2970600453810911	T	T	T
0.8207049709301127	0.0126395566869239	0.5030548651991283	T	T	T
0.8333333332986896	0.1666666667013104	0.0000000000000000	F	F	F
0.8334196917660144	0.1665847851205807	0.1975211699185914	T	T	T
0.8340194041287351	0.1659919234768235	0.3951311345369222	T	T	T
0.8333333332986896	0.3333333332986896	0.0984529120410897	F	F	F
0.8333376562001350	0.3333376449218383	0.2965113034617938	T	T	T

0.8333315508358695	0.3333401346085882	0.4911740806265508	T	T	T
0.8333333332986896	0.5000000000000000	0.0000000000000000	F	F	F
0.8332525683748422	0.5000824468285330	0.1975199051572185	T	T	T
0.8326526249609989	0.5006870191675528	0.3951279665846947	T	T	T
0.0000000000000000	0.6666666667013104	0.0000000000000000	F	F	F
0.9999185109685310	0.6667494142252063	0.1975214349682519	T	T	T
0.9993145112776837	0.6673564862157666	0.3951347386385775	T	T	T
0.1666666667013104	0.6666666667013104	0.0984529120410897	F	F	F
0.1666600993034817	0.6666700029010675	0.2965122276404738	T	T	T
0.1666608444995939	0.6666743393120144	0.4911784896552229	T	T	T
0.3333333332986896	0.6666666667013104	0.0000000000000000	F	F	F
0.3334101818664085	0.6665874780325068	0.1975202617937404	T	T	T
0.3340053286634417	0.6659923286504518	0.3951253151791413	T	T	T
0.5000000000000000	0.6666666667013104	0.0984529120410897	F	F	F
0.5001798804273695	0.6664864350325506	0.2970542949011478	T	T	T
0.4873769186463189	0.6793006089878525	0.5030402773411942	T	T	T
0.6666666667013104	0.6666666667013104	0.0000000000000000	F	F	F
0.6666666484830496	0.6666682407348444	0.1976000985905878	T	T	T
0.6666630487140229	0.6666711084687703	0.3968137366115091	T	T	T
0.8333333332986896	0.6666666667013104	0.0984529120410897	F	F	F
0.8331511931572748	0.6668529899643663	0.2970579318330380	T	T	T
0.8459427209690691	0.6540538824377528	0.5030580530307552	T	T	T
0.0000000000000000	0.8333333332986896	0.0984529120410897	F	F	F
0.9998135626612071	0.8335212101241354	0.2970631363292331	T	T	T
0.0126077514423476	0.8207145479381276	0.5030737332510780	T	T	T
0.1666666667013104	0.8333333332986896	0.0000000000000000	F	F	F
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0.1659765710602322	0.8340190238311379	0.3951367725376619	T	T	T
0.3333333332986896	0.8333333332986896	0.0984529120410897	F	F	F
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0.3333297838857586	0.8333405703794680	0.4911732023960884	T	T	T
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0.5000797183824705	0.8332546314553099	0.1975193879253423	T	T	T
0.5006744698576233	0.8326608400917828	0.3951207734278320	T	T	T
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0.6668507055836981	0.8331542043127483	0.2970558108462931	T	T	T
0.6540403621201851	0.8459707880747427	0.5030394495358221	T	T	T
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0.8333330737497811	0.8333362584234473	0.1976017058346193	T	T	T
0.8333289257976590	0.8333402957936085	0.3968258922048101	T	T	T
0.1666666667013104	0.1666666667013104	0.0984529120410897	F	F	F
0.1666670620272925	0.1666682632484944	0.2982678807174831	T	T	T
0.1666699593119005	0.1666678147532242	0.4940630878316912	T	T	T
0.1666666667013104	0.0000000000000000	0.0000000000000000	F	F	F
0.1663648536688771	0.0003009343454473	0.1984006664153450	T	T	T
0.1660790500221166	0.0005830420630443	0.3989829123607027	T	T	T
0.0000000000000000	0.1666666667013104	0.0000000000000000	F	F	F
0.0003013969957759	0.1663670842738647	0.1983994356143580	T	T	T
0.0005850383967633	0.1660903292230179	0.3989832764799502	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529120410897	F	F	F
-0.0000000493441894	0.0000004099529844	0.2982675326752738	T	T	T
0.9999799785618700	-0.0000003273714541	0.4940642646266523	T	T	T
0.1666666667013104	0.5000000000000000	0.0984529120410897	F	F	F
0.1672453863828470	0.4994209077196904	0.2965282831185372	T	T	T
0.1627092202773706	0.5039657589026425	0.4906263168327104	T	T	T
0.1666666667013104	0.3333333332986896	0.0000000000000000	F	F	F
0.1669659432110716	0.3330336735913620	0.1984001422139750	T	T	T
0.1672494460976561	0.3327563032468533	0.3989812702972417	T	T	T
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0.0000011942589379	0.5000049850955250	0.3946946250346169	T	T	T
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0.9960478129666194	0.3372968942677181	0.4906321572119258	T	T	T
0.5000000000000000	0.166666667013104	0.0984529120410897	F	F	F
0.4994191491712022	0.1672507744504813	0.2965237197790428	T	T	T
0.5039547495696755	0.1627160497567143	0.4906164660548400	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
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0.4999939439198156	0.0000075368580637	0.3946831820668070	T	T	T
0.333333332986896	0.166666667013104	0.0000000000000000	F	F	F
0.3330321123869318	0.1669682491342483	0.1983982807837851	T	T	T
0.3327496988634905	0.1672504187729278	0.3989765502030800	T	T	T
0.333333332986896	0.0000000000000000	0.0984529120410897	F	F	F
0.3327480201450086	0.0005837511833988	0.2965251177531444	T	T	T
0.3372835700781686	0.9960447455308783	0.4906189503156532	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120410897	F	F	F
0.4999980225094471	0.5000019127471601	0.2982582479409983	T	T	T
0.4999925543801875	0.5000000698049057	0.4940367368122234	T	T	T
0.5000000000000000	0.333333332986896	0.0000000000000000	F	F	F
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0.4994158087728785	0.3339166811865305	0.3989722814961109	T	T	T
0.333333332986896	0.5000000000000000	0.0000000000000000	F	F	F
0.3336308871438945	0.4997015455753026	0.1983986973949339	T	T	T
0.3339102945229455	0.4994247305409165	0.3989730275543482	T	T	T
0.333333332986896	0.333333332986896	0.0984529120410897	F	F	F
0.3333322177111495	0.3333353512442243	0.2982628713260693	T	T	T
0.3333346675706843	0.3333424913393503	0.4940471902448382	T	T	T
0.666666667013104	0.166666667013104	0.0000000000000000	F	F	F
0.6666679832756049	0.1666677781589385	0.1979412374164451	T	T	T
0.6666679962617669	0.1666743221259822	0.3946850613096642	T	T	T
0.666666667013104	0.0000000000000000	0.0984529120410897	F	F	F
0.6672479850272002	0.9994234674322047	0.2965231218889535	T	T	T
0.6627032776718241	0.0039722866991912	0.4906109089757414	T	T	T
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0.6663668431534293	0.5003015398694113	0.1983953875536250	T	T	T
0.6660834935245151	0.5005853267979097	0.3989693858168707	T	T	T
0.666666667013104	0.333333332986896	0.0984529120410897	F	F	F
0.6660871238466939	0.3339159677924939	0.2965223959247521	T	T	T
0.6706197599341873	0.3293839525190062	0.4906123462082856	T	T	T
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0.8293772861603664	0.1706357512464770	0.4906245419220066	T	T	T
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0.8336349083231372	0.9997008604070368	0.1983981229205271	T	T	T
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0.8327555603150707	0.5005840292250884	0.2965259202661926	T	T	T
0.8372850405666830	0.4960503142744945	0.4906215122520968	T	T	T
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0.8333367336175418	0.3333342780260879	0.1979422473061279	T	T	T
0.8333384110292639	0.3333384987060868	0.3946912101664819	T	T	T
0.0000000000000000	0.666666667013104	0.0984529120410897	F	F	F
0.9994179189645215	0.6672506902802589	0.2965290151615553	T	T	T
0.0039439195529693	0.6627173250696281	0.4906304085097163	T	T	T
0.166666667013104	0.666666667013104	0.0000000000000000	F	F	F
0.1666646941766505	0.6666684050839706	0.1979438563272376	T	T	T
0.1666592449172742	0.6666720655881572	0.3946934804991019	T	T	T
0.333333332986896	0.666666667013104	0.0984529120410897	F	F	F
0.3339080510003060	0.6660890234873227	0.2965246028342903	T	T	T

0.3293706717634315	0.6706332308179940	0.4906162787118739	T	T	T
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0.5005735697517230	0.6660925637227236	0.3989677191552207	T	T	T
0.6666666667013104	0.6666666667013104	0.0984529120410897	F	F	F
0.6666647593137333	0.6666696623031756	0.2982566608403505	T	T	T
0.6666406067643649	0.6666573420852545	0.4940336193517038	T	T	T
0.8333333332986896	0.6666666667013104	0.0000000000000000	F	F	F
0.8330335822303596	0.6669682356999642	0.1983974427256799	T	T	T
0.8327478248516820	0.6672537186054180	0.3989751686553704	T	T	T
0.0000000000000000	0.8333333332986896	0.0000000000000000	F	F	F
0.9996995064815395	0.8336345926225303	0.1984006393790050	T	T	T
0.9994123131823641	0.8339190975962267	0.3989831903548401	T	T	T
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0.1660817185402724	0.8339174879749652	0.2965300326057079	T	T	T
0.1706120239242831	0.8293809584143167	0.4906318463111035	T	T	T
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0.3333291048361276	0.8333352271634438	0.1979422561504008	T	T	T
0.3333240720325812	0.8333395481516715	0.3946881115447674	T	T	T
0.5000000000000000	0.8333333332986896	0.0984529120410897	F	F	F
0.5005778954682522	0.8327559976638018	0.2965230662857383	T	T	T
0.4960370454048981	0.8373005533408986	0.4906108051888712	T	T	T
0.6666666667013104	0.8333333332986896	0.0000000000000000	F	F	F
0.6669664829266013	0.8330355404344011	0.1983968078913508	T	T	T
0.6672419915708494	0.8327591070490515	0.3989705918899561	T	T	T
0.8333330000000032	0.8333333332986896	0.0984529120410897	F	F	F
0.8333326260861688	0.8333351940248509	0.2982625943455943	T	T	T
0.8333008948790170	0.8333228667675817	0.4940500205901452	T	T	T
0.9437234993853335	0.0563715750041093	0.5730299212865740	T	T	T
0.0562444538008690	0.9436605635857382	0.5730360064360452	T	T	T
0.1104172105477576	0.2230244218710388	0.5730382280822629	T	T	T
0.2229397842883592	0.1103051216124314	0.5730283396371635	T	T	T
0.2770855627716665	0.3896925316727191	0.5730202371480118	T	T	T
0.3896120913307289	0.2769818789815609	0.5730128072150316	T	T	T
0.4437361484222799	0.5563574698271183	0.5730052685488635	T	T	T
0.5562856031698126	0.4436709372005821	0.5730035156948379	T	T	T
0.6103743702293715	0.7230263345129612	0.5729984596192232	T	T	T
0.7229528656686436	0.6103583181132131	0.5730090158708235	T	T	T
0.7770307497838184	0.8897102441982138	0.5730111727469798	T	T	T
0.8895860518628562	0.7770244962458556	0.5730288065680742	T	T	T
0.9999876842096361	0.0000108820004136	0.5509298381337329	T	T	T
0.1666815949919481	0.1666549383920791	0.5509259773293329	T	T	T
0.3333342714837024	0.3333377932531406	0.5509118588973462	T	T	T
0.4999942701236449	0.5000038988430822	0.5509005045791197	T	T	T
0.6666435969943039	0.6666862825564142	0.5508983364665815	T	T	T
0.8333071191839285	0.8333478838363318	0.5509171034696150	T	T	T

T3-pbc-0CO2 (-2447.2539 eV)

1.0000000000000000

19.2439999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.2439999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 24.4329999999999998

Ca O

192 192

Selective dynamics

Direct

0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F

0.0000001437415571 0.0000001773703641 0.1975618234908186 T T T

0.0000002881752029 0.9999998740055723 0.3957601213892530 T T T

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0.0000000415070200	0.1250011399656800	0.4934351271298926	T	T	T
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0.1250012565229556	0.0000000579301777	0.2966230121289371	T	T	T
0.1250015735109641	0.9999998652277368	0.4934354073756275	T	T	T
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0.1250006820734734	0.1250008304171980	0.1975612667678079	T	T	T
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0.0000001838120691	0.2499998364526345	0.3957598747851396	T	T	T
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0.0000001023526889	0.3749988268540768	0.2966230943992449	T	T	T
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0.1250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.1250008091336019	0.3749993626119899	0.1975613333379458	T	T	T
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0.2500000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.2500000019486625	0.1250031232363297	0.2966192531533295	T	T	T
0.2500002803774121	0.1250026151792073	0.4934371508614027	T	T	T
0.3750000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.3749987934768473	0.0000000976787293	0.2966228241301259	T	T	T
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0.3750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.3749993631790414	0.1250008092188980	0.1975612581978198	T	T	T
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0.2500000755295963	0.3749968744351557	0.2966194293320260	T	T	T
0.2500000313443068	0.3749974013391388	0.4934369451953630	T	T	T
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0.3749970101557189	0.2500001496972437	0.2966193092749305	T	T	T
0.3749973733604666	0.2500000550340116	0.4934370652422599	T	T	T
0.3750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.3749994038365725	0.3749995132705071	0.1975611349326559	T	T	T
0.3750000598333607	0.3750000561627320	0.3957590501484937	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0000001140920506	0.5000001621361214	0.1975618274700648	T	T	T
0.0000002296813685	0.4999998473101068	0.3957601466759613	T	T	T
0.0000000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.0000001315137707	0.6250014091987418	0.2966230552365902	T	T	T
0.0000000332583121	0.6250011029323016	0.4934351761806841	T	T	T
0.1250000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.1250012763136878	0.5000000362842276	0.2966230213536358	T	T	T
0.1250015768169550	0.4999998504766729	0.4934353471495714	T	T	T
0.1250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.1250006528934662	0.6250008928214047	0.1975612718732452	T	T	T
0.1250004514061810	0.6250000485013775	0.3957591613015036	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0000000077968920	0.7500001396983033	0.1975627516371889	T	T	T
0.0000001371753369	0.7499998123678840	0.3957598710420658	T	T	T

0.0000000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.0000001149520891	0.8749988515543521	0.2966230520209632	T	T	T
0.0000000567158607	0.8749987779371664	0.4934353057691978	T	T	T
0.1250000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.1250031276046811	0.7500000739027848	0.2966195097934692	T	T	T
0.1250029870058048	0.7499997716415031	0.4934377161678139	T	T	T
0.1250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.1250008350373282	0.8749994109613036	0.1975612974709060	T	T	T
0.1250003266412467	0.8749994911346971	0.3957592956174737	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2499999268655822	0.5000001594648334	0.1975626181554357	T	T	T
0.2500001384956899	0.4999999770340063	0.3957595043424026	T	T	T
0.2500000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.2500000086122110	0.6250030841892880	0.2966192226422041	T	T	T
0.2500003050788022	0.6250026270284864	0.4934371103200368	T	T	T
0.3750000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.3749988082629420	0.5000001098326418	0.2966228136683911	T	T	T
0.3749987280438276	0.4999999359917105	0.4934357072964544	T	T	T
0.3750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.3749993634592644	0.6250007994966303	0.1975612706415233	T	T	T
0.3749998399741155	0.6249999139915490	0.3957589037170983	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2500001958872939	0.7500000912256772	0.1975618180735934	T	T	T
0.2500001998884144	0.7499998032386670	0.3957587708048438	T	T	T
0.2500000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.2500001325394283	0.8749969117553466	0.2966193983404273	T	T	T
0.2500001285267204	0.8749973314167040	0.4934369700254024	T	T	T
0.3750000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.3749970703944137	0.7500001070802887	0.2966192954696121	T	T	T
0.3749973784013683	0.7500000991911638	0.4934370929358960	T	T	T
0.3750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.3749994080218113	0.8749995590306493	0.1975611462719030	T	T	T
0.3750001103315930	0.8750000320709582	0.3957591198318671	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5000000767022046	0.0000000760651206	0.1975618423748495	T	T	T
0.5000002582327580	0.9999999223237647	0.3957601159111738	T	T	T
0.5000000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.5000001114215498	0.1250013633748205	0.2966230453461801	T	T	T
0.5000000078214075	0.1250011252276932	0.4934351113417284	T	T	T
0.6250000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.6250012553830397	-0.0000000031883811	0.2966229992383924	T	T	T
0.6250015634665660	0.9999998325813318	0.4934353318885729	T	T	T
0.6250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.6250006901081379	0.1250008651785225	0.1975612728514886	T	T	T
0.6250003837897723	0.1250000273606722	0.3957591177479726	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.5000000222122728	0.2500001070322285	0.1975627766253666	T	T	T
0.5000001241483654	0.2499997781513144	0.3957598438977256	T	T	T
0.5000000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.5000000892250904	0.3749988470389903	0.2966230743128992	T	T	T
0.5000000581811945	0.3749988147769310	0.4934353241624813	T	T	T
0.6250000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.6250031063428040	0.2500000580106354	0.2966195437137591	T	T	T
0.6250029599486786	0.2499997834846256	0.4934376933372374	T	T	T
0.6250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.6250008964400332	0.3749994193899889	0.1975613333266061	T	T	T
0.6250002936939590	0.3749994635668238	0.3957592861324046	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7499999493659656	0.0000001887502933	0.1975625850927290	T	T	T
0.7500001242754574	0.0000000007352938	0.3957594975819809	T	T	T

0.7500000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.7499999866789997	0.1250031281841781	0.2966192416484199	T	T	T
0.7500002877175725	0.1250026068322591	0.4934371630634828	T	T	T
0.8750000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.8749987820829906	0.0000000779453231	0.2966228624971861	T	T	T
0.8749987577187105	0.9999999179497556	0.4934357126995267	T	T	T
0.8750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.8749993442718113	0.1250007594732997	0.1975612510191437	T	T	T
0.8749998331608593	0.1249998674291227	0.3957589371054659	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7500002177451411	0.2500001474966571	0.1975618193877955	T	T	T
0.7500001759813260	0.2499998186396740	0.3957588229406968	T	T	T
0.7500000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.7500000810008350	0.3749969066939612	0.2966193701965530	T	T	T
0.7500001172820875	0.3749973287826843	0.4934369386208323	T	T	T
0.8750000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.8749970331499490	0.2500001370333069	0.2966193007489107	T	T	T
0.8749974112584491	0.2500000631537229	0.4934370786056274	T	T	T
0.8750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.8749994535130062	0.3749995104710429	0.1975611249230311	T	T	T
0.8750000995304706	0.3750000107679993	0.3957590763996736	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
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0.5000002954521469	0.4999998950405520	0.3957601107514094	T	T	T
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0.5000000999140304	0.6250013777345472	0.2966230320612872	T	T	T
0.5000000685539974	0.6250011849610390	0.4934351115225232	T	T	T
0.6250000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.6250012598734725	0.5000000536881283	0.2966230329016031	T	T	T
0.6250016570612257	0.4999998197784150	0.4934353341494238	T	T	T
0.6250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
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0.6250004779388402	0.6250000135033386	0.3957591147391404	T	T	T
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0.5000001436533883	0.7499998295803266	0.3957598863173225	T	T	T
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0.5000001251548070	0.8749988167058692	0.2966230472494331	T	T	T
0.5000000696306930	0.8749987994218992	0.4934353662787186	T	T	T
0.6250000000000000	0.7500000000000000	0.0984529120451825	F	F	F
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0.6250029544706371	0.7499998079491349	0.4934377030546381	T	T	T
0.6250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.6250008261963412	0.8749994334007015	0.1975613256598755	T	T	T
0.6250002190316168	0.8749995167607199	0.3957592810552907	T	T	T
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0.7499999391825153	0.5000001361177024	0.1975625903660471	T	T	T
0.7500001621352069	0.4999999676605890	0.3957595278842105	T	T	T
0.7500000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.7500000248286933	0.6250031317462436	0.2966192392669524	T	T	T
0.7500002665517252	0.6250025871804770	0.4934371134382095	T	T	T
0.8750000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.8749987836793948	0.5000001429911430	0.2966227757855172	T	T	T
0.8749987076967701	0.4999999322528281	0.4934357162287777	T	T	T
0.8750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.8749993583892319	0.6250008226317263	0.1975612528536287	T	T	T
0.8749999039470627	0.6249998805120808	0.3957589756271031	T	T	T
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0.7500002097530186	0.7500001538573856	0.1975617876763769	T	T	T
0.7500001848456725	0.7499998341842554	0.3957588291496356	T	T	T

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0.7500000450772348	0.8749972926227009	0.4934369873248621	T	T	T
0.8750000000000000	0.7500000000000000	0.0984529120451825	F	F	F
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0.8749974331078995	0.7500000305208463	0.4934370430544585	T	T	T
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0.8749994513525708	0.8749994660653977	0.1975611597586159	T	T	T
0.8750000906715588	0.8749999924837537	0.3957590817177670	T	T	T
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0.1250002788155147	0.1250003764234877	0.2964481496321598	T	T	T
0.1250003011297142	0.1250000814967344	0.4926334822089058	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
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0.1249978125723480	0.9999998239777182	0.3961285196497269	T	T	T
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0.0000000100297272	0.1249977972302408	0.3961284972827708	T	T	T
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0.0000002582618260	0.9999998322242593	0.4926342714777664	T	T	T
0.1250000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.1250002995267004	0.3750000067760975	0.2964482111758771	T	T	T
0.125000222252331	0.3749997888540563	0.4926335495391359	T	T	T
0.1250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.1249983460062100	0.2500002190239572	0.1976233560276875	T	T	T
0.1249982649455466	0.2499996842405093	0.3961305146902706	T	T	T
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0.0000000398174514	0.3750021080581061	0.3961286557431027	T	T	T
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0.9999999548771349	0.2500003122842984	0.2964513594225764	T	T	T
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0.3749996940477177	0.1250002282468424	0.2964479848589709	T	T	T
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0.3750019749161762	0.0000001377983229	0.1976249078530957	T	T	T
0.3750023154609590	0.0000001680945682	0.3961285722763593	T	T	T
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0.3750019660641057	0.2500001953778201	0.1976230172856432	T	T	T
0.3750019379976052	0.2499999213193017	0.3961301091447014	T	T	T
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0.2500001097943129	0.3750020357859872	0.1976230228351316	T	T	T
0.2500002199285786	0.3750017489133843	0.3961301322159387	T	T	T
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0.2500000235976372	0.2500000232167013	0.2964496625554591	T	T	T
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0.1250002674723206	0.6250003420424806	0.2964481517160860	T	T	T
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0.1249982593307737	0.5000002762179033	0.1976249452541947	T	T	T
0.1249978149321904	0.4999998454989174	0.3961285330109257	T	T	T
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0.0000001427143540	0.5000001584513578	0.2964498228609573	T	T	T
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0.1249982528017226	0.7499996687860085	0.3961305489889146	T	T	T
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0.5000000555537829	0.1249977583418727	0.3961284879865858	T	T	T
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0.6250002858985034	0.3749997966463860	0.4926335600329898	T	T	T

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0.5000000399705393	0.3750021191765463	0.3961286663601626	T	T	T
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0.4999999308074447	0.2500002805226675	0.2964513718064590	T	T	T
0.5000000107164370	0.249999997338703	0.4926350673827105	T	T	T
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0.8749997157869503	0.1250002514141388	0.2964479753535542	T	T	T
0.8749996616691100	0.1250000785372208	0.4926337659150077	T	T	T
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0.8750019774034611	0.0000001105757560	0.1976248802143452	T	T	T
0.8750023023409792	0.0000001796273976	0.3961285998167302	T	T	T
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0.75000000181716716	0.1249980526814721	0.1976233263323881	T	T	T
0.7500001549679807	0.1249981969145939	0.3961301301693785	T	T	T
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0.7500001625822761	0.9999997990949963	0.4926350219138567	T	T	T
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0.8749997902716879	0.3749998927499913	0.2964480912256951	T	T	T
0.8749999256425783	0.3749999051458915	0.4926337119552454	T	T	T
0.8750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.8750019989744934	0.2500001935454229	0.1976229926789826	T	T	T
0.8750019537159689	0.2499999223617649	0.3961300801747775	T	T	T
0.7500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.7500001544367785	0.3750020565049921	0.1976230146439522	T	T	T
0.7500002574825512	0.3750017412281668	0.3961301321702217	T	T	T
0.7500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.7500000483343437	0.2500000537628282	0.2964496689375447	T	T	T
0.7499993117411229	0.2499995175388063	0.4926324487051101	T	T	T
0.6250000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.6250002753852061	0.6250003454255807	0.2964481555681029	T	T	T
0.6250003360573264	0.6250001244870540	0.4926335057497974	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.6249982610315299	0.5000002947140687	0.1976249119400033	T	T	T
0.6249978489788669	0.4999998317714672	0.3961285328402827	T	T	T
0.5000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.5000000202210295	0.6249982371068775	0.1976251705224644	T	T	T
0.5000000600195880	0.6249977583393796	0.3961285211306403	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.5000001315760443	0.5000001547821872	0.2964498345404067	T	T	T
0.5000002974804238	0.4999998481966487	0.4926342286839968	T	T	T
0.6250000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.6250002813183685	0.8750000040610878	0.2964482105798561	T	T	T
0.6250002781556968	0.8749997803272280	0.4926335428149724	T	T	T
0.6250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.6249983459952907	0.7500002253530592	0.1976233337627900	T	T	T
0.6249982550437644	0.7499996926784692	0.3961304865090332	T	T	T
0.5000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.5000000431962979	0.8750020826638857	0.1976249535893014	T	T	T
0.5000000489781092	0.8750021558618859	0.3961286521841583	T	T	T
0.5000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.4999999521382696	0.7500003143586983	0.2964513551364202	T	T	T
0.4999999911409922	0.7499999717619654	0.4926350736028555	T	T	T
0.8750000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.8749996953292195	0.6250002383924453	0.2964479915439626	T	T	T
0.8749996952577748	0.6250001094376386	0.4926337540342294	T	T	T

0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8750019905306060	0.5000001555166294	0.1976248881641958	T	T	T
0.8750023014439204	0.5000001645251314	0.3961285749280130	T	T	T
0.7500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.7500000269580177	0.6249980563077701	0.1976233168806731	T	T	T
0.7500001838206126	0.6249981781133055	0.3961301137933763	T	T	T
0.7500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.7500000230172220	0.5000000413548342	0.2964515605408487	T	T	T
0.7500001265055335	0.4999998169250603	0.4926349817719931	T	T	T
0.8750000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.8749997733674424	0.8749999131913970	0.2964481037186676	T	T	T
0.8749999462323940	0.8749999285262294	0.4926337401716354	T	T	T
0.8750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.8750019697339138	0.7500001447819119	0.1976230219885596	T	T	T
0.8750019238235360	0.7499999100240466	0.3961300936744696	T	T	T
0.7500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.7500000865202107	0.8750020726029825	0.1976229967196799	T	T	T
0.7500002257382018	0.8750017586251286	0.3961301349645959	T	T	T
0.7500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.7500000345872547	0.7500000267716173	0.2964496461519703	T	T	T
0.7499992505336878	0.7499995122843014	0.4926324394758118	T	T	T

T3-pbc-1CO2 (-2471.6705 eV)

1.0000000000000000

19.2439999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.2439999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 24.4329999999999998

Ca O C

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Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0000551223221663	0.0000021133080602	0.1980273207228712	T	T	T
0.0005718920273974	0.9999460935516178	0.3975981871222437	T	T	T
0.0000000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.9998671156926054	0.1250034214589469	0.2975023654194950	T	T	T
0.9925476325785235	0.1250188688703555	0.4957707278088074	T	T	T
0.1250000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.1249995786374488	0.9998348873876785	0.2976969340607549	T	T	T
0.1250142032393893	0.9932086175388515	0.5005808364165705	T	T	T
0.1250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.1250001744929738	0.1249999820749747	0.1980473734023763	T	T	T
0.1249986610024664	0.1250024347791355	0.3962287535849671	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0000520822160157	0.2499994866052622	0.1980302425043483	T	T	T
0.0005662626234640	0.2500657125148785	0.3975943725556874	T	T	T
0.0000000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.0000457819130243	0.3749088089251941	0.2974096719473941	T	T	T
0.9987308300347809	0.3758672855735106	0.4946323320206560	T	T	T
0.1250000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.1250002473530625	0.2501668199307034	0.2977002266878577	T	T	T
0.1249751171251201	0.2567843709620819	0.5005976753295041	T	T	T
0.1250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.1250001002984650	0.3749444790341457	0.1979761093029824	T	T	T
0.1249966306189658	0.3749193223758980	0.3970469563731397	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2499442214013908	-0.0000005923841986	0.1980331809597130	T	T	T
0.2494255917545044	0.9999383398232753	0.3975980823518646	T	T	T
0.2500000000000000	0.1250000000000000	0.0984529120451825	F	F	F

0.2501311293477302	0.1250031359212115	0.2975089448777422	T	T	T
0.2574456029449609	0.1249773385405808	0.4957863576941647	T	T	T
0.3750000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.3748433826151110	0.9998984672078065	0.2973662398263546	T	T	T
0.3760464801087518	0.9986371637365700	0.4943603808280009	T	T	T
0.3750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.3749345151968125	0.1250001938472374	0.1979306946362809	T	T	T
0.3757054734267178	0.1250009643006924	0.3962713023221981	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2499447968061465	0.2499984043394186	0.1980322537086907	T	T	T
0.2494165746971639	0.2500572673450722	0.3976172602980747	T	T	T
0.2500000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.2499495976568369	0.3749014960920888	0.2974174007656501	T	T	T
0.2512541201232841	0.3758619802723069	0.4946491994034637	T	T	T
0.3750000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.3748385660862086	0.2500996669194521	0.2973721616106154	T	T	T
0.3760333277893054	0.2513576471056311	0.4943755191362674	T	T	T
0.3750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.3749260329878827	0.3749757806771932	0.1978876099204939	T	T	T
0.3750984364411993	0.3751320206205063	0.3963962033649477	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0000462405472292	0.4999621324009086	0.1979108305027708	T	T	T
0.0000098764812221	0.5001086539810025	0.3966094763961959	T	T	T
0.0000000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.0000534360359811	0.6250061854784477	0.2971818952655582	T	T	T
0.9997957928379544	0.6250020588487161	0.4945123670703847	T	T	T
0.1250000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.1250005884405818	0.4999463436205869	0.2973292089614905	T	T	T
0.1249927218358319	0.5004056101344083	0.4947300355249161	T	T	T
0.1250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.1250005614514024	0.6250021766112158	0.1979122120739612	T	T	T
0.1249958937612985	0.6250020039369423	0.3966491538043643	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0000468757341220	0.7500410880762115	0.1979105601474642	T	T	T
0.0000154467710155	0.7499017063983241	0.3966139748552983	T	T	T
0.0000000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.0000458781935787	0.8750942450102489	0.2974106518207609	T	T	T
0.9987400485336584	0.8741436323748302	0.4946383605694070	T	T	T
0.1250000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.1250030605183291	0.7500573947730966	0.2973339409438491	T	T	T
0.1249969435144300	0.7495972322201628	0.4947385138333629	T	T	T
0.1250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.1250000220556418	0.8750544376376581	0.1979745258292864	T	T	T
0.1249993003723243	0.8750818387430909	0.3970458718371561	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2499521415225102	0.4999606317490584	0.1979118378245484	T	T	T
0.2499812604225468	0.5001044243503295	0.3966150040894669	T	T	T
0.2500000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.2499423571627122	0.6250066992401563	0.2971895288680799	T	T	T
0.2501947934276643	0.6250003793526688	0.4945174101904659	T	T	T
0.3750000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.3749399057363718	0.5000265755314054	0.2971251658539431	T	T	T
0.3753997974352947	0.5004011782832902	0.4943765147654783	T	T	T
0.3750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.3749387954744781	0.6250014792356138	0.1978406674073608	T	T	T
0.3750334063342379	0.6250014723574239	0.3964420099576655	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2499523490089391	0.7500393671761754	0.1979110646720177	T	T	T
0.2499843953690748	0.7498954791047644	0.3966256391316427	T	T	T
0.2500000000000000	0.8750000000000000	0.0984529120451825	F	F	F

0.2499509477954943	0.8750859487683285	0.2974141438189675	T	T	T
0.2512721927198678	0.8741331937606013	0.4946397829859517	T	T	T
0.3750000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.3749383723754279	0.7499729745535181	0.2971295875011996	T	T	T
0.3754104296749469	0.7495957701097417	0.4943826559501948	T	T	T
0.3750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.3749265171322446	0.8750214398817957	0.1978865797545911	T	T	T
0.3751065183897487	0.8748628608560886	0.3963900754504037	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.4999307083336482	0.9999872599695597	0.1978686544562097	T	T	T
0.5001979619952304	0.9998655905012324	0.3964456787430576	T	T	T
0.5000000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.5000810642950039	0.1250022200241817	0.2970762212073455	T	T	T
0.5005585547003255	0.1249978534419436	0.4944719536443219	T	T	T
0.6250000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.6250030281177460	0.9999697888260964	0.2970646308882688	T	T	T
0.6250042475922882	0.9997671885189167	0.4943826666615062	T	T	T
0.6250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.6250003798959163	0.1250009980215336	0.1978068040257730	T	T	T
0.6249997746784099	0.1250000112848703	0.3964509015778880	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4999294731736755	0.2500119847331275	0.1978667039757467	T	T	T
0.5001912829681457	0.2501308870819400	0.3964507680180405	T	T	T
0.5000000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.4999940251134061	0.3750125491013525	0.2970796009322138	T	T	T
0.5004346049144447	0.3754471568694753	0.4943390716458090	T	T	T
0.6250000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.6250005410116887	0.2500305508341350	0.2970688834315911	T	T	T
0.6249997933395549	0.2502309283739084	0.4943879447393942	T	T	T
0.6250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.6249993948097925	0.3749866322963422	0.1978128776703264	T	T	T
0.6249973576169660	0.3751257207676189	0.3963709285144815	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7500686483892617	0.9999881967761677	0.1978649003145872	T	T	T
0.7498085100071701	0.9998691563626053	0.3964443494462970	T	T	T
0.7500000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.7499141025429362	0.1250050780567344	0.2970779955315162	T	T	T
0.7494418578795413	0.1250041286652633	0.4944691061915966	T	T	T
0.8750000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.8751537093596028	0.9999033438795649	0.2973624668206782	T	T	T
0.8739614571235294	0.9986532017279361	0.4943643753303419	T	T	T
0.8750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.8750619681624077	0.1250019592601840	0.1979262162936009	T	T	T
0.8742908262401987	0.1250059328496708	0.3962619221966470	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7500667904256985	0.2500125673614705	0.1978660817505369	T	T	T
0.7498005479418014	0.2501394316767575	0.3964497895218451	T	T	T
0.7500000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.7499990828861259	0.3750150489628773	0.2970799826939978	T	T	T
0.7495548469033594	0.3754588888494806	0.4943404492368079	T	T	T
0.8750000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.8751466871191684	0.2501035325167889	0.2973635461743633	T	T	T
0.8739524198913433	0.2513703942027956	0.4943662767302884	T	T	T
0.8750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.8750691466666318	0.3749775196921136	0.1978849484252495	T	T	T
0.8748892138394527	0.3751405745016100	0.3963878617076538	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4999568905686379	0.4999901910726083	0.1978254974816930	T	T	T
0.5000495430451294	0.5000908380975566	0.3963680771512073	T	T	T
0.5000000000000000	0.6250000000000000	0.0984529120451825	F	F	F

0.4999706686508349	0.6250033825597592	0.2970509361321285	T	T	T
0.5002078999266028	0.6250022008482912	0.4942962792090562	T	T	T
0.6250000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.6250002569223939	0.5000162882650495	0.2970334836898718	T	T	T
0.6249975189568476	0.5002447194483578	0.4942727431627890	T	T	T
0.6250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.6250005783449355	0.6250016943228256	0.1978055217486392	T	T	T
0.6250004806198639	0.6250045018192850	0.3963257058188557	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.4999573564381282	0.7500096603051203	0.1978219266880277	T	T	T
0.5000533475081386	0.7499110630223467	0.3963638029486129	T	T	T
0.5000000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.4999976899983507	0.8749800873793158	0.2970773657319279	T	T	T
0.5004424656587314	0.8745436248701171	0.4943371231227663	T	T	T
0.6250000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.6250036069923118	0.7499854822789350	0.2970363595041007	T	T	T
0.6250059907335085	0.7497659193956806	0.4942723959500924	T	T	T
0.6250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.6250015520241311	0.8750108521939312	0.1978130631636832	T	T	T
0.6250031484925423	0.8748762858318406	0.3963696618638780	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7500406071554160	0.4999913639694130	0.1978206883581982	T	T	T
0.7499454424648468	0.5000958804374731	0.3963622533820568	T	T	T
0.7500000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.7500272451368083	0.6250056586442460	0.2970534245293115	T	T	T
0.7497951196467744	0.6250078110659999	0.4942947311413122	T	T	T
0.8750000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.8750497526868523	0.5000298457764784	0.2971210847593330	T	T	T
0.8745856075139744	0.5004061850078213	0.4943748791125595	T	T	T
0.8750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.8750570292290843	0.6250030215678074	0.1978399933242251	T	T	T
0.8749645613310993	0.6250050034927008	0.3964387516084659	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7500422877394326	0.7500106330084874	0.1978238380216067	T	T	T
0.7499493959491602	0.7499125715373922	0.3963657284654329	T	T	T
0.7500000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.7500033682599889	0.8749820779289375	0.2970812019515245	T	T	T
0.7495683494346913	0.8745541328661200	0.4943368019545891	T	T	T
0.8750000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.8750526911380914	0.7499751539016190	0.2971281060167542	T	T	T
0.8745955610546499	0.7496078057830617	0.4943756980779642	T	T	T
0.8750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.8750701998949192	0.8750223155729118	0.1978857078812753	T	T	T
0.8748961885744468	0.8748712675209814	0.3963891123260400	T	T	T
0.1250000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.1250004657920170	0.1250010300377244	0.2987055152643234	T	T	T
0.1249894239810579	0.1249944633026166	0.4995294609276573	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1249983783640826	0.0001902409807326	0.1982826636946109	T	T	T
0.1249954769122506	0.0009054747670594	0.3981178057505353	T	T	T
0.0000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.0001880819899505	0.1249987266169125	0.1983815720436701	T	T	T
0.0006338593330099	0.1250009311808716	0.3989347344712169	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.0001060191536259	0.0002106188069065	0.2972735427740023	T	T	T
0.9982727360904955	0.9997760617702732	0.4930603067490826	T	T	T
0.1250000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.1249969733381447	0.3748310522905883	0.2974153479572986	T	T	T
0.1249880086498080	0.3767382644291275	0.4942503136926207	T	T	T
0.1250000000000000	0.2500000000000000	0.0000000000000000	F	F	F

0.1249982307558778	0.2498122077070079	0.1982948399391128	T	T	T
0.1249943531310963	0.2490974025205070	0.3981215054081935	T	T	T
0.0000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.0000675471631294	0.3749381686688517	0.1981002832298768	T	T	T
0.9999850388605981	0.3752643510627405	0.3971790898987284	T	T	T
0.0000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.0000986854259212	0.2497886032889616	0.2972739027838305	T	T	T
0.9982491919576706	0.2502533771702305	0.4930420036855576	T	T	T
0.3750000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.3747849711489449	0.1249998696536306	0.2973582290817987	T	T	T
0.3761374955125756	0.1249885951293276	0.4936937721592918	T	T	T
0.3750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3749322657129918	0.0000581496374234	0.1980583323514651	T	T	T
0.3753937003470680	-0.0000016518036840	0.3969085382977448	T	T	T
0.2500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.2498181152140145	0.1249994542534823	0.1983963808036649	T	T	T
0.2493576114920412	0.1249964083729246	0.3989569390233140	T	T	T
0.2500000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.2498899596062827	0.0001987095441137	0.2972768932992379	T	T	T
0.2517276359196132	0.9997464100743892	0.4930433157811360	T	T	T
0.3750000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.3749509826398644	0.3750007820504691	0.2970675882779743	T	T	T
0.3755093906860510	0.3754853965546192	0.4935516761195649	T	T	T
0.3750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.3749302108345192	0.2499417558556998	0.1980542976922542	T	T	T
0.3753808340060309	0.2499975024608700	0.3969216010817949	T	T	T
0.2500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.2499303422663987	0.3749355511850495	0.1981003833606874	T	T	T
0.2500042505292172	0.3752538168204183	0.3971921840904763	T	T	T
0.2500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.2498925017171636	0.2497911203493880	0.2972877198952237	T	T	T
0.2517135747186268	0.2502392229858468	0.4930788182654905	T	T	T
0.1250000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.1249996819354472	0.6250037871356504	0.2971056185234699	T	T	T
0.1249915326932871	0.6249957743485908	0.4937596286897207	T	T	T
0.1250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1249998450900592	0.4999208112768923	0.1980717525810147	T	T	T
0.1249941047512235	0.5000246072179172	0.3970357469016383	T	T	T
0.0000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.0000326581208025	0.6250007649207192	0.1980120453799603	T	T	T
0.9999767321929371	0.6250034251416929	0.3969490301931734	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.0000305485023489	0.4999710273310897	0.2970738977809549	T	T	T
0.9995877172344263	0.5002353420870743	0.4936813235297098	T	T	T
0.1250000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.1249997777305450	0.8751704223933326	0.2974134137997631	T	T	T
0.1249934047810694	0.8732551048660460	0.4942488476967718	T	T	T
0.1250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.1249994466675514	0.7500814205027518	0.1980672911780650	T	T	T
0.1249962003791646	0.7499783676704470	0.3970454036997531	T	T	T
0.0000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.0000673544172197	0.8750655452976372	0.1981002713265415	T	T	T
0.9999892188660270	0.8747542137593945	0.3971836974800576	T	T	T
0.0000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.0000323257740691	0.7500377168126778	0.2970850881454254	T	T	T
0.9995928340118984	0.7497819864321937	0.4936862570167703	T	T	T
0.3750000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.3749616847555858	0.6250030122373310	0.2969844706793728	T	T	T
0.3752691315455788	0.6249954311394320	0.4935734434107641	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F

0.3749606855796900	0.4999751731383087	0.1979842000175295	T	T	T
0.3750960471360836	0.5000790727103872	0.3968408879972177	T	T	T
0.2500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.2499657638574712	0.6249991534847064	0.1980060582009915	T	T	T
0.2500156116257683	0.6249979810424229	0.3969504165591839	T	T	T
0.2500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.2499645232312485	0.4999670850880196	0.2970864809858404	T	T	T
0.2503974546227882	0.5002296775643830	0.4936865561963358	T	T	T
0.3750000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.3749522072252658	0.8749904281939881	0.2970644247276742	T	T	T
0.3755201320774055	0.8745067590865340	0.4935517908859964	T	T	T
0.3750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.3749600348859210	0.7500239000429046	0.1979756414708601	T	T	T
0.3751039839393990	0.7499229107884827	0.3968410039024091	T	T	T
0.2500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.2499290943255088	0.8750624900432232	0.1980999587062184	T	T	T
0.2500108302602870	0.8747398503459748	0.3971917699304325	T	T	T
0.2500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.2499650422469437	0.7500335836335347	0.2970870532839133	T	T	T
0.2504085552194149	0.7497599094132898	0.4936916500219711	T	T	T
0.6250000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.6250019789373622	0.1250029833235217	0.2969905154998023	T	T	T
0.6249988868770835	0.1249986004901940	0.4935770456128473	T	T	T
0.6250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6249971980374375	0.0000248189778988	0.1979591999051373	T	T	T
0.6250026131408608	0.9999525589401511	0.3968173901513876	T	T	T
0.5000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.4999204590908770	0.1249987910601589	0.1980342941778217	T	T	T
0.5001013680797369	0.1249984376726798	0.3969036014636618	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.5000060770625151	0.0000266627484288	0.2969907218685676	T	T	T
0.5003763111080392	0.9997572677576800	0.4935825037795593	T	T	T
0.6250000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.6249997858268288	0.3749944482900627	0.2969435306839007	T	T	T
0.6249910296526564	0.3752437637057127	0.4935124196419624	T	T	T
0.6250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.6249956989120991	0.2499744711993951	0.1979518064908360	T	T	T
0.6249944544454110	0.2500469713011939	0.3968183376441164	T	T	T
0.5000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.4999622415695219	0.3749826906112698	0.1979752517597685	T	T	T
0.5000920560512649	0.3751143897340362	0.3968181335332382	T	T	T
0.5000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.5000014858996568	0.2499725280874199	0.2969977141367505	T	T	T
0.5003655097721843	0.2502281698679755	0.4935911333021517	T	T	T
0.8750000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.8752095715664745	0.1250019569365078	0.2973495828584547	T	T	T
0.8738569258511821	0.1250007349652601	0.4936865916759577	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.8750694449939853	0.0000596611335143	0.1980543749354028	T	T	T
0.8746149683801102	0.0000054765315536	0.3969069338157898	T	T	T
0.7500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.7500772796413483	0.1250002166437751	0.1980264484052372	T	T	T
0.7499026673840415	0.1250003093009266	0.3969007104094880	T	T	T
0.7500000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.7499931613856310	0.0000280948396841	0.2969925092816141	T	T	T
0.7496368442932727	0.9997658248388200	0.4935832737167111	T	T	T
0.8750000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.8750395959343563	0.3750082786593752	0.2970620720886954	T	T	T
0.8744747081184644	0.3754966507995565	0.4935489770316584	T	T	T
0.8750000000000000	0.2500000000000000	0.0000000000000000	F	F	F

0.8750657612698201	0.2499410838410262	0.1980507894959869	T	T	T
0.8746058942095959	0.2500063950705143	0.3969070877400753	T	T	T
0.7500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.7500358249002793	0.3749829505999910	0.1979658111911461	T	T	T
0.7499029644674886	0.3751264757196244	0.3968130927907986	T	T	T
0.7500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.7499903544741087	0.2499758164277592	0.2969914115154151	T	T	T
0.7496228958283099	0.2502477964036096	0.4935900611974572	T	T	T
0.6250000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.6250022419119952	0.6250041843272534	0.2969037769891872	T	T	T
0.6250011692660364	0.6250049426402144	0.4934632406117321	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.6249951916081939	0.4999865865389336	0.1979312995734299	T	T	T
0.6249971419490457	0.5000605364062761	0.3967421968662627	T	T	T
0.5000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.4999734382391001	0.6249963045606665	0.1979430845723377	T	T	T
0.5000392355362612	0.6250007103393866	0.3967635690509041	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.4999827630846854	0.4999961744333087	0.2969404770960163	T	T	T
0.5002103695913855	0.5001748340032940	0.4935258661794433	T	T	T
0.6250000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.6250043018722173	0.8749995043585215	0.2969426789645426	T	T	T
0.6250032003004676	0.8747621180195341	0.4935078124471988	T	T	T
0.6250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.6249979429055854	0.7500142303280103	0.1979242295324123	T	T	T
0.6249999925673037	0.7499461821365627	0.3967360081611274	T	T	T
0.5000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.4999639152493890	0.8750210862339246	0.1979731166102714	T	T	T
0.5000959159931182	0.8748874145752505	0.3968133460589337	T	T	T
0.5000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.4999850952925154	0.7500019962917794	0.2969402785915729	T	T	T
0.5002185057783625	0.7498306350558527	0.4935224787135433	T	T	T
0.8750000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.8750302067699354	0.6250053511081342	0.2969829571932374	T	T	T
0.8747326905578316	0.6250008029329354	0.4935654519903329	T	T	T
0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8750411564174884	0.4999774097979097	0.1979803249386146	T	T	T
0.8749019124179782	0.5000834041406275	0.3968354419576711	T	T	T
0.7500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.7500261239888603	0.6249993486255541	0.1979355657574004	T	T	T
0.7499602865512555	0.6250022099150043	0.3967569638846242	T	T	T
0.7500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.7500113936497521	0.4999990692006590	0.2969386299864947	T	T	T
0.7497875304763395	0.5001825663780605	0.4935197817829952	T	T	T
0.8750000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.8750428724862737	0.8749970303099559	0.2970630790681636	T	T	T
0.8744884510043296	0.8745217167102429	0.4935471763015639	T	T	T
0.8750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.8750409469928370	0.7500260290634165	0.1979745542631969	T	T	T
0.8749082662274308	0.7499300373563489	0.3968370064372985	T	T	T
0.7500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.7500379920998871	0.8750201404646943	0.1979655543177011	T	T	T
0.7499091891120148	0.8748922817447903	0.3968109554587106	T	T	T
0.7500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.7500147987488675	0.7500041727103026	0.2969374593037751	T	T	T
0.7497881755397980	0.7498291798195665	0.4935189810518528	T	T	T
0.1247984556979334	0.1842060426926097	0.5799085953545637	T	T	T
0.1251900306202120	0.0657608380794859	0.5799009750658765	T	T	T
0.1249917049842115	0.1249902524933100	0.5570974458628382	T	T	T

T3-pbc-2CO2 (-2496.1767 eV)

1.0000000000000000
 19.2439999999999998 0.0000000000000000 0.0000000000000000
 0.0000000000000000 19.2439999999999998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 24.4329999999999998

Ca O C

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Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0002558394497049	0.0002546593298816	0.1981335502543778	T	T	T
0.0016098019071647	0.0016036416928115	0.3987751985284709	T	T	T
0.0000000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.0002023684827388	0.1253335510142130	0.2979520694815976	T	T	T
0.9925785979107923	0.1286652439927879	0.4989410637831483	T	T	T
0.1250000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.1253298220887533	0.0001972858818927	0.2979596949144442	T	T	T
0.1286533135235148	0.9925720219107357	0.4989796366517221	T	T	T
0.1250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.1250818478732931	0.1250828045954619	0.1981922898855384	T	T	T
0.1261428961005043	0.1261342694107790	0.3971888102927352	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
-0.0000055748961391	0.2500924277946632	0.1980159010867713	T	T	T
-0.0002331434919463	0.2510059199707972	0.3970358069171970	T	T	T
0.0000000000000000	0.3750000000000000	0.0984529120451825	F	F	F
-0.0004287741114677	0.3754260555536381	0.2971298937290601	T	T	T
0.9951851923282319	0.3798023055340354	0.4930367114147171	T	T	T
0.1250000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.1246137784657324	0.2503834577469846	0.2978289622059822	T	T	T
0.1132638538282133	0.2617211688319430	0.5050132351053143	T	T	T
0.1250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.1249083161376410	0.3750051034575101	0.1980169285793177	T	T	T
0.1240091941146954	0.3752283925915045	0.3970391605377123	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2500859148917559	0.9999916796299809	0.1980155532136068	T	T	T
0.2509923718042635	0.9997566298767100	0.3970385885960185	T	T	T
0.2500000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.2503793034903062	0.1246133233666272	0.2978237239865469	T	T	T
0.2617271873993816	0.1132787902113412	0.5049704514771144	T	T	T
0.3750000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.3754181993849612	0.9995652103742076	0.2971209965162919	T	T	T
0.3798062808028557	0.9951993414135818	0.4930215505892183	T	T	T
0.3750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.3750012488185173	0.1249095871118125	0.1980094754696537	T	T	T
0.3752355716325361	0.1240068007925170	0.3970016481949782	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2499108993388676	0.2499163926187053	0.1981802848165997	T	T	T
0.2488518004413160	0.2488596069038067	0.3971439563810587	T	T	T
0.2500000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.2496635768576689	0.3748084968460987	0.2979355823995696	T	T	T
0.2463778612766459	0.3824246056323148	0.4989037853047201	T	T	T
0.3750000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.3748028208542916	0.2496691976282228	0.2979263125239363	T	T	T
0.3824306820182569	0.2463478087159633	0.4988727756510357	T	T	T
0.3750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.3747409214533755	0.3747475351706442	0.1981155361748166	T	T	T
0.3733902530503223	0.3733917291312682	0.3987107998098363	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
-0.0000890891616416	0.5001474296199430	0.1977643244152932	T	T	T

-0.0009221700122661	0.5012865695920357	0.3956566578360231	T	T	T
0.0000000000000000	0.6250000000000000	0.0984529120451825	F	F	F
-0.0001246425512737	0.6255740027245379	0.2968893953916860	T	T	T
0.9988728458728955	0.6263485880093496	0.4941685361791128	T	T	T
0.1250000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.1246854245295052	0.5001363964742733	0.2972166729760494	T	T	T
0.1219529706058933	0.5024005490507766	0.4940975267425571	T	T	T
0.1250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.1249729277797136	0.6250691174090186	0.1978197838529444	T	T	T
0.1247069412666862	0.6255577719593303	0.3962803981753459	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0000909066710313	0.7503415227820404	0.1978631780035753	T	T	T
0.0001072931308035	0.7506661067711894	0.3965171563330293	T	T	T
0.0000000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.0003563322725314	0.8757408422696039	0.2976392831053949	T	T	T
0.9997253856543136	0.8749558082492856	0.4949603303145763	T	T	T
0.1250000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.1250932609469066	0.7502521113908985	0.2971324673114766	T	T	T
0.1251984213579874	0.7498269966748158	0.4945703195624251	T	T	T
0.1250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.1251096873305087	0.8752289828292524	0.1979855750108517	T	T	T
0.1257049137685941	0.8750382244889431	0.3968093830142617	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2498790332903564	0.4997878345907855	0.1979728250357909	T	T	T
0.2492773713269013	0.4999522940211166	0.3967625370064984	T	T	T
0.2500000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.2498917824831778	0.6247641340097696	0.2971152451090268	T	T	T
0.2498117844234078	0.6251589738408401	0.4945522951785239	T	T	T
0.3750000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.3746325246207338	0.4992657279999455	0.2976029321457770	T	T	T
0.3752586357178980	0.5000142848375360	0.4949040275666053	T	T	T
0.3750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.3748979433100897	0.6246656664079000	0.1978490937868089	T	T	T
0.3748850228060678	0.6243358076072377	0.3964822816879765	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2500151970735123	0.7499376922175294	0.1978203219230991	T	T	T
0.2502836857873462	0.7494326929102486	0.3962708170500578	T	T	T
0.2500000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.2503065078242138	0.8748553313674385	0.2972216271868034	T	T	T
0.2530535303604861	0.8725517989247243	0.4940984987343748	T	T	T
0.3750000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.3751110607730619	0.7494207078738906	0.2968736368618727	T	T	T
0.3761182560282849	0.7486216965452716	0.4941378575775128	T	T	T
0.3750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.3750782569664454	0.8748547884409529	0.1977555542176416	T	T	T
0.3759116246758826	0.8736950746598104	0.3956382444676260	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5001423659715226	0.9999092824342901	0.1977566581194877	T	T	T
0.5012888880382556	0.9990757793724627	0.3956359556448001	T	T	T
0.5000000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.5001372926490371	0.1246853988267362	0.2971964633115607	T	T	T
0.5024054283294677	0.1219524263494988	0.4940638270299937	T	T	T
0.6250000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.6255735440906132	-0.0001240112790494	0.2968744756561232	T	T	T
0.6263479290250654	0.9988843016051313	0.4941505876524834	T	T	T
0.6250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.6250701188542155	0.1249752921502239	0.1978123472395778	T	T	T
0.6255593520034964	0.1247105577428808	0.3962553975526181	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4997828791740526	0.2498827662382753	0.1979662990198858	T	T	T

0.4999569209270559	0.2492800255657860	0.3967394147860384	T	T	T
0.5000000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.4992608013317784	0.3746411487060035	0.2975955155238982	T	T	T
0.5000094579246194	0.3752518718128853	0.4948923493125622	T	T	T
0.6250000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.6247632358518532	0.2498965685574585	0.2970998603887502	T	T	T
0.6251561620597514	0.2498075898794117	0.4945331049536785	T	T	T
0.6250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.6246660410620875	0.3749036039531796	0.1978459396099898	T	T	T
0.6243332397159551	0.3748880004281353	0.3964715357292296	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7503458729256354	0.0000922839698701	0.1978579066651327	T	T	T
0.7506627112784294	0.0001127394669416	0.3965029133025712	T	T	T
0.7500000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.7502521770069462	0.1250988968701107	0.2971184399726831	T	T	T
0.7498284951840625	0.1252087141985576	0.4945487840298345	T	T	T
0.8750000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.8757423864856023	0.0003571170336451	0.2976328987627697	T	T	T
0.8749516850689871	0.9997447341346399	0.4949462176572672	T	T	T
0.8750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.8752309908112053	0.1251132013011693	0.1979802514948378	T	T	T
0.8750369554212389	0.1257124233763368	0.3967829515169559	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7499423752822141	0.2500204948665088	0.1978146664312407	T	T	T
0.7494286871940303	0.2502908644735077	0.3962559526135915	T	T	T
0.7500000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.7494218387291919	0.3751194761582592	0.2968681369595511	T	T	T
0.7486143160782218	0.3761127906931736	0.4941335569024778	T	T	T
0.8750000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.8748592182341256	0.2503174305842176	0.2972154655482460	T	T	T
0.8725480107295613	0.2530496941151318	0.4940817552452444	T	T	T
0.8750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.8748588589951057	0.3750853003486955	0.1977570124631375	T	T	T
0.8736958572377777	0.3759194122751391	0.3956407401522825	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4997334626113106	0.4997372705415862	0.1978918495953291	T	T	T
0.4993775926850915	0.4993833509106935	0.3965607089868163	T	T	T
0.5000000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.4998294415732517	0.6245564648515124	0.2970200229116289	T	T	T
0.5002461853064657	0.6245674416745444	0.4943213796509312	T	T	T
0.6250000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.6245545881893003	0.4998347080914619	0.2970170780778583	T	T	T
0.6245629052374970	0.5002407542968323	0.4943171058418412	T	T	T
0.6250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.6248996200972470	0.6248999647248998	0.1977417921899095	T	T	T
0.6247972928549914	0.624799008625605	0.3962254567844533	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.5000362581654473	0.7497895488114743	0.1977131091710006	T	T	T
0.5004287114170326	0.7492329225581010	0.3960640928412106	T	T	T
0.5000000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.5004515968459775	0.8745392773797450	0.2967529313125414	T	T	T
0.5019652346835820	0.8730224382365702	0.4938898818936439	T	T	T
0.6250000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.6251910254256501	0.7498176552999872	0.2968806269809020	T	T	T
0.6255315927797497	0.7494434211890632	0.4941606537730640	T	T	T
0.6250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.6252117071302418	0.8749670729617307	0.1977154428193822	T	T	T
0.6257619102961930	0.8745658372243975	0.3960803884505694	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7497924578601005	0.5000414026621407	0.1977144025381505	T	T	T

0.7492322532093207	0.5004312336853887	0.3960661489206451	T	T	T
0.7500000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.7498174339459575	0.6251910811136770	0.2968857246067274	T	T	T
0.7494322717932848	0.6255328483632193	0.4941667107631229	T	T	T
0.8750000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.8745438944817913	0.5004567174793116	0.2967599133682189	T	T	T
0.8730121701514338	0.5019632188471054	0.4939029797263312	T	T	T
0.8750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.8749679804551986	0.6252121135170198	0.1977192742852783	T	T	T
0.8745627977069323	0.6257591555508659	0.3960917361927173	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7501130460491737	0.7501110793034936	0.1977546695683059	T	T	T
0.7501992653017314	0.7501990187618687	0.3962338195361410	T	T	T
0.7500000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.7504570520521997	0.8751648679330766	0.2970440199543432	T	T	T
0.7504006177235302	0.8747427163401933	0.4943494152335048	T	T	T
0.8750000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.8751650370442746	0.7504539423807670	0.2970492887580014	T	T	T
0.8747314110752142	0.7504015258004445	0.4943558207842489	T	T	T
0.8750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.8752813592712166	0.8752777669905052	0.1979063814509279	T	T	T
0.8756037145784310	0.8756066221616421	0.3966039550223920	T	T	T
0.1250000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.1253104342706801	0.1253100307406655	0.2988333970602216	T	T	T
0.1286991175471291	0.1286225019816370	0.4952154935879949	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1251452001453482	0.0003119057018766	0.1984704547708815	T	T	T
0.1262613830520765	0.0008567908695627	0.3992254336136901	T	T	T
0.0000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.0003145117009117	0.1251478129646395	0.1984686123811099	T	T	T
0.0008662019012356	0.1262652813612992	0.3992300321530369	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.0006810133878978	0.0006811240301075	0.2978064556721198	T	T	T
0.0018610629213215	0.0018825075507672	0.4950960720985871	T	T	T
0.1250000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.1247618485784090	0.3749837070876407	0.2972037975502482	T	T	T
0.1194605763447965	0.3797251245730803	0.4919229765294033	T	T	T
0.1250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.1251242795517423	0.2498823490551071	0.1985399244159909	T	T	T
0.1247774363973935	0.2502266281206711	0.3993510661283959	T	T	T
0.0000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
-0.0000879828784826	0.3750927660298591	0.1979572034177368	T	T	T
-0.0017545311889420	0.3767482076373873	0.3959173825842169	T	T	T
0.0000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.0000168588624730	0.2502435096657707	0.2972111407233229	T	T	T
0.9952686390100496	0.2555311180118257	0.4919359830927067	T	T	T
0.3750000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.3749824231717532	0.1247642101352401	0.2971877943037574	T	T	T
0.3797417500603458	0.1194783581881677	0.4918760072406070	T	T	T
0.3750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3750875689642412	-0.0000916401997182	0.1979525508763893	T	T	T
0.3767455139736065	-0.0017552007909164	0.3959021683534774	T	T	T
0.2500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.2498778871549605	0.1251250793493912	0.1985364297770927	T	T	T
0.2502297600296290	0.1247788207837678	0.3993465360475142	T	T	T
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0.2502372553632679	0.0000126375713913	0.2972106652338821	T	T	T
0.2555365945943839	0.9952779103399739	0.4919468174486563	T	T	T
0.3750000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.3743166141403880	0.3743223939015227	0.2977681890412220	T	T	T

0.3731359115084079	0.3731150116934201	0.4950313271903075	T	T	T
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0.3746904501426028	0.2498580799704737	0.1984556453507562	T	T	T
0.3741378916965075	0.2487513940008542	0.3991734267811546	T	T	T
0.2500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.2498532966741248	0.3746943998301177	0.1984582356158326	T	T	T
0.2487511605992243	0.3741375717814084	0.3991821875067031	T	T	T
0.2500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.2496843812518816	0.2496865995302785	0.2988185002765586	T	T	T
0.2463420463602921	0.2463775339279738	0.4951738711636553	T	T	T
0.1250000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.1249109539644457	0.6252856481473522	0.2969148906526455	T	T	T
0.1242333976245375	0.6259549867624209	0.4934533242548251	T	T	T
0.1250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1249549855962804	0.5000079788437757	0.1980340091132131	T	T	T
0.1242773596835006	0.5010887412653620	0.3966227134567834	T	T	T
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-0.0000285826104019	0.6252682269525961	0.1979156262753846	T	T	T
-0.0004395153991958	0.6260271710776956	0.3965808951396473	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
-0.0003591325174293	0.5005859255106508	0.2966849545565278	T	T	T
0.9976407345119911	0.5026939312940774	0.4929294879211605	T	T	T
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0.1252726834707310	0.8754479512310052	0.2974854731768720	T	T	T
0.1262515769095231	0.8738867236837217	0.4942711721262112	T	T	T
0.1250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.1250496160445616	0.7502083547850339	0.1980395072250032	T	T	T
0.1251464840468446	0.7503450716642928	0.3969439809921876	T	T	T
0.0000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.0002230546071736	0.8753492576081154	0.1982013822719100	T	T	T
0.0006528354452373	0.8757687195530119	0.3976802702856803	T	T	T
0.0000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.0001253044919513	0.7505923376759051	0.2970813950008195	T	T	T
0.9998386945981669	0.7508619457035087	0.4937032437721690	T	T	T
0.3750000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.3748566924156537	0.6243996200620705	0.2970519096726722	T	T	T
0.3751603709931761	0.6241011352577946	0.4936630792857691	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3747722613620567	0.4996638063166389	0.1981791368455492	T	T	T
0.3743299506709192	0.4992339367364887	0.3976314536165499	T	T	T
0.2500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.2499388235249334	0.6248041336758374	0.1980325315042727	T	T	T
0.2498494678493819	0.6246389452884470	0.3969273545236559	T	T	T
0.2500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.2497208623789014	0.4995664942267163	0.2974530359793753	T	T	T
0.2487634275033879	0.5011046848447693	0.4942213978193474	T	T	T
0.3750000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.3753620927556701	0.8743914557809432	0.2966724275321616	T	T	T
0.3773404295702107	0.8722856625579392	0.4929114212758150	T	T	T
0.3750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.3750249326290178	0.7497366427708606	0.1978957943380674	T	T	T
0.3754370371926843	0.7489728979403373	0.3965525225874088	T	T	T
0.2500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.2500353560160284	0.8749961962272914	0.1980374017537575	T	T	T
0.2507077780416719	0.8738994893808978	0.3966222741464921	T	T	T
0.2500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.2500810057192189	0.7497148330505762	0.2969070232045087	T	T	T
0.2507609128287620	0.7490323157310348	0.4934519255725283	T	T	T
0.6250000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.6252853792765957	0.1249154737212378	0.2968998176271405	T	T	T

0.6259562026840686	0.1242396548542918	0.4934197063205922	T	T	T
0.6250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6252682382686571	-0.0000271959524758	0.1979054121281047	T	T	T
0.6260269923051054	0.9995650720898536	0.3965635227420513	T	T	T
0.5000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.5000051661741566	0.1249554148486437	0.1980270192760350	T	T	T
0.5010930525054453	0.1242785563479601	0.3965912934600534	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.5005842254742358	-0.0003620447094611	0.2966688302946667	T	T	T
0.5026966489352689	0.9976467583289176	0.4929105897574318	T	T	T
0.6250000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.6243979741879691	0.3748631204254806	0.2970432493844716	T	T	T
0.6240975248351989	0.3751527667265973	0.4936521952557278	T	T	T
0.6250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.6248038194280378	0.2499430507412379	0.1980238423104277	T	T	T
0.6246358071785563	0.2498511081650366	0.3969122399078515	T	T	T
0.5000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.4996594963847056	0.3747759920735070	0.1981759779118956	T	T	T
0.4992311304265407	0.3743332599141505	0.3976210401123377	T	T	T
0.5000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.4995647283055172	0.2497227610096768	0.2974384931517948	T	T	T
0.5010997228670958	0.2487569892985131	0.4942016657028848	T	T	T
0.8750000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.8754529125016803	0.1252795062703295	0.2974749708043310	T	T	T
0.8738882142709239	0.1262619251204386	0.4942468164871798	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.8753504513817462	0.0002218580384689	0.1981975027128540	T	T	T
0.8757644727661658	0.0006581014973445	0.3976636703191093	T	T	T
0.7500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.7502114734993699	0.1250523746916380	0.1980343382459366	T	T	T
0.7503498488876830	0.1251553368818465	0.3969220722784100	T	T	T
0.7500000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.7505903790519627	0.0001295421311062	0.2970702336567111	T	T	T
0.7508596883381300	0.9998480477391182	0.4936895704480838	T	T	T
0.8750000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.8743956953184541	0.3753724483973843	0.2966731027766625	T	T	T
0.8722758746809284	0.3773355075812285	0.4929127018885587	T	T	T
0.8750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.8749979972228914	0.2500421607263681	0.1980339275363044	T	T	T
0.8738993932569847	0.2507148321296546	0.3966093204659262	T	T	T
0.7500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.7497395073978120	0.3750314584912592	0.1978939828291454	T	T	T
0.7489721546212297	0.3754408624441010	0.3965480215085707	T	T	T
0.7500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.7497122868927957	0.2500880597952378	0.2968958046072226	T	T	T
0.7490304733075241	0.2507614832354880	0.4934387427287998	T	T	T
0.6250000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.6248331279135673	0.6248350738704715	0.2968618732519324	T	T	T
0.6248042037877930	0.6248061633961911	0.4934568789513791	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.6247493162613675	0.4998972034635567	0.1979520450040009	T	T	T
0.6243376581039013	0.4998858162410782	0.3968022185294483	T	T	T
0.5000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.4998942063719539	0.6247486260273055	0.1979543315627832	T	T	T
0.4998824892953830	0.6243401015318382	0.3968078133415337	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.4995419052504297	0.4995476566601413	0.2971804191666090	T	T	T
0.4994019226454903	0.4994019872495601	0.4937743206935538	T	T	T
0.6250000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.6254660407496999	0.8748226359463760	0.2967889982628324	T	T	T

0.6261577659172345	0.8741140999041638	0.4933089112598586	T	T	T
0.6250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.6250799748115994	0.7499240951758636	0.1978711144876945	T	T	T
0.6253446475506663	0.7496583095490366	0.3966066263150876	T	T	T
0.5000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.5001694121181537	0.8748239866555766	0.1978492352247708	T	T	T
0.5009906592356803	0.8739968823854581	0.3963575874213345	T	T	T
0.5000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.5001709296552990	0.7495434092762379	0.2967791788329260	T	T	T
0.5008754961087398	0.7488272455094027	0.4933009303097056	T	T	T
0.8750000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.8748242397383499	0.6254654296463047	0.2967982661972930	T	T	T
0.8741007607102987	0.6261586655294595	0.4933225206571968	T	T	T
0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8748265107925363	0.5001748955155672	0.1978529460304951	T	T	T
0.8739961903202987	0.5009954666548239	0.3963668146397165	T	T	T
0.7500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.7499246430463709	0.6250816586389019	0.1978753442007910	T	T	T
0.7496573387737379	0.6253439161592635	0.3966140671079832	T	T	T
0.7500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.7495435353693045	0.5001743895830201	0.2967812716528422	T	T	T
0.7488174218879652	0.5008735958424967	0.4933046356552626	T	T	T
0.8750000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.8754667412260606	0.8754641296245844	0.2972216548660329	T	T	T
0.8755683716164846	0.8755791305474216	0.4938249742779323	T	T	T
0.8750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.8751150617201255	0.7502607360376432	0.1979594496966459	T	T	T
0.8750987369837020	0.7506454455491803	0.3968349759481640	T	T	T
0.7500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.7502643154758484	0.8751158058849601	0.1979566877643592	T	T	T
0.7506479476917632	0.8751016083432803	0.3968309503964305	T	T	T
0.7500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.7501734546908965	0.7501751733135568	0.2968770924739138	T	T	T
0.7501601909653380	0.7501662044272681	0.4934782807101057	T	T	T
0.0774629660841713	0.1618796287185054	0.5735335640866570	T	T	T
0.1615525671605937	0.0772554566440884	0.5735962818362299	T	T	T
0.2134777042014070	0.2977746442593060	0.5735570975364687	T	T	T
0.2975909960014425	0.2131595521656363	0.5735145699039796	T	T	T
0.1224239311644012	0.1224390139853376	0.5511846553720816	T	T	T
0.2526157990530790	0.2525760420286751	0.5511357356336517	T	T	T

T3-pbc-3CO2 (-2520.5892 eV)

1.0000000000000000

19.2439999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.2439999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 24.4329999999999998

Ca O C

192 198 3

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0003875660632471	0.0003871833783735	0.1980595998739485	T	T	T
0.0018656404369614	0.0018636199536654	0.3984905774001796	T	T	T
0.0000000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.0005449205649536	0.1255529159182082	0.2979282163548842	T	T	T
0.9924588448104747	0.1284413459692853	0.4988858237939370	T	T	T
0.1250000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.1255509568499851	0.0005405371260146	0.2979328725132806	T	T	T
0.1284283163241180	0.9924672175540065	0.4989054095582982	T	T	T

0.1250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.1252700194968892	0.1252685488600036	0.1982355433827592	T	T	T
0.1266764583188362	0.1266745956939369	0.3974838109696854	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0001793477924079	0.2501739941987600	0.1980308133314082	T	T	T
-0.0000711040408365	0.2512805886084821	0.3970730487000945	T	T	T
0.0000000000000000	0.3750000000000000	0.0984529120451825	F	F	F
-0.0003325806518299	0.3755284615805662	0.2971669086866944	T	T	T
0.9946743952506930	0.3803838996130260	0.4931864590822356	T	T	T
0.1250000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.1250378140568492	0.2506189584916850	0.2982086326994571	T	T	T
0.1125273796659954	0.2614557648978350	0.5051884424495313	T	T	T
0.1250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.1249395121026361	0.3750578626304457	0.1980382335395047	T	T	T
0.1242471349754549	0.3757529371548036	0.3974450038895179	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2501698774627495	0.0001758691141997	0.1980305984268739	T	T	T
0.2512736247797448	0.9999209724981357	0.3970731289223648	T	T	T
0.2500000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.2506180766242189	0.1250355150530376	0.2982056223565780	T	T	T
0.2614640296420083	0.1125372137592492	0.5051491040188527	T	T	T
0.3750000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.3755255599161713	0.9996629319389765	0.2971604354566976	T	T	T
0.3803829998339044	0.9946762009567293	0.4931808430506600	T	T	T
0.3750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.3750561196499004	0.1249382939615591	0.1980337758655304	T	T	T
0.3757560952018280	0.1242470697313300	0.3974289496046006	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2499979662131548	0.2499986695769975	0.1983270017794494	T	T	T
0.2500100737281161	0.2500134404047225	0.3986418460219924	T	T	T
0.2500000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.2493806060125158	0.3749689543955359	0.2981911930387169	T	T	T
0.2385683509272390	0.3874478915184393	0.5051201898644687	T	T	T
0.3750000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.3749689632809684	0.2493821309066068	0.2981856682499411	T	T	T
0.3874539955308685	0.2385682907686850	0.5051138786856241	T	T	T
0.3750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.3747274972365762	0.3747297398562124	0.1982196354418116	T	T	T
0.3733412540760317	0.3733429415212246	0.3974148045299654	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
-0.0001666694101567	0.5001687230608545	0.1976851924365645	T	T	T
-0.0015860822829040	0.5015948068808881	0.3952269888977308	T	T	T
0.0000000000000000	0.6250000000000000	0.0984529120451825	F	F	F
-0.0004431422653456	0.6257442078263551	0.2966011628007664	T	T	T
0.9977325604141420	0.6274105195522034	0.4937731558847214	T	T	T
0.1250000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.1244711277079906	0.5003400229892835	0.2971628506186764	T	T	T
0.1196394479153308	0.5053191298846890	0.4931859260086982	T	T	T
0.1250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.1249019096975952	0.6251386774979859	0.1977071134368227	T	T	T
0.1240545268322132	0.6263050574746158	0.3955478876967266	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0000266852764212	0.7504303434834910	0.1977250151278455	T	T	T
-0.0002405124474675	0.7510551390463218	0.3960849164463642	T	T	T
0.0000000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.0003918256797392	0.8759553245461328	0.2974022087123844	T	T	T
0.9994711486972597	0.8752580324655393	0.4946455458858554	T	T	T
0.1250000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.1249585483006907	0.7505962695211015	0.2968302252667105	T	T	T
0.1242539900748431	0.7508933390662548	0.4942051866032279	T	T	T

0.1250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.1251497054874506	0.8754006613710811	0.1978789416832496	T	T	T
0.1256545078672815	0.8754482596186083	0.3965047340789225	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2498174031873982	0.4998255033737642	0.1980188098143714	T	T	T
0.2487209749188984	0.5000815168875908	0.3970454531639098	T	T	T
0.2500000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.2496311988506293	0.6249057958333873	0.2970565535771518	T	T	T
0.2471246937864597	0.6271555539700432	0.4939953883474072	T	T	T
0.3750000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.3744438777106734	0.4994686301618816	0.2978853744851519	T	T	T
0.3715771745883416	0.5075058309096814	0.4988293737889790	T	T	T
0.3750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.3748346688894810	0.6246119865920297	0.1978596645643288	T	T	T
0.3743405537589107	0.6245507946599954	0.3964524059596390	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2499891418805575	0.7500078084219496	0.1977375770549853	T	T	T
0.2499966694158664	0.7499986056170762	0.3959119754960289	T	T	T
0.2500000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.2503512915652682	0.8751036041932162	0.2970698728956511	T	T	T
0.2528994952361450	0.8728309360025477	0.4940138706196139	T	T	T
0.3750000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.3750244204900358	0.7494139807844775	0.2968097328571459	T	T	T
0.3757613360191912	0.7490883022685056	0.4941758084698601	T	T	T
0.3750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.3750857106469648	0.8748693210378400	0.1977023661548040	T	T	T
0.3759423007819882	0.8736965918098504	0.3955388056429263	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5001674681351147	0.9998307124530817	0.1976812660522257	T	T	T
0.5015931104507878	-0.0015870671658746	0.3952186439848179	T	T	T
0.5000000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.5003412918681728	0.1244691355046800	0.2971532463087268	T	T	T
0.5053181434012881	0.1196400711212244	0.4931694248566435	T	T	T
0.6250000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.6257433517475698	0.9995553586855789	0.2965963956615026	T	T	T
0.6274086354873885	0.9977388145129252	0.4937678862176772	T	T	T
0.6250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.6251393027088462	0.1249031650021054	0.1977047077656509	T	T	T
0.6263077111265304	0.1240556105870824	0.3955381853150544	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4998252801865684	0.2498189005458362	0.1980148432560369	T	T	T
0.5000821901744688	0.2487210047970295	0.3970324717915303	T	T	T
0.5000000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.4994669282662159	0.3744485476834971	0.2978817262675646	T	T	T
0.5075058209518453	0.3715668144029835	0.4988191683472171	T	T	T
0.6250000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.6249066145856248	0.2496343363851489	0.2970501479216185	T	T	T
0.6271559830323060	0.2471181480517230	0.4939864148952535	T	T	T
0.6250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.6246116506627091	0.3748383119017110	0.1978576767826982	T	T	T
0.6245514104844936	0.3743412509676652	0.3964501388263640	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7504298480849767	0.0000284786564981	0.1977237190783161	T	T	T
0.7510543440153165	0.9997623148409746	0.3960775900070053	T	T	T
0.7500000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.7505987662171356	0.1249638361615537	0.2968249492827283	T	T	T
0.7508965092658634	0.1242565730316637	0.4941955680193464	T	T	T
0.8750000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.8759553003556652	0.0003952864068698	0.2973979663145259	T	T	T
0.8752557155537959	0.9994759199908915	0.4946395735002881	T	T	T

0.8750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.8754025306490760	0.1251541343808258	0.1978759962830939	T	T	T
0.8754511382375297	0.1256581322220030	0.3964955617037174	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7500089909976250	0.2499939349294183	0.1977353628803428	T	T	T
0.7500019753002001	0.2500007170093028	0.3959048181725596	T	T	T
0.7500000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.7494147752740112	0.3750286944530166	0.2968091032927263	T	T	T
0.7490847431145803	0.3757588215512581	0.4941767953970024	T	T	T
0.8750000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.8751088381081771	0.2503579077893269	0.2970670333189827	T	T	T
0.8728289737980349	0.2529054176562030	0.4940082531510254	T	T	T
0.8750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.8748721726901796	0.3750903480487440	0.1977029039173971	T	T	T
0.8736973801148290	0.3759458129699403	0.3955402384082241	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4996112715626085	0.4996147903295795	0.1980305450151979	T	T	T
0.4981389862101104	0.4981415555673613	0.3984331217593378	T	T	T
0.5000000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.4996078624413384	0.6240526640803804	0.2973616741250927	T	T	T
0.5005113275318898	0.6247214736606100	0.4946032914350895	T	T	T
0.6250000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.6240515974176040	0.4996093144845565	0.2973630607842465	T	T	T
0.6247171101569285	0.5005097452131766	0.4946048708118576	T	T	T
0.6250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.6247179713627287	0.6247183871955699	0.1977613959490228	T	T	T
0.6243601074313659	0.6243609709806994	0.3961791198499120	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.4999659115789012	0.7495833990378471	0.1977088793944850	T	T	T
0.5002364607485954	0.7489427263650161	0.3960512604990477	T	T	T
0.5000000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.5004406508373744	0.8742637721731054	0.2965879935509705	T	T	T
0.5022654250761819	0.8725774863611396	0.4937538767046925	T	T	T
0.6250000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.6250014551127628	0.7495373232870486	0.2967850742358711	T	T	T
0.6255903570873422	0.7492947979572294	0.4940231840633241	T	T	T
0.6250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.6251939864408896	0.8748130167012089	0.1975996933678180	T	T	T
0.6258626271140505	0.8741372812821445	0.3957734438583049	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7495853140119804	0.4999689919340562	0.1977090868679078	T	T	T
0.7489415062450127	0.5002375211276573	0.3960542021657577	T	T	T
0.7500000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.7495370540853673	0.6250004588750009	0.2967848460196867	T	T	T
0.7492880527140379	0.6255928684179077	0.4940250238097055	T	T	T
0.8750000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.8742661645987728	0.5004431392653680	0.2965896957695753	T	T	T
0.8725733229468315	0.5022674322520767	0.4937559146679798	T	T	T
0.8750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.8748144739641974	0.6251942351120627	0.1976001315067534	T	T	T
0.8741347937572383	0.6258642694709947	0.3957737522587171	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7500077121437805	0.7500065942464449	0.1976561475439714	T	T	T
0.7499973905552838	0.7499980925055432	0.3959398719159095	T	T	T
0.7500000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.7504690322606202	0.8750044041406166	0.2967983659428660	T	T	T
0.7506858255024537	0.8743892870209647	0.4940359231644337	T	T	T
0.8750000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.8750037958342569	0.7504699431581155	0.2967984800473762	T	T	T
0.8743834820603581	0.7506890785542882	0.4940375802197201	T	T	T

0.8750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.8752885636341856	0.8752900256883567	0.1977792681607783	T	T	T
0.8756349879750606	0.8756378773254819	0.3962061231468907	T	T	T
0.1250000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.1256541717059895	0.1256549249499483	0.2990871616637744	T	T	T
0.1305181513434621	0.1304740713342504	0.4958735095703943	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1252572085530549	0.0005049318442824	0.1984964187281035	T	T	T
0.1264972718408840	0.0013205052633373	0.3992494393126095	T	T	T
0.0000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.0005063044127703	0.1252589159628744	0.1984951181274588	T	T	T
0.0013209547676820	0.1264997236197110	0.3992657662548184	T	T	T
0.0000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.0008961952294362	0.0008992711245203	0.2976962220929765	T	T	T
0.0020260502931932	0.0020407902903742	0.4947632416003687	T	T	T
0.1250000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.1248656911273594	0.3751377328386875	0.2975332605739303	T	T	T
0.1187538236072857	0.3812595312059640	0.4930695256094723	T	T	T
0.1250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.1252786796903962	0.2500191037194653	0.1987093904894753	T	T	T
0.1250210312097107	0.2508360682065843	0.4001001790732966	T	T	T
0.0000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
-0.0000170945803576	0.3751248134939313	0.1980071807765937	T	T	T
-0.0016854084601668	0.3769905660648900	0.3960713640600259	T	T	T
0.0000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.0002996386484086	0.2504015949351637	0.2972849232343147	T	T	T
0.9952202825087028	0.2559032178826463	0.4920205583722252	T	T	T
0.3750000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.3751376679704351	0.1248636833086780	0.2975232705689187	T	T	T
0.3812646411772957	0.1187575959023276	0.4930502858736651	T	T	T
0.3750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3751214189095401	-0.0000192607644843	0.1980018811897230	T	T	T
0.3769874136120205	-0.0016858456657596	0.3960647370675022	T	T	T
0.2500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.2500182394682661	0.1252771233127795	0.1987068114790604	T	T	T
0.2508391855734345	0.1250187168655589	0.4000986876419839	T	T	T
0.2500000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.2504015326168811	0.0002966176487352	0.2972841091123807	T	T	T
0.2558963753257297	0.9952289239816711	0.4920298704308034	T	T	T
0.3750000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.3743556884048780	0.3743552359039531	0.2990414211589977	T	T	T
0.3696186961891418	0.3696317443765537	0.4957834439879057	T	T	T
0.3750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.3747209100623866	0.2499754099873909	0.1986935440365279	T	T	T
0.3749914927961581	0.2491757831532937	0.4000631358828390	T	T	T
0.2500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.2499752111081888	0.3747225029304400	0.1986985132445594	T	T	T
0.2491729687072105	0.3749926129123114	0.4000724624046061	T	T	T
0.2500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.2500034763895191	0.2500033135392018	0.2992347899461257	T	T	T
0.2501328104967458	0.2501333075736423	0.4949184213277411	T	T	T
0.1250000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.1246088105668842	0.6255928587737946	0.2966515437340264	T	T	T
0.1225636834919960	0.6277294720002258	0.4928465524337790	T	T	T
0.1250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1248727024897991	0.5000177287837028	0.1980031125871245	T	T	T
0.1230088560640264	0.5016870073100581	0.3960612004796199	T	T	T
0.0000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
-0.0001578326075782	0.6253417197271240	0.1978204227777960	T	T	T
0.9989495089654493	0.6264854258586281	0.3962014437648360	T	T	T

0.0000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
-0.0006946688310703	0.5007007234059139	0.2964650478033568	T	T	T
0.9964578061429342	0.5035380401767675	0.4925383814480435	T	T	T
0.1250000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.1252985916474283	0.8757780958171983	0.2973344957009186	T	T	T
0.1259230491732194	0.8742772663435869	0.4939975996516914	T	T	T
0.1250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.1249877685168308	0.7503514443067276	0.1979454219771336	T	T	T
0.1247376988144785	0.7509603468055878	0.3965318802977463	T	T	T
0.0000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.0002415567866337	0.8754652092430971	0.1981306180617837	T	T	T
0.0006252221631427	0.8760629811357248	0.3973665201478466	T	T	T
0.0000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
-0.0000324430173536	0.7507935565148948	0.2968450524917854	T	T	T
0.9991556022964114	0.7515199597515766	0.4933471571806879	T	T	T
0.3750000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.3746920683750120	0.6242286922460152	0.2972960735135841	T	T	T
0.3740783661287785	0.6257129508247763	0.4939424794071191	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3747316273140731	0.4995027792365903	0.1984674918859177	T	T	T
0.3735042491703269	0.4986812412653798	0.3992011120246425	T	T	T
0.2500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.2499182143846327	0.6248684240251406	0.1979930151800890	T	T	T
0.2492915385978939	0.6257121545271532	0.3964459982472445	T	T	T
0.2500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.2495968196153477	0.4997100838307140	0.2972665872288436	T	T	T
0.2441140186773846	0.5047714483783330	0.4919903101376305	T	T	T
0.3750000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.3753813447344508	0.8744166568476957	0.2966476036635280	T	T	T
0.3774448160999666	0.8722613248084551	0.4928535887650222	T	T	T
0.3750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.3749955113408943	0.7496626836093377	0.1979305501332914	T	T	T
0.3752573781601875	0.7490476698013113	0.3965074031084049	T	T	T
0.2500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.2500669374911240	0.8751407560079757	0.1980004906805314	T	T	T
0.2507036290566719	0.8742919018013063	0.3964640941450620	T	T	T
0.2500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.2499911118119739	0.7500043508029651	0.2967010512118813	T	T	T
0.2500090163292006	0.7499909526773983	0.4931259129280644	T	T	T
0.6250000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.6255945525363681	0.1246095417304188	0.2966479014797970	T	T	T
0.6277315069243362	0.1225658791077982	0.4928365149453527	T	T	T
0.6250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6253408079484502	-0.0001562897592206	0.1978169903411078	T	T	T
0.6264825624430380	0.9989519980937567	0.3961963567028136	T	T	T
0.5000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.5000196552531923	0.1248717422654160	0.1979998794532432	T	T	T
0.5016855542660330	0.1230094963081148	0.3960483136031552	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.5007000774040606	-0.0006992078091554	0.2964581355351241	T	T	T
0.5035378980771347	0.9964626301878163	0.4925311228741308	T	T	T
0.6250000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.6242276495785462	0.3746933747048849	0.2972958699670979	T	T	T
0.6257081840524015	0.3740715640038376	0.4939437056768157	T	T	T
0.6250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.6248685389355726	0.2499181180258558	0.1979885853059226	T	T	T
0.6257151025198050	0.2492914179078433	0.3964372225047016	T	T	T
0.5000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.4995012098057656	0.3747365037660839	0.1984669984121316	T	T	T
0.4986820011187003	0.3735061287723910	0.3992014255984637	T	T	T

0.5000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.4997120909515295	0.2496001091181269	0.2972569494711463	T	T	T
0.5047699709527126	0.2441114576255032	0.4919737197206203	T	T	T
0.8750000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.8757864076485092	0.1253045494149098	0.2973307425550030	T	T	T
0.8742713230935888	0.1259288698603350	0.4939966091411983	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.8754645311656510	0.0002451973149190	0.1981274395734667	T	T	T
0.8760639151016389	0.0006293981773463	0.3973594108543511	T	T	T
0.7500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.7503527748205108	0.1249918073077358	0.1979444514611294	T	T	T
0.7509683238491131	0.1247407880903041	0.3965241345821748	T	T	T
0.7500000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.7507910721388462	-0.0000306663881029	0.2968395745152239	T	T	T
0.7515170690187685	0.9991581864470054	0.4933344651334756	T	T	T
0.8750000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.8744180588663424	0.3753850681955470	0.2966487721636780	T	T	T
0.8722589856958826	0.3774471450401364	0.4928534067997987	T	T	T
0.8750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.8751435248374101	0.2500717914788015	0.1979971803487678	T	T	T
0.8742950507708865	0.2507064908794687	0.3964585337621776	T	T	T
0.7500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.7496635849836309	0.3750008610098166	0.1979303349427226	T	T	T
0.7490461119703729	0.3752601979982710	0.3965077424051425	T	T	T
0.7500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.7500057688633347	0.2499973138376426	0.2966947532304112	T	T	T
0.7499889166489249	0.2500105330029141	0.4931171186174603	T	T	T
0.6250000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.6245154148694982	0.6245152364403281	0.2969777069410725	T	T	T
0.6244074179137216	0.6244107997285070	0.4934383093539145	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.6245428549931185	0.4997509652525945	0.1981020613298772	T	T	T
0.6239320503832344	0.4993722873757720	0.3973263167649258	T	T	T
0.5000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.4997485366323613	0.6245429531897299	0.1981030787086961	T	T	T
0.4993743046217284	0.6239332708784311	0.3973240007265604	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.4991068161086460	0.4991099377344299	0.2976482026114425	T	T	T
0.4979653715171667	0.4979629504202828	0.4947158753472269	T	T	T
0.6250000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.6254693750807732	0.8745345205686392	0.2966368202590096	T	T	T
0.6264952363734877	0.8734960680362841	0.4930793506224601	T	T	T
0.6250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.6249887194282671	0.7497496594452708	0.1978668606867506	T	T	T
0.6251611445939798	0.7492743182423817	0.3965115263062894	T	T	T
0.5000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.5001521366357328	0.8746655278955694	0.1978094768294034	T	T	T
0.5010447550403595	0.8735207351173572	0.3961837672580053	T	T	T
0.5000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.5000260767196605	0.7492118265486977	0.2968163935028790	T	T	T
0.5008365352684552	0.7484654932228361	0.4933033789411027	T	T	T
0.8750000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.8745342784008552	0.6254704134649023	0.2966345856485177	T	T	T
0.8734896779673078	0.6265000428242478	0.4930771230540503	T	T	T
0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8746697371990392	0.5001544847594466	0.1978096356487756	T	T	T
0.8735193374052386	0.5010480340921105	0.3961859599449639	T	T	T
0.7500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.7497500553752973	0.6249891503135065	0.1978682213988579	T	T	T
0.7492700239211327	0.6251606914769224	0.3965111660544937	T	T	T

0.7500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.7492131324085394	0.5000279100311339	0.2968180216754203	T	T	T
0.7484621546492874	0.5008370252290568	0.4933085027794548	T	T	T
0.8750000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.8754865395392173	0.8754907098013953	0.2970002796027031	T	T	T
0.8755734365653358	0.8755765474710266	0.4934642371075333	T	T	T
0.8750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.8750160880210381	0.7502665915523670	0.1978783761490831	T	T	T
0.8748364268816828	0.7507265107965380	0.3965223158216942	T	T	T
0.7500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.7502663177299603	0.8750155019603704	0.1978799207292533	T	T	T
0.7507234848862313	0.8748365833345970	0.3965200299664779	T	T	T
0.7500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.7500027394906222	0.7500013327452946	0.2967185557201175	T	T	T
0.7499884415643977	0.7499930013607771	0.4932217636490057	T	T	T
0.0752774226876268	0.1596999792008693	0.5735718781333091	T	T	T
0.1594530239765888	0.0751806794149148	0.5736155734605181	T	T	T
0.2077954217840038	0.2921798635101754	0.5736999138789015	T	T	T
0.2921131384901763	0.2076792857415584	0.5736873793870434	T	T	T
0.3404006495166994	0.4247125773686636	0.5735443868573384	T	T	T
0.4246642455511710	0.3402761646125579	0.5735242303057353	T	T	T
0.1215259520841206	0.1215442273008027	0.5515172574913925	T	T	T
0.2500025719025627	0.2499977209019081	0.5509068178199521	T	T	T
0.3784578719798732	0.3784364632226406	0.5514418464243517	T	T	T

T3-pbc-4CO2 (-2544.9525 eV)

1.0000000000000000

19.2439999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.2439999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 24.4329999999999998

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Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0003959884011571	0.0003960102893893	0.1979296045101585	T	T	T
0.0018584306583875	0.0018613909813444	0.3980776112982855	T	T	T
0.0000000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.0007794689343068	0.1255762447566011	0.2977239936502731	T	T	T
0.9927298338453556	0.1279299884730163	0.4986328118806262	T	T	T
0.1250000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.1255757831748987	0.0007801612977193	0.2977221046911054	T	T	T
0.1279178727399733	0.9927331922507939	0.4986348695784928	T	T	T
0.1250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.1253871210731404	0.1253870265742699	0.1981601373412675	T	T	T
0.1269606047192979	0.1269608864221082	0.3974367188529897	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0003471932892749	0.2502074532909194	0.1979382700137112	T	T	T
0.0003589807096780	0.2512021707535709	0.3968277593318121	T	T	T
0.0000000000000000	0.3750000000000000	0.0984529120451825	F	F	F
-0.0000641929493717	0.3755383350947897	0.2970365219782229	T	T	T
0.9950107297781871	0.3802474176919178	0.4930876067994953	T	T	T
0.1250000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.1253838159240315	0.2508011479707475	0.2981894647339034	T	T	T
0.1122814423844870	0.2612945148968391	0.5051887354934419	T	T	T
0.1250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.1251386810281756	0.3751171990193760	0.1980628648670327	T	T	T
0.1244954353328355	0.3759915774856817	0.3974888933883151	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F

0.2502076544626474	0.0003457757465968	0.1979386146260033	T	T	T
0.2511992007365338	0.0003591425282991	0.3968291102838598	T	T	T
0.2500000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.2508011690915138	0.1253826316950541	0.2981899030690031	T	T	T
0.2612969219994377	0.1122858741146942	0.5051741352504764	T	T	T
0.3750000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.3755363262164796	0.9999349290163734	0.2970374663234404	T	T	T
0.3802450056858702	0.9950133327711698	0.4930892204204028	T	T	T
0.3750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.3751176396774498	0.1251375879026745	0.1980632978965617	T	T	T
0.3759939582405584	0.1244944191231356	0.3974859978902341	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2501824035202767	0.2501816479981269	0.1983662769937494	T	T	T
0.2505906138804512	0.2505900237706852	0.3988541719474575	T	T	T
0.2500000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.2498132742988558	0.3752032680366608	0.2985691973250728	T	T	T
0.2380241338540211	0.3869699126135208	0.5053179375465553	T	T	T
0.3750000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.3752021710293576	0.2498136050425721	0.2985681148362828	T	T	T
0.3869714568085317	0.2380210679633275	0.5053127032395300	T	T	T
0.3750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.3748218549759076	0.3748215114747704	0.1983582470535872	T	T	T
0.3744617486397437	0.3744612278919988	0.3988123137684330	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
-0.0001228517355414	0.5001449549325088	0.1976437584085490	T	T	T
-0.0015371649118715	0.5015820535331171	0.3951333822690469	T	T	T
0.0000000000000000	0.6250000000000000	0.0984529120451825	F	F	F
-0.0006753209918761	0.6256757724216425	0.2964224488221740	T	T	T
0.9973600477834331	0.6276439333182353	0.4936001074461996	T	T	T
0.1250000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.1246105489761349	0.5003953600765794	0.2972107862475403	T	T	T
0.1192408757524594	0.5057729699295155	0.4933555382116699	T	T	T
0.1250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.1248534610714070	0.6251297279139758	0.1976416263407456	T	T	T
0.1234179825935845	0.6265445420748523	0.3951295065065621	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
-0.0000900991707019	0.7503641564780353	0.1976089808428007	T	T	T
-0.0006536980243877	0.7511233105278692	0.3957256088694437	T	T	T
0.0000000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.0002348726920111	0.8759520743902856	0.2971340663898957	T	T	T
0.9991127241975438	0.8754609091532212	0.4943179476360711	T	T	T
0.1250000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.1246785804599565	0.7507203721975975	0.2965436406935159	T	T	T
0.1231069844872805	0.7518789496864381	0.4937882586257444	T	T	T
0.1250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.1251041882766613	0.8754643681636961	0.1977460702866824	T	T	T
0.1253097650060511	0.8758245981444898	0.3960705175327950	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2498786173731986	0.4998680278539708	0.1980595259170005	T	T	T
0.2490056447952462	0.5005334526980408	0.3974645555774032	T	T	T
0.2500000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.2494538536741974	0.6250832015704200	0.2970253825748158	T	T	T
0.2447752032881973	0.6299706774083182	0.4930743513608171	T	T	T
0.3750000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.3742049879824888	0.4996362562217436	0.2981684675212711	T	T	T
0.3637126501250109	0.5126421539037860	0.5051189459210977	T	T	T
0.3750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.3747901936424544	0.6246609554110083	0.1979294382216190	T	T	T
0.3738060050294976	0.6246521891947763	0.3968018345003175	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F

0.2499316979333939	0.7500626546520754	0.1976363184021570	T	T	T
0.2493571223912170	0.7507239473042518	0.3952222634673910	T	T	T
0.2500000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.2502204327466607	0.8754420088866540	0.2967876464848771	T	T	T
0.2519287692534940	0.8739089352115087	0.4936624496909852	T	T	T
0.3750000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.3747766164310675	0.7495626087353200	0.2967789892040599	T	T	T
0.3730723559304244	0.7510800272703667	0.4936472694197209	T	T	T
0.3750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.3750543095757468	0.8749475458260032	0.1976349378047267	T	T	T
0.3756379465034962	0.8742797370270666	0.3952249500933794	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5001453429367754	0.9998762756271494	0.1976446600198219	T	T	T
0.5015796188679782	-0.0015362052538645	0.3951336120858531	T	T	T
0.5000000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.5003961251770739	0.1246110299749195	0.2972087548136850	T	T	T
0.5057740007114334	0.1192415011245178	0.4933535170478208	T	T	T
0.6250000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.6256750301899087	-0.0006749595914677	0.2964227751892147	T	T	T
0.6276419477511557	0.9973593444316177	0.4935993192839247	T	T	T
0.6250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.6251300669996362	0.1248532944632506	0.1976407447778714	T	T	T
0.6265450599693549	0.1234178076010842	0.3951269526306728	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4998686870038404	0.2498789619446963	0.1980593869404041	T	T	T
0.5005338556139959	0.2490053506099340	0.3974616378233223	T	T	T
0.5000000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.4996373334813935	0.3742046991735153	0.2981681178620901	T	T	T
0.5126436584298187	0.3637099933289832	0.5051183571584341	T	T	T
0.6250000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.6250847279338749	0.2494545026959489	0.2970247687322424	T	T	T
0.6299721217574854	0.2447764962595520	0.4930708122885977	T	T	T
0.6250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.6246606821114846	0.3747912886351154	0.1979302032955974	T	T	T
0.6246535716924775	0.3738055831004065	0.3968018099354363	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7503632047506184	-0.0000900881411736	0.1976088887513842	T	T	T
0.7511226660746576	0.9993448189008656	0.3957242947684042	T	T	T
0.7500000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.7507203174204891	0.1246785545792296	0.2965410631174342	T	T	T
0.7518738795723419	0.1231060731493501	0.4937872028179522	T	T	T
0.8750000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.8759522415528311	0.0002350861085205	0.2971337390193033	T	T	T
0.8754612178618114	0.9991137368952655	0.4943178711201345	T	T	T
0.8750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.8754650419766203	0.1251047931267034	0.1977459446740092	T	T	T
0.8758204888610908	0.1253111205741275	0.3960706702172361	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7500630986937078	0.2499329891509862	0.1976357807573745	T	T	T
0.7507245464444098	0.2493575299111402	0.3952206248042674	T	T	T
0.7500000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.7495634869907885	0.3747777276274609	0.2967785206947229	T	T	T
0.7510793786232471	0.3730745309589632	0.4936463296359636	T	T	T
0.8750000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.8754432870489915	0.2502208435253703	0.2967868925127345	T	T	T
0.8739057074277033	0.2519328061632041	0.4936603900740920	T	T	T
0.8750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.8749484013087028	0.3750545426434351	0.1976345984505284	T	T	T
0.8742789046376774	0.3756389737398216	0.3952238968895562	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F

0.4996168058248961	0.4996171324712919	0.1981501698817057	T	T	T
0.4980654952526490	0.4980640482519947	0.3973784220505032	T	T	T
0.5000000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.4994238146269855	0.6242356344025225	0.2976966908927596	T	T	T
0.4970622465424773	0.6322334045798956	0.4986031081138807	T	T	T
0.6250000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.6242353893697542	0.4994249357100993	0.2976965103781553	T	T	T
0.6322330233986871	0.4970624637498891	0.4986034028971104	T	T	T
0.6250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.6246060857832609	0.6246068296497426	0.1979174710047288	T	T	T
0.6231414174914026	0.6231426334975555	0.3980577339969585	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.4998938159567978	0.7495425465037904	0.1977402138135548	T	T	T
0.4996851767154000	0.7491767677296758	0.3960587225720737	T	T	T
0.5000000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.5003185212667862	0.8742886399621422	0.2965394457137311	T	T	T
0.5018935013248522	0.8731183092773893	0.4937903367031448	T	T	T
0.6250000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.6247606502456586	0.7490403624357926	0.2971234131749054	T	T	T
0.6258722132560132	0.7495196347466587	0.4943073317699017	T	T	T
0.6250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.6250895489225036	0.8746360148935012	0.1976037943693497	T	T	T
0.6256450281796854	0.8738760778710892	0.3957244128925838	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7495419848569514	0.4998941287807439	0.1977398390281440	T	T	T
0.7491751350727318	0.4996873273292851	0.3960576894504071	T	T	T
0.7500000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.7490405448042015	0.6247622499148850	0.2971220053233840	T	T	T
0.7495191363485932	0.6258751180659266	0.4943051402820576	T	T	T
0.8750000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.8742881333169494	0.5003193981715831	0.2965390686325554	T	T	T
0.8731163646126412	0.5018956952877559	0.4937882085197594	T	T	T
0.8750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.8746369337815212	0.6250904899581460	0.1976029908818225	T	T	T
0.8738749614242921	0.6256492096898549	0.3957238791437041	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7498150807772550	0.7498160252650620	0.1976766636581180	T	T	T
0.7495602701660836	0.7495632259545622	0.3958957512697825	T	T	T
0.7500000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.7502617903746451	0.8747321511378287	0.2966811951824842	T	T	T
0.7507242858630443	0.8742628328303605	0.4938733618165670	T	T	T
0.8750000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.8747320316270003	0.7502638381491716	0.2966810743738514	T	T	T
0.8742610587220152	0.7507274089845037	0.4938737042310709	T	T	T
0.8750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.8751764944675413	0.8751777130060545	0.1976769942340111	T	T	T
0.8754221313984302	0.8754232196175744	0.3959020818423980	T	T	T
0.1250000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.1258562294262736	0.1258571539919332	0.2990482066527692	T	T	T
0.1314496588711444	0.1314348632899667	0.4962174792707702	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1252791118256652	0.0006072749049620	0.1984343666332527	T	T	T
0.1264328582782350	0.0016933129774451	0.3990401508990428	T	T	T
0.0000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.0006074594276950	0.1252793821242632	0.1984362184493871	T	T	T
0.0016895572168799	0.1264376557089494	0.3990417618398423	T	T	T
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0.0009099938996962	0.0009108552472425	0.2975038305365529	T	T	T
0.0020045999871788	0.0020102105335774	0.4943964802205081	T	T	T
0.1250000000000000	0.3750000000000000	0.0984529120451825	F	F	F

0.1251351978328928	0.3752611535637635	0.2976132285219522	T	T	T
0.1188404143138368	0.3815146670007618	0.4931543206649726	T	T	T
0.1250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.1254599201373439	0.2501053615082264	0.1987486735132403	T	T	T
0.1255267120160652	0.2510186216980689	0.4003031591857085	T	T	T
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0.0001291861887820	0.3751347038968704	0.1979863515550414	T	T	T
-0.0012639099122432	0.3769720342626162	0.3959387773400575	T	T	T
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0.0006332270341901	0.2504053568047625	0.2971777860143606	T	T	T
0.9956329562528898	0.2556032405341436	0.4917760365951560	T	T	T
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0.3752613383268730	0.1251352701468222	0.2976121360235846	T	T	T
0.3815121280685801	0.1188389521725489	0.4931504270332616	T	T	T
0.3750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3751353014305215	0.0001275760039011	0.1979873738518755	T	T	T
0.3769690227669159	-0.0012650765517379	0.3959411227138963	T	T	T
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0.2501052096284589	0.1254591618494734	0.1987500318994667	T	T	T
0.2510200835020201	0.1255246599983856	0.4003020933182495	T	T	T
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0.2504042318797526	0.0006320498566328	0.2971780276211405	T	T	T
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0.3747135401955867	0.3747130919479666	0.2993987882204901	T	T	T
0.3722610622995626	0.3722732958969641	0.4951389174799691	T	T	T
0.3750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.3748545799679411	0.2501404187064357	0.1988527773708885	T	T	T
0.3756600504682579	0.2493807046742169	0.4004938735344264	T	T	T
0.2500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.2501406969024761	0.3748536965964531	0.1988531598622162	T	T	T
0.2493806422556097	0.3756594197754601	0.4004945472769674	T	T	T
0.2500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.2502970517270214	0.2502975246340134	0.2994320289544887	T	T	T
0.2532847401270746	0.2532639852313698	0.4952023152871293	T	T	T
0.1250000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.1243075592812980	0.6256591853357578	0.2964507351849957	T	T	T
0.1214096877747603	0.6284850590146450	0.4925063312823343	T	T	T
0.1250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1249720669390196	0.5000251609397681	0.1980687463810395	T	T	T
0.1231039000291787	0.5018989371435952	0.3962489116639324	T	T	T
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-0.0002775065533285	0.6252752848845750	0.1977799178722354	T	T	T
0.9985097060143184	0.6264867150380926	0.3959942696828805	T	T	T
0.0000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
-0.0006452611931041	0.5006789620131861	0.2964528491100167	T	T	T
0.9965115710366781	0.5035943734378400	0.4925109716495931	T	T	T
0.1250000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.1251375984655594	0.8759763583415496	0.2970932221400151	T	T	T
0.1251928417062018	0.8748375336077461	0.4936111818558561	T	T	T
0.1250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.1248857955030604	0.7503838570734856	0.1978549810979197	T	T	T
0.1241492372164810	0.7513757461867011	0.3961335669832364	T	T	T
0.0000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.0001694634952293	0.8754407389867884	0.1980411132379728	T	T	T
0.0003520474741219	0.8761224032256647	0.3970442915612582	T	T	T
0.0000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
-0.0002987567704472	0.7507650850403912	0.2966469535345275	T	T	T
0.9985697248278681	0.7518075524505959	0.4930299230647347	T	T	T
0.3750000000000000	0.6250000000000000	0.0984529120451825	F	F	F

0.3745870713485226	0.6243795652610618	0.2971525585930915	T	T	T
0.3694066849111178	0.6293413254415883	0.4917477191107520	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3749000702264658	0.4995438831344534	0.1987295860939995	T	T	T
0.3739898448864635	0.4995162207933993	0.4002258524895355	T	T	T
0.2500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.2498585522249766	0.6248808003711486	0.1979720164032509	T	T	T
0.2480260993419318	0.6262814131766793	0.3959212401745089	T	T	T
0.2500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.2497332908359754	0.4998844521072836	0.2975842544335968	T	T	T
0.2434953218689050	0.5061598759696421	0.4931280586778258	T	T	T
0.3750000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.3752721828607735	0.8747151602938926	0.2964607248134172	T	T	T
0.3766925022386655	0.8732522933948647	0.4925376727643651	T	T	T
0.3750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.3749776018105569	0.7497417729703140	0.1979129459796485	T	T	T
0.3747066923399453	0.7500856257353290	0.3960630505643135	T	T	T
0.2500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.2500148753774482	0.8752744616584521	0.1979141599231089	T	T	T
0.2502826313573184	0.8749329798156290	0.3960790447931413	T	T	T
0.2500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.2497197313562552	0.7502993377509420	0.2964630200934495	T	T	T
0.2483086305012085	0.7517445535133596	0.4925312768242007	T	T	T
0.6250000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.6256606216333629	0.1243075303329654	0.2964482960444866	T	T	T
0.6284853366416847	0.1214093857074116	0.4925092172933778	T	T	T
0.6250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6252756871798505	-0.0002792495409024	0.1977816358342416	T	T	T
0.6264864283546002	0.9985108064732500	0.3959931069938393	T	T	T
0.5000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.5000264553278888	0.1249714614971967	0.1980684492903676	T	T	T
0.5019024268620127	0.1231041725923362	0.3962467000289431	T	T	T
0.5000000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.5006779838198787	-0.0006439823563175	0.2964535049583568	T	T	T
0.5035930746240648	0.9965129860470361	0.4925101279285131	T	T	T
0.6250000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.6243805355724100	0.3745888320328949	0.2971528683360667	T	T	T
0.6293403609409215	0.3694061236402774	0.4917473308214783	T	T	T
0.6250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.6248817559712432	0.2498603112980268	0.1979727661116862	T	T	T
0.6262842646509426	0.2480250700709272	0.3959187948087926	T	T	T
0.5000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.4995449862784159	0.3749000223443658	0.1987293875549598	T	T	T
0.4995169141432248	0.3739878179020699	0.4002292873408761	T	T	T
0.5000000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.4998848190815410	0.2497340834162801	0.2975841864722794	T	T	T
0.5061637570039601	0.2434942408082489	0.4931227012553224	T	T	T
0.8750000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.8759742233096394	0.1251381343500536	0.2970933849032465	T	T	T
0.8748445860735600	0.1251966058809310	0.4936070048525777	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.8754405058965836	0.0001708836116200	0.1980414600779511	T	T	T
0.8761209239973045	0.0003519439976667	0.3970461773051572	T	T	T
0.7500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.7503838682499887	0.1248861183544517	0.1978538228702268	T	T	T
0.7513705406016894	0.1241479196271249	0.3961318114075155	T	T	T
0.7500000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.7507668262633755	-0.0002982027767924	0.2966465352542095	T	T	T
0.7518063342142899	0.9985712065810323	0.4930299765952825	T	T	T
0.8750000000000000	0.3750000000000000	0.0984529120451825	F	F	F

0.8747161544094486	0.3752724700529905	0.2964600121701247	T	T	T
0.8732499033721018	0.3766918251808624	0.4925381992615958	T	T	T
0.8750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.8752757285025562	0.2500154423960734	0.1979144460197556	T	T	T
0.8749315659266095	0.2502846562685959	0.3960787051204182	T	T	T
0.7500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.7497405516596503	0.3749778548162996	0.1979123910094719	T	T	T
0.7500866396590909	0.3747076725133494	0.3960619490683713	T	T	T
0.7500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.7503028594299362	0.2497199407302018	0.2964620253228117	T	T	T
0.7517437562231551	0.2483090453832996	0.4925302276056784	T	T	T
0.6250000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.6240833004915318	0.6240841753738821	0.2974890220679109	T	T	T
0.6229982673288439	0.6229981400165755	0.4943830600688170	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.6243988719639909	0.4997234466392065	0.1984221369788043	T	T	T
0.6233371694997430	0.4985765945876489	0.3990159443673545	T	T	T
0.5000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.4997226912417371	0.6243997635282590	0.1984202497833260	T	T	T
0.4985755897593774	0.6233378267742287	0.3990120247264750	T	T	T
0.5000000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.4991548753959806	0.4991533123953185	0.2990151842990850	T	T	T
0.4937281931636243	0.4937324596225494	0.4961298932263313	T	T	T
0.6250000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.6252956020666797	0.8742153712471775	0.2966471211872369	T	T	T
0.6264183939489748	0.8731810862691708	0.4930344670601606	T	T	T
0.6250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.6248255225199808	0.7495566392662643	0.1980292862312755	T	T	T
0.6246364627714938	0.7488850889341507	0.3970355733051762	T	T	T
0.5000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.5001049535723475	0.8746259496614067	0.1978567622901057	T	T	T
0.5008361473680664	0.8736295690537157	0.3961386582002673	T	T	T
0.5000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.4998539695740733	0.7490510631045605	0.2970772261640569	T	T	T
0.4997917382625707	0.7501430893416779	0.4936018553643243	T	T	T
0.8750000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.8742159215802860	0.6252977612161507	0.2966461848747456	T	T	T
0.8731799807879739	0.6264204037534340	0.4930319444503276	T	T	T
0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8746257373664699	0.5001045983164811	0.1978569958866005	T	T	T
0.8736280149496495	0.5008366692907444	0.3961375226355816	T	T	T
0.7500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.7495565583717241	0.6248258076079618	0.1980265252391939	T	T	T
0.7488837340382549	0.6246400306479928	0.3970337860350109	T	T	T
0.7500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.7490498750814122	0.4998546047880313	0.2970763326310578	T	T	T
0.7501417325388604	0.4997933128408545	0.4936008075216444	T	T	T
0.8750000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.8753101910489748	0.8753115907590183	0.2968502165291427	T	T	T
0.8753844848198552	0.8753882607704259	0.4932241158886321	T	T	T
0.8750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.8748556994624158	0.7501412392580731	0.1978680310843785	T	T	T
0.8744454562731226	0.7505363123351890	0.3964124519609131	T	T	T
0.7500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.7501380878720745	0.8748565519597654	0.1978677678031482	T	T	T
0.7505326408921095	0.8744479406532508	0.3964116922231368	T	T	T
0.7500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.7496832179135464	0.7496845145798271	0.2968457409941148	T	T	T
0.7496110939946883	0.7496141646054535	0.4932319187830079	T	T	T
0.0743173153319744	0.1586729512552346	0.5735636860251153	T	T	T

0.1585403131869414	0.0742556596331818	0.5735901893916269	T	T	T
0.2051605829337296	0.2895630308895173	0.5737025145140040	T	T	T
0.2895096356548201	0.2051072635648564	0.5737140839078017	T	T	T
0.3351941440158800	0.4195960258960806	0.5736987298701359	T	T	T
0.4195581918115620	0.3351299497069120	0.5736895726034679	T	T	T
0.4662346691447479	0.5505635285340076	0.5735580925482056	T	T	T
0.5505452606198276	0.4662028331418416	0.5735544601377537	T	T	T
0.1211807912579602	0.1212094954121768	0.5517050751047284	T	T	T
0.2491527525378401	0.2491359472863385	0.5510777650255320	T	T	T
0.3758122264491645	0.3758111000612004	0.5510494340301819	T	T	T
0.5037487160204497	0.5037439892683120	0.5516624330584761	T	T	T

T3-pbc-8CO2 (-2641.8273 eV)

1.0000000000000000

19.243999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.243999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 24.432999999999998

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Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0000009331964887	0.0000031086956055	0.1980671272489019	T	T	T
-0.0000187868774562	-0.0000147272213604	0.3981514578812845	T	T	T
0.0000000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.0001178710839037	0.1248698565854634	0.2979329982714338	T	T	T
0.9891381642275097	0.1358623958640001	0.5044204585398163	T	T	T
0.1250000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.1248644263714666	0.0001182343361889	0.2979329879673707	T	T	T
0.1358560275036030	0.9891387531226645	0.5044294561513925	T	T	T
0.1250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.1250004794030987	0.1250013613984033	0.1980727261670243	T	T	T
0.1249932876395664	0.1249963316287170	0.3981544504312964	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0002387923912994	0.2497591137650999	0.1977029729720773	T	T	T
0.0001463743957924	0.2498533296079148	0.3964030567543524	T	T	T
0.0000000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.0002841935333093	0.3747186738152841	0.2963159201456204	T	T	T
0.9969777583265097	0.3780363479663170	0.4922279114281614	T	T	T
0.1250000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.1251308887490390	0.2498790883472232	0.2979394380672396	T	T	T
0.1141349134418665	0.2608740711477841	0.5044300998747769	T	T	T
0.1250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.1252388573641003	0.3747632344843209	0.1976975007878519	T	T	T
0.1251516636207331	0.3748588318628801	0.3964086903887721	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2497557428213711	0.0002380182147423	0.1977029706787746	T	T	T
0.2498455980455575	0.0001453821153534	0.3964037299785595	T	T	T
0.2500000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.2498765064557521	0.1251301304677116	0.2979394931044519	T	T	T
0.2608652300240955	0.1141365843128868	0.5044248354457594	T	T	T
0.3750000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.3747124990283246	0.0002823763366226	0.2963139476758000	T	T	T
0.3780313142567737	0.9969791369803980	0.4922266855095881	T	T	T
0.3750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.3747606932389470	0.1252360711288493	0.1976969275408477	T	T	T
0.3748521695973358	0.1251528447287726	0.3964061736693955	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2499978193061104	0.2499973855689575	0.1980676071389653	T	T	T

0.2500135777719525	0.2500154511091960	0.3981597822977236	T	T	T
0.2500000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.2501272365732325	0.3748757207502886	0.2979262745124126	T	T	T
0.2391438368240965	0.3858666328022240	0.5044071612261034	T	T	T
0.3750000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.3748745701524570	0.2501261999564945	0.2979243529169402	T	T	T
0.3858618008705320	0.2391401689121936	0.5044101834605762	T	T	T
0.3750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.3749998363003034	0.3749999537918034	0.1980621407310206	T	T	T
0.3750167014992491	0.3750172519318013	0.3981164804704539	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0000092243985348	0.4999922934080897	0.1973469141679215	T	T	T
0.0000077697880410	0.4999956393340838	0.3936564183488452	T	T	T
0.0000000000000000	0.6250000000000000	0.0984529120451825	F	F	F
-0.0002655205679899	0.6252709741462474	0.2962992873951949	T	T	T
0.0029995874694146	0.6219781488098812	0.4922069255464020	T	T	T
0.1250000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.1252771428139692	0.4997252947806146	0.2963102179872408	T	T	T
0.1219754815080607	0.5030236045668327	0.4922248579488218	T	T	T
0.1250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.1249997583589277	0.6250010882066503	0.1973379431025532	T	T	T
0.1249970550119490	0.6250010122960127	0.3936597930458310	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
-0.0002313987554764	0.7502374573929563	0.1976927562339500	T	T	T
-0.0001438212729240	0.7501483167305362	0.3963750838761311	T	T	T
0.0000000000000000	0.8750000000000000	0.0984529120451825	F	F	F
-0.0001285564934025	0.8751258712041418	0.2979203091280876	T	T	T
0.0108552298625869	0.8641521910875480	0.5044094041317231	T	T	T
0.1250000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.1247250658676172	0.7502746474821554	0.2963063103649279	T	T	T
0.1280139180839061	0.7469743924977299	0.4922231333347441	T	T	T
0.1250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.1247616624066116	0.8752348364673941	0.1976965496590637	T	T	T
0.1248443659902998	0.8751417633565407	0.3964067613355119	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2502337753479594	0.4997662322168921	0.1976930078756563	T	T	T
0.2501417821611910	0.4998568088937859	0.3963748935358943	T	T	T
0.2500000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.2502606876353129	0.6247371332904709	0.2962945208766670	T	T	T
0.2469899058827703	0.6280196074214950	0.4922026616355480	T	T	T
0.3750000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.3751200419985898	0.4998806789025058	0.2978962820757899	T	T	T
0.3641616655130070	0.5108494416854147	0.5043461258718418	T	T	T
0.3750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.375222528925180	0.6247723272688943	0.1976795754525683	T	T	T
0.3751347270990720	0.6248657430470980	0.3963420841881553	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2499889816282297	0.7500080605392213	0.1973357405162752	T	T	T
0.2499881369040191	0.7500072947987511	0.3936567744691752	T	T	T
0.2500000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.2497134347892898	0.8752760375325781	0.2963112464950332	T	T	T
0.2530219341110899	0.8719720312288002	0.4922270946384140	T	T	T
0.3750000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.3752481598951542	0.7497421204500189	0.2962818897517697	T	T	T
0.3719943892871030	0.7530134856222659	0.4921862998311043	T	T	T
0.3750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.3749887786535469	0.8750067460038212	0.1973391751260988	T	T	T
0.3749856670798604	0.8750103160083937	0.3936540618962824	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.4999889893388586	0.0000076047222313	0.1973455795977715	T	T	T

0.4999884930479926	0.0000097762692091	0.3936513190955846	T	T	T
0.5000000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.4997206198244604	0.1252763718045538	0.2963071708706696	T	T	T
0.5030205348168070	0.1219786890749161	0.4922198734269015	T	T	T
0.6250000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.6252670221030220	-0.0002641570134997	0.2962954299500823	T	T	T
0.6219728774609372	0.0030060317708360	0.4922031408894844	T	T	T
0.6250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.6249987427699644	0.1250007320979409	0.1973360092870916	T	T	T
0.6249964413373362	0.1250009012742496	0.3936531278868788	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4997656432670332	0.2502326702518408	0.1976917084082836	T	T	T
0.4998526763768393	0.2501415316838859	0.3963709679375436	T	T	T
0.5000000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.4998793924176828	0.3751211198562940	0.2978941378688788	T	T	T
0.5108458928091150	0.3641569715377862	0.5043346931394505	T	T	T
0.6250000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.6247351585861276	0.2502637896327751	0.2962904880909156	T	T	T
0.6280176953755575	0.2469900546760032	0.4921993188119972	T	T	T
0.6250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.6247718738522379	0.3752248394342760	0.1976786550246827	T	T	T
0.6248661777816463	0.3751352828747522	0.3963380123938773	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7502347095287450	-0.0002280919854455	0.1976913902311181	T	T	T
0.7501441700636640	-0.0001374931295625	0.3963701500326914	T	T	T
0.7500000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.7502730522677864	0.1247313400459082	0.2963015623480973	T	T	T
0.7469694584690411	0.1280173493608666	0.4922159042384187	T	T	T
0.8750000000000000	0.0000000000000000	0.0984529120451825	F	F	F
0.8751226427666896	-0.0001240485122925	0.2979171925350748	T	T	T
0.8641497896451079	0.0108665680470152	0.5044073441214023	T	T	T
0.8750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.8752352191116969	0.1247666845341494	0.1976950130456123	T	T	T
0.8751399353372548	0.1248513120073243	0.3964011252628670	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7500080541474671	0.2499935977714225	0.1973343882676011	T	T	T
0.7500062127744593	0.2499926490395265	0.3936523242134029	T	T	T
0.7500000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.7497426155469930	0.3752533410422434	0.2962803909834999	T	T	T
0.7530116851338060	0.3719970282983365	0.4921855466055957	T	T	T
0.8750000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.8752764613065023	0.2497200727860599	0.2963084142797012	T	T	T
0.8719695847509945	0.2530275434295649	0.4922234040794058	T	T	T
0.8750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.8750087852895959	0.3749926809843027	0.1973382220970601	T	T	T
0.8750097397563991	0.3749922424563516	0.3936539043078478	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4999949219613088	0.4999969103014643	0.1980430996033989	T	T	T
0.5000117976719642	0.5000136466337666	0.3980627743310813	T	T	T
0.5000000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.5001131478744804	0.6248851980179970	0.2978777701924669	T	T	T
0.4891591748378266	0.6358385006736383	0.5042953089309508	T	T	T
0.6250000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.6248834870276166	0.5001164015861864	0.2978785285435531	T	T	T
0.6358351482674179	0.4891566397974934	0.5042887013295309	T	T	T
0.6250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.6250001973812050	0.6250015827989692	0.1980443816490064	T	T	T
0.6249964317450610	0.6249997981742134	0.3980466365246805	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.5002200385852156	0.7497763184958398	0.1976786032947120	T	T	T

0.5001311499280996	0.7498657286677123	0.3963272559842397	T	T	T
0.5000000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.5002562461204335	0.8747417224680779	0.2962850779811421	T	T	T
0.4969900215946618	0.8780102793919695	0.4921892177388026	T	T	T
0.6250000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.6251135624885038	0.7498848574565682	0.2978833762581103	T	T	T
0.6141552059948161	0.7608444999930467	0.5042972324687908	T	T	T
0.6250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.6252278380135817	0.8747746333656037	0.1976807084541808	T	T	T
0.6251350753987458	0.8748618131030492	0.3963445848181419	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7497763087144019	0.5002223334235700	0.1976782656587955	T	T	T
0.7498638975266940	0.5001355565839976	0.3963274102345515	T	T	T
0.7500000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.7498825093262741	0.6251164287553720	0.2978829885035454	T	T	T
0.7608346748232324	0.6141585282059076	0.5043035472040859	T	T	T
0.8750000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.8747421856844143	0.5002616528305700	0.2962864606356996	T	T	T
0.8780061497063689	0.4969948606283362	0.4921903261847247	T	T	T
0.8750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.8747742679560430	0.6252298763456057	0.1976809556140525	T	T	T
0.8748563710753640	0.6251424473232760	0.3963487170466546	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7500044569852482	0.7500052752066982	0.1980478216539051	T	T	T
0.7499849790209412	0.7499902062962766	0.3980660597000760	T	T	T
0.7500000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.7501183529205213	0.8748842702925089	0.2978961384038907	T	T	T
0.7391532983206257	0.8858584887010500	0.5043393816808188	T	T	T
0.8750000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.8748802170579204	0.7501225370617817	0.2978974711806373	T	T	T
0.8858473259144577	0.7391576519136835	0.5043498046750438	T	T	T
0.8750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.8749975958006598	0.8749999273644974	0.1980622727253697	T	T	T
0.8749854914202984	0.8749904433182919	0.3981149765965440	T	T	T
0.1250000000000000	0.1250000000000000	0.0984529120451825	F	F	F
0.1249962559811354	0.1249981367272718	0.2991146300436970	T	T	T
0.1249687065341137	0.1249729605654772	0.4948828961758578	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1246847272646993	0.0003099962895461	0.1987000330628715	T	T	T
0.1248701940694704	0.0001042696610011	0.4002016779689755	T	T	T
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0.0001009088477413	0.1248791047897777	0.4002026984651288	T	T	T
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0.1250000000000000	0.3750000000000000	0.0984529120451825	F	F	F
0.1255138435517296	0.3744934314425073	0.2970904773568994	T	T	T
0.1203188160451750	0.3796958955768496	0.4920816898151072	T	T	T
0.1250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.1253143977529726	0.2496873314597271	0.1987051830134867	T	T	T
0.1251084542201688	0.2498921468381514	0.4002147332322504	T	T	T
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0.3744885042492688	0.1255101764363986	0.2970874242225799	T	T	T

0.3796847007582940	0.1203211820676666	0.4920782647563838	T	T	T
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0.3747372150291107	0.0002636650846374	0.1977966257759629	T	T	T
0.3753571682077452	-0.0003556919519391	0.3951282636936094	T	T	T
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0.2498892763526581	0.1251085603892852	0.4002154106061102	T	T	T
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0.2494908444338755	0.0005029202800577	0.2970853068190793	T	T	T
0.2546806872091478	0.9953121946271782	0.4920771688410840	T	T	T
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0.3750033050843275	0.3750004768963763	0.2990765909899052	T	T	T
0.3752236496102294	0.3752185502426998	0.4948223914171819	T	T	T
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0.3746872967007301	0.2503042576416907	0.1986951657517538	T	T	T
0.3749061282427539	0.2501169838405372	0.4001840501806695	T	T	T
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0.2503077150842380	0.3746884138280849	0.1986964712723305	T	T	T
0.2501161261090936	0.3749117052890995	0.4001931586888771	T	T	T
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0.2499968911204878	0.2500002255172761	0.2991244916179142	T	T	T
0.2501351078747126	0.2501238568661503	0.4948726287112435	T	T	T
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0.1249989933022192	0.6250005735221681	0.2957595150803101	T	T	T
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0.1252558848468284	0.4997401347587218	0.1977961123378022	T	T	T
0.1246254628293466	0.5003670491725617	0.3951183233534765	T	T	T
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0.1244834607932026	0.8755063316105692	0.2970827869997755	T	T	T
0.1296842176429165	0.8703046010744233	0.4920828679308441	T	T	T
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0.1247361586110176	0.7502588795291294	0.1977867158640405	T	T	T
0.1253697392649231	0.7496340644826653	0.3951086298032832	T	T	T
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-0.0003077368012402	0.8753112762775396	0.1986973474995045	T	T	T
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0.0046745942800946	0.7453139536496914	0.4920464920140312	T	T	T
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0.3754916479967932	0.6245034860888921	0.2970397904434195	T	T	T
0.3703089083920789	0.6296984852434850	0.4920002000478170	T	T	T
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0.3753022633779727	0.4996929835566096	0.1986820154736740	T	T	T
0.3751226420235002	0.4999090138037341	0.4001335727589099	T	T	T
0.2500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.2502478416510327	0.6247450757746941	0.1977814753233187	T	T	T
0.2496154429299024	0.6253778836607191	0.3950928799940372	T	T	T
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0.2504935159629338	0.4995072475773985	0.2970703663742182	T	T	T
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0.3749808167005127	0.8750174218583024	0.2957562682078521	T	T	T

0.3750050163668543	0.8749969210603726	0.4910621001765856	T	T	T
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0.3752435946843013	0.7497534730045404	0.1977720325893587	T	T	T
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0.2503559365358571	0.8746375733112589	0.3951196297156108	T	T	T
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0.2499832397904303	0.7500074497045881	0.2957489955964668	T	T	T
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0.6249982388584842	0.1250015641651785	0.2957566021789840	T	T	T
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0.4997403708757957	0.1252540365861173	0.1977943170999154	T	T	T
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0.6245010913313847	0.3754920813878845	0.2970396564634983	T	T	T
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0.6247436754531396	0.2502479324631865	0.1977804775548390	T	T	T
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0.4996940962390298	0.3753041305417495	0.1986819274474187	T	T	T
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0.4995056950846755	0.2504939706350045	0.2970680804257985	T	T	T
0.5046906696584268	0.2453192733997757	0.4920425893336255	T	T	T
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0.7496319095570296	0.1253741402570928	0.3951043461969709	T	T	T
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0.8750169777674514	0.3749844445857959	0.2957552928437431	T	T	T
0.8749946100971345	0.3750109789037023	0.4910618945725534	T	T	T
0.8750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.8752646591749650	0.2497376311509307	0.1977867303505609	T	T	T
0.8746361808131675	0.2503599183513790	0.3951173673057959	T	T	T
0.7500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.7497544718726072	0.3752478380929846	0.1977713052056685	T	T	T
0.7503852381665903	0.3746101951393536	0.3950751329503329	T	T	T
0.7500000000000000	0.2500000000000000	0.0984529120451825	F	F	F
0.7500069582692822	0.2499904939499528	0.2957470007205487	T	T	T
0.7499910768638955	0.2500022089041469	0.4910498603937216	T	T	T
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0.6249966367095141	0.6249988406751052	0.2990383963769332	T	T	T

0.6249940965716136	0.6249980720974772	0.4947332881780453	T	T	T
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0.6246926268583695	0.5002988837633141	0.1986644786602019	T	T	T
0.6248993932050028	0.5000961580428460	0.4000993887015445	T	T	T
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0.5002968803817621	0.6246936234718433	0.1986641743290476	T	T	T
0.5000967714450343	0.6249016080064861	0.4000973433385373	T	T	T
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0.4999963464527238	0.4999987180170400	0.2990479612479007	T	T	T
0.5001521269077741	0.5001519435151451	0.4947715174668017	T	T	T
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0.6254972647707331	0.8745099151969079	0.2970479851056779	T	T	T
0.6203038869968670	0.8796911895828952	0.4920131988929271	T	T	T
0.6250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.6253037332710734	0.7497038813925841	0.1986677104573774	T	T	T
0.6250873850028223	0.7499046150293130	0.4001024321572340	T	T	T
0.5000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.5002432309375010	0.8747598656579618	0.1977794322380732	T	T	T
0.4996169037409142	0.8753914250497117	0.3950810247048739	T	T	T
0.5000000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.5004770976739916	0.7495216639328047	0.2970347051478205	T	T	T
0.4953164414335816	0.7546836203791911	0.4919845409791183	T	T	T
0.8750000000000000	0.6250000000000000	0.0984529120451825	F	F	F
0.8745082220434781	0.6255011299652804	0.2970491432906008	T	T	T
0.8796819490312013	0.6203108568795751	0.4920191158191634	T	T	T
0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8747605597574151	0.5002458373952303	0.1977795960358203	T	T	T
0.8753893846435684	0.4996214215997341	0.3950820380583702	T	T	T
0.7500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.7497037287006806	0.6253057446919610	0.1986675579640648	T	T	T
0.7498978040257203	0.6250911078626832	0.4000999760417895	T	T	T
0.7500000000000000	0.5000000000000000	0.0984529120451825	F	F	F
0.7495205652124582	0.5004813142937478	0.2970349853535265	T	T	T
0.7546795685446753	0.4953175435306229	0.4919843026106508	T	T	T
0.8750000000000000	0.8750000000000000	0.0984529120451825	F	F	F
0.8749966301856912	0.8750014328546968	0.2990712504268328	T	T	T
0.8748006236539342	0.8748101389395559	0.4948276373565855	T	T	T
0.8750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.8746972139727628	0.7503063330412042	0.1986826282548622	T	T	T
0.8748947163812932	0.7500951117911410	0.4001399064209416	T	T	T
0.7500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.7503028972499883	0.8746984804562897	0.1986835286136213	T	T	T
0.7500872195887028	0.8749009768236466	0.4001400353192275	T	T	T
0.7500000000000000	0.7500000000000000	0.0984529120451825	F	F	F
0.7500026681682854	0.7500049034435463	0.2990597322670875	T	T	T
0.7498415592279598	0.7498502662081606	0.4947575485372901	T	T	T
0.0827940910838372	0.1672904406593845	0.5737165737871713	T	T	T
0.1672488992582897	0.0827598573334384	0.5737170675716640	T	T	T
0.2077067128288304	0.2921919853032316	0.5737189915698027	T	T	T
0.2921590466742393	0.2077005964114566	0.5737266073730547	T	T	T
0.3326988353571790	0.4171618833064791	0.5736777334932998	T	T	T
0.4171213716347422	0.3326528835575041	0.5736762337185564	T	T	T
0.4577280605536266	0.5421802756925546	0.5736279204563552	T	T	T
0.5421639528439683	0.4576848645113167	0.5736169150141645	T	T	T
0.5827746515559281	0.6672458229528510	0.5735875497684321	T	T	T
0.6672262605563443	0.5827597135322288	0.5735861753457622	T	T	T
0.7078428373010600	0.7923239751415900	0.5736050674618012	T	T	T
0.7922779484914314	0.7078364011281669	0.5736152865349712	T	T	T
0.8328714947227783	0.9173466937868110	0.5736808231390513	T	T	T
0.9172997543878284	0.8328432704900106	0.5736838468354006	T	T	T

0.9578648824207613	0.0423432967908155	0.5737303857832085	T	T	T
0.0423126511489324	0.9578428876388299	0.5737286424014804	T	T	T
0.1250041596217440	0.1250083308509850	0.5514564113753947	T	T	T
0.2499910583802133	0.2499957264658187	0.5514514900111203	T	T	T
0.3750017373687979	0.3749993806477124	0.5513908285406791	T	T	T
0.5000083438247143	0.4999953592262902	0.5513393449290683	T	T	T
0.6249976493011429	0.6250010307511801	0.5512963686964425	T	T	T
0.7499939540247671	0.7500126366098211	0.5513238171940540	T	T	T
0.8750016961424333	0.8750100331445771	0.5513969238638582	T	T	T
0.0000199785841350	0.0000275728487737	0.5514605165533714	T	T	T

MS1-pbc-0CO2 (-1320.8711 eV)

1.0000000000000000

19.2439999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 9.6219999999999999 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.2439999999999998

Ca O

104 104

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0004350193151147	0.0000000163893671	0.1654403969479613	T	T	T
-0.0006133577286723	0.0000000398248969	0.3323334326752732	T	T	T
0.0000000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.0005258256797029	0.2500000278259440	0.2487252796286843	T	T	T
-0.0076010650962666	0.2500000093998718	0.4195098467700603	T	T	T
0.1250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.1251810023760460	-0.0000000356511441	0.2491361608239219	T	T	T
0.1242361190948592	0.0000000542961015	0.4140966439809950	T	T	T
0.1250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.1251811211795965	0.2499999947401608	0.1656464397919885	T	T	T
0.1237567005800757	0.2500000193859780	0.3327042070044276	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0004350182975456	0.4999999457769098	0.1654403950902706	T	T	T
-0.0006133606259897	0.4999999589819080	0.3323333985302158	T	T	T
0.0000000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.0005257678017847	0.7500000298905976	0.2487252871195639	T	T	T
-0.0076011588189268	0.7499999106135500	0.4195097491926275	T	T	T
0.1250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.1251810004839890	0.4999999954911507	0.2491361428874538	T	T	T
0.1242360813371269	0.4999998206153614	0.4140966558918834	T	T	T
0.1250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.1251810677993970	0.7499999981239621	0.1656464367077265	T	T	T
0.1237566682804268	0.7500000371817680	0.3327041988779882	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2498212010999529	-0.0000000092672973	0.1656438686673522	T	T	T
0.2512533288880853	0.0000000468094835	0.3327050716008199	T	T	T
0.2500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.2498200348079847	0.2500000455869146	0.2491350798067807	T	T	T
0.2507909348950310	0.2499999721278329	0.4140999790202120	T	T	T
0.3750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.3744771841036328	0.0000000261310376	0.2487231107868708	T	T	T
0.3826019212819355	0.0000000363728503	0.4195092248312324	T	T	T
0.3750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.3745703034318982	0.2500000037452827	0.1654389155876425	T	T	T
0.3756186412671414	0.2500000500420565	0.3323316196591414	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2498212325296825	0.4999999545614033	0.1656438693141043	T	T	T
0.2512532932222389	0.5000000964912273	0.3327050684522984	T	T	T

0.2500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.2498200244507797	0.7500000437302312	0.2491350529038712	T	T	T
0.2507909816449957	0.7500000163468615	0.4140999206868414	T	T	T
0.3750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.3744771830922460	0.4999999599288478	0.2487230835968872	T	T	T
0.3826019394356535	0.5000000205611577	0.4195092170699084	T	T	T
0.3750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.3745703116590914	0.7499999224205560	0.1654389023206901	T	T	T
0.3756186336632421	0.7499999899059947	0.3323316080985986	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.4995272464571026	-0.0000000247210670	0.1650649413627255	T	T	T
0.4998616269068817	0.0000000263097378	0.3301692637451847	T	T	T
0.5000000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.4994137751094543	0.2500001072670018	0.2476125594109635	T	T	T
0.5058474720957612	0.2500000887003125	0.4108589072929119	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4995272648641299	0.4999999505881086	0.1650649021380653	T	T	T
0.4998616246681507	0.5000000623600186	0.3301692457631256	T	T	T
0.5000000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.4994137874716501	0.7500000337418973	0.2476125475562458	T	T	T
0.5058474368246965	0.7500000156763467	0.4108589419122237	T	T	T
0.6250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.6247160570553797	0.0000000728907005	0.2470037463384397	T	T	T
0.6263364109456162	-0.0000000984542031	0.4110820347149083	T	T	T
0.6250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.6248421296120965	0.2499999502644422	0.1648086511095314	T	T	T
0.6255742728716418	0.2500000435330318	0.3290380904800706	T	T	T
0.6250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.6247160824822215	0.4999999096681828	0.2470037183656846	T	T	T
0.6263364025710481	0.5000000169108585	0.4110819641770895	T	T	T
0.6250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.6248421143437197	0.7499999246209693	0.1648086746686207	T	T	T
0.6255742565412840	0.7500001428009976	0.3290380704412842	T	T	T
0.0098829640678177	-0.0000002505636216	0.4989688776227844	T	T	T
0.0098829029285253	0.4999998678671991	0.4989689120316214	T	T	T
0.1270795356097833	0.2499997750468987	0.4958602366102185	T	T	T
0.1270794513793908	0.7499998697679812	0.4958600448405878	T	T	T
0.2479419054872858	-0.0000000694336848	0.4958702222084218	T	T	T
0.2479418479432953	0.4999998245524768	0.4958702189877164	T	T	T
0.3651423297141858	0.2499999035632420	0.4989822310428478	T	T	T
0.3651422570947038	0.7499999040515877	0.4989822910878450	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7501594597574627	-0.0000000168689954	0.1648052657057525	T	T	T
0.7494299787103790	0.0000000578549423	0.3290355465378288	T	T	T
0.7500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.7502862044753111	0.2500000867772210	0.2469998293531926	T	T	T
0.7486600239017642	0.2499998817732765	0.4110803886927909	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7501594386480448	0.4999999449856919	0.1648052641481474	T	T	T
0.7494299724889733	0.4999999851247682	0.3290355233278569	T	T	T
0.7500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.7502862052876115	0.7500000330232007	0.2469998704031713	T	T	T
0.7486600449341116	0.7500000053979454	0.4110803423985821	T	T	T
0.8750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.8755879931093961	0.0000000339868196	0.2476083467264448	T	T	T
0.8691493146989856	-0.0000000305777719	0.4108531150062224	T	T	T
0.8750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.8754734954255480	0.2499999695632997	0.1650594833512290	T	T	T
0.8751431880387793	0.2500000331117354	0.3301609066368457	T	T	T
0.8750000000000000	0.5000000000000000	0.0822561893037914	F	F	F

0.8755879896391298	0.4999999310985226	0.2476083399965411	T	T	T
0.8691492777907057	0.4999999052138804	0.4108531086491640	T	T	T
0.8750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.87547344498433941	0.7499999388921992	0.1650594728235042	T	T	T
0.8751431307129267	0.7500000498901861	0.3301609061558052	T	T	T
0.1250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.1251631369315221	0.2499999887939134	0.2488280514130138	T	T	T
0.1256218613645027	0.2499999465813826	0.4147668572028133	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1249930876539204	-0.0000000477133225	0.1656436360667902	T	T	T
0.1239767941934184	0.0000000236265969	0.3322079141758630	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0002877069617228	0.2499999797452582	0.1654783361322223	T	T	T
-0.0002265809865466	0.2500000116563521	0.3318035156769385	T	T	T
0.0000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.0000582137297623	0.0000000066748627	0.2489617711683218	T	T	T
-0.0058063464459396	-0.0000000767194496	0.4194469826620912	T	T	T
0.1250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.1251630840893639	0.7500000294669041	0.2488280313355258	T	T	T
0.1256218794367734	0.7499998738916568	0.4147667573299647	T	T	T
0.1250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1249930931726737	0.4999999567051839	0.1656436420627277	T	T	T
0.1239767991995342	0.5000000433651605	0.3322079107188126	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0002876333674659	0.7499999511724479	0.1654783281912705	T	T	T
-0.0002266241912021	0.7500000329815208	0.3318034884940926	T	T	T
0.0000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.0000582200656387	0.5000000180698833	0.2489617776303909	T	T	T
-0.0058064582152857	0.4999998381908208	0.4194470175934326	T	T	T
0.3750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.3749470073095824	0.2500000595858393	0.2489661941356320	T	T	T
0.3808092784417965	0.2500000520493180	0.4194520789993686	T	T	T
0.3750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3747123522394083	0.0000000301741528	0.1654846093775607	T	T	T
0.3752272972192581	0.0000000972628147	0.3318157536206685	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2500070939321919	0.2499999523306663	0.1656422257549126	T	T	T
0.2510187174836271	0.2500000616734300	0.3322091713676242	T	T	T
0.2500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.2498420413499398	0.0000000156668321	0.2488314962177836	T	T	T
0.2493876612951381	-0.0000000120962007	0.4147724784847891	T	T	T
0.3750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.3749470215047827	0.7500000464921897	0.2489661909721264	T	T	T
0.3808093012507516	0.7500000011327858	0.4194521457015598	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3747123088224542	0.4999999872636213	0.1654846173279259	T	T	T
0.3752272780156568	0.5000000902814951	0.3318157607457443	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2500070392741771	0.7499999615885854	0.1656422121553156	T	T	T
0.2510187392552539	0.7500000731240714	0.3322091495902310	T	T	T
0.2500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.2498420500377622	0.5000000742150298	0.2488314967222484	T	T	T
0.2493876043463505	0.4999999447350767	0.4147724920228720	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4996546564985455	0.2500002353244863	0.1651509422052022	T	T	T
0.5000447441802872	0.2500000482230084	0.3308676328559781	T	T	T
0.5000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.4998420339026932	0.0000000661311349	0.2473934020708327	T	T	T
0.5050591063895681	0.0000000860220463	0.4099280028746499	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F

0.4996545808866010	0.7500000864835454	0.1651509075753273	T	T	T
0.5000447165380127	0.7500000568240152	0.3308676647087884	T	T	T
0.5000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.4998420673908919	0.5000000199516718	0.2473934374909075	T	T	T
0.5050591060034739	0.5000000810627661	0.4099279803820031	T	T	T
0.6250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.6247952817486893	0.2499999477378464	0.2470351844430392	T	T	T
0.6263151770120369	0.2499999694729719	0.4104144575026717	T	T	T
0.6250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6249541741577079	-0.0000000797025462	0.1648350584378154	T	T	T
0.6254776011595127	0.0000001137224142	0.3296193492875600	T	T	T
0.6250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.6247952348408128	0.7500000205021460	0.2470351738749267	T	T	T
0.6263151976579484	0.7500000012199918	0.4104144319787073	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.6249541968061842	0.4999999319912357	0.1648350471591410	T	T	T
0.6254776040172693	0.5000000656788623	0.3296193067839231	T	T	T
0.0098390994066215	0.2499997433879707	0.4976435537713784	T	T	T
0.0098390731025973	0.7499997681706012	0.4976434034896520	T	T	T
0.1253987221775100	-0.0000002240585700	0.4956421895954800	T	T	T
0.1253986998431553	0.4999997947761058	0.4956422056187503	T	T	T
0.2496288788684876	0.2499998587648317	0.4956472989720780	T	T	T
0.2496287836398907	0.7499999012162268	0.4956472519787258	T	T	T
0.3651917451394504	0.0000000270955316	0.4976541139807004	T	T	T
0.3651916358435202	0.5000000855500347	0.4976541006025239	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7500463953318955	0.2499999631718869	0.1648334758605089	T	T	T
0.7495285888129954	0.2500000202126668	0.3296186038850119	T	T	T
0.7500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.7502071002974606	0.0000001031297637	0.2470335727425931	T	T	T
0.7486768298874332	0.0000000010015184	0.4104151059648588	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7500463730832714	0.7499999490916228	0.1648335085493597	T	T	T
0.7495285480274002	0.7500001082914418	0.3296186078335099	T	T	T
0.7500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.7502071130573483	0.5000000282177141	0.2470335761622208	T	T	T
0.7486767941722978	0.4999999061690929	0.4104150555714059	T	T	T
0.8750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.8751553594052542	0.2500000104413134	0.2473874587392824	T	T	T
0.8699292445920658	0.2499998530171471	0.4099265197591227	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.8753466944275318	-0.0000000600310715	0.1651493664953752	T	T	T
0.8749596478967541	0.0000001085024644	0.3308682230712299	T	T	T
0.8750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.8751553525202902	0.7500000440367304	0.2473874791451982	T	T	T
0.8699291999659515	0.7499998473240589	0.4099264638056930	T	T	T
0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8753466931581181	0.4999999668087833	0.1651493619223265	T	T	T
0.8749596324598814	0.4999999804961616	0.3308682196965110	T	T	T

MS1-pbc-1CO2 (-1346.4795 eV)

1.0000000000000000

19.2439999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 9.6219999999999999 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.2439999999999998

Ca O C

104 106 1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0002984724094325	0.9999998657279900	0.1655226066676632	T	T	T
0.9991396072152029	0.9999999692722361	0.3324694657108404	T	T	T
0.0000000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.0002411923686897	0.2499961629863186	0.2489244068922667	T	T	T
0.9927977537767565	0.2500615794992332	0.4200935269319014	T	T	T
0.1250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.1249417187753714	-0.0000000202150354	0.2490431203387811	T	T	T
0.1243763907772574	0.0000004069687014	0.4137128839028342	T	T	T
0.1250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.1251083163172036	0.2499551491065415	0.1656652379116847	T	T	T
0.1238414453646490	0.2498116673976495	0.3326235565467981	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0003018968657793	0.4999999206328846	0.1655087909741808	T	T	T
0.9992437627623165	0.4999999314313749	0.3325181607710744	T	T	T
0.0000000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.0002412067936049	0.7500037362008205	0.2489244108471046	T	T	T
0.9927978332981700	0.7499387773515085	0.4200932875776764	T	T	T
0.1250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.1249063146241675	0.4999999508341973	0.2489619159281370	T	T	T
0.1246019509167831	0.5000003807124963	0.4137309193478895	T	T	T
0.1250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.1251082929094942	0.7500446661934471	0.1656652694895082	T	T	T
0.1238414480213731	0.7501886983954303	0.3326235879928323	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2498807973660317	0.999999849400286	0.1655883391172723	T	T	T
0.2509710673220590	0.0000005459720870	0.3319928826599386	T	T	T
0.2500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.2499697983123076	0.2498009511860846	0.2489066195348878	T	T	T
0.2522097690195731	0.2492571359247536	0.4137166617705874	T	T	T
0.3750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.3751668483779077	0.0000003001243963	0.2483607573649657	T	T	T
0.3825117991666556	0.0000009214440642	0.4158106728390188	T	T	T
0.3750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.3748489094731001	0.2499499211150937	0.1653351958380720	T	T	T
0.3769588664688637	0.2486133907781568	0.3313464323318774	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2498553653494735	0.4999999321754011	0.1655547901670935	T	T	T
0.2505838407168343	0.5000001293801908	0.3314681736434994	T	T	T
0.2500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.2499698852937544	0.7501992969755347	0.2489065479205170	T	T	T
0.2522098125447357	0.7507433602342358	0.4137167001884630	T	T	T
0.3750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.3750200646667482	0.4999999140767763	0.2481953434538977	T	T	T
0.3809143721849707	0.5000003798909800	0.4119244280946526	T	T	T
0.3750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.3748488948390915	0.7500501062316144	0.1653351620323759	T	T	T
0.3769591849691509	0.7513870682545865	0.3313464902644047	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.4998785653759466	0.0000000894639364	0.1650583023255976	T	T	T
0.5010860382713300	0.0000002700065197	0.3312226443868266	T	T	T
0.5000000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.5001540408731444	0.2494859462729458	0.2477861599500610	T	T	T
0.5058154877323581	0.2549865092835247	0.4153068158617152	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4999000014308008	0.4999998755863831	0.1650346676565787	T	T	T
0.5014838810918467	0.5000002571202093	0.3294480435416676	T	T	T
0.5000000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.5001540737571120	0.7505142443680310	0.2477860002296529	T	T	T
0.5058155414546287	0.7450132989305805	0.4153079470503485	T	T	T

0.6250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.6249318486895334	0.9999999340477285	0.2474763770153549	T	T	T
0.6255436445959697	0.0000010875873197	0.4121787665447681	T	T	T
0.6250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.6250254028753954	0.2499474644748805	0.1649167266358816	T	T	T
0.6248221806268482	0.2501537957399610	0.3301306321667310	T	T	T
0.6250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.6252170458470619	0.4999999641641242	0.2472369636714721	T	T	T
0.6256883886312513	0.4999992444956139	0.4125353571242903	T	T	T
0.6250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.6250254690825242	0.7500523651754112	0.1649166644923454	T	T	T
0.6248222450021848	0.7498462597919195	0.3301310089966106	T	T	T
0.0115740363085128	0.0000004976422011	0.4995407599380668	T	T	T
0.0124198528577281	0.5000001246572275	0.4995250250485390	T	T	T
0.1292863685964483	0.2496003345431469	0.4956164249078809	T	T	T
0.1292863303900464	0.7504004313876863	0.4956165480560501	T	T	T
0.2482590236631523	0.0000018227987189	0.4948625597611087	T	T	T
0.2483589563742228	0.5000003870540798	0.4948659016868573	T	T	T
0.3716066042956601	0.2321214567252146	0.4979791635853467	T	T	T
0.3716074109372809	0.7678804086068316	0.4979796847725790	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7501881978492970	0.9999998405390246	0.1649840666933430	T	T	T
0.7490847004845501	0.9999997817685417	0.3298238334076549	T	T	T
0.7500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.7501441441476788	0.2499617325292147	0.2475948994476877	T	T	T
0.7483465626579110	0.2499978181855372	0.4119332152313390	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7502807593314784	0.4999999247370179	0.1649437070138385	T	T	T
0.7490723511210128	0.4999999878322313	0.3298109141561877	T	T	T
0.7500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.7501440089340823	0.7500379216371896	0.2475949516617314	T	T	T
0.7483466950418123	0.7500020205549476	0.4119335474160273	T	T	T
0.8750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.8752741770568017	0.9999998742854079	0.2479834666977967	T	T	T
0.8691339286172307	0.0000001802016441	0.4115403268493975	T	T	T
0.8750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.8753543520020158	0.2499823562383778	0.1652320334140382	T	T	T
0.8749374480147916	0.2500536502578868	0.3308251049204757	T	T	T
0.8750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.8753091460587002	0.499999795777508	0.2479944744090609	T	T	T
0.8691319028792837	0.4999996149890905	0.4116251238085973	T	T	T
0.8750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.8753543226133993	0.7500173816708730	0.1652320745921873	T	T	T
0.8749374061688604	0.7499460279270970	0.3308250635300545	T	T	T
0.1250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.1250837462041170	0.2500622970719933	0.2489498611461198	T	T	T
0.1267610561769960	0.2503948959116992	0.4148401505074109	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1249710197249119	0.9999999262778451	0.1657610318814316	T	T	T
0.1239905564036698	0.0000001331229845	0.3322025027565065	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0003674918254196	0.2500052825483587	0.1656546155690518	T	T	T
0.0000002728498862	0.2500684140849085	0.3323523703276408	T	T	T
0.0000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.9999414007142298	0.9999998186610243	0.2492553176891883	T	T	T
0.9949614190628785	0.0000002853271649	0.4203099922013046	T	T	T
0.1250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.1250836281036442	0.7499375459081846	0.2489499053595878	T	T	T
0.1267611791734245	0.7496059406981028	0.4148401757862245	T	T	T
0.1250000000000000	0.5000000000000000	0.0000000000000000	F	F	F

0.1249922557521600	0.4999999152603253	0.1657752334431838	T	T	T
0.1244062148760745	0.5000001114509041	0.3323939716283153	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0003675161009333	0.7499944768719837	0.1656546412941312	T	T	T
0.0000003207515009	0.7499314821918622	0.3323524479892988	T	T	T
0.0000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.0000435137263806	0.4999999154062575	0.2493060810474718	T	T	T
0.9956021664739148	0.5000000836999594	0.4203199427103065	T	T	T
0.3750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.3751717848763761	0.2499896097183202	0.2487264952689939	T	T	T
0.3793594553353307	0.2507236596509450	0.4179494994035076	T	T	T
0.3750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3746938260339655	0.0000000587901264	0.1654846330084211	T	T	T
0.3750810583340292	0.0000004651883010	0.3316842901013652	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2499797093870016	0.2500020036025922	0.1656780130497784	T	T	T
0.2511156866378502	0.2502839665119215	0.3319150924234900	T	T	T
0.2500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.2499283040551971	0.0000001524063688	0.2487924417296603	T	T	T
0.2496010931050029	0.0000004893364800	0.4143668927153200	T	T	T
0.3750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.3751718228648371	0.7500106242576976	0.2487264424242566	T	T	T
0.3793599011267203	0.7492775594520493	0.4179503848590462	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3746400655486236	0.4999999558247950	0.1654663350035502	T	T	T
0.3745624345037137	0.5000001540474515	0.3315949410315289	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2499796953153833	0.7499979340436072	0.1656780007496934	T	T	T
0.2511157415222353	0.7497167853263252	0.3319149782308460	T	T	T
0.2500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.2499150932176465	0.5000000561071273	0.2488135306154625	T	T	T
0.2524563035594212	0.5000003843035544	0.4153462914888250	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4997560747544854	0.2498671630591609	0.1650645625179905	T	T	T
0.4999827439017317	0.2496333400213648	0.3308102694811708	T	T	T
0.5000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.5000746209373094	0.0000002017625172	0.2473990615898044	T	T	T
0.5042477405804473	0.0000004938109448	0.4106233045313739	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.4997561052807455	0.7501327925299665	0.1650644913960581	T	T	T
0.4999827479392439	0.7503671070396777	0.3308102832880301	T	T	T
0.5000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.5000403010180442	0.4999998942882558	0.2469106067531222	T	T	T
0.5028845657462683	0.5000003708814135	0.4068537643216825	T	T	T
0.6250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.6250526040281238	0.2499732465195930	0.2472636334316936	T	T	T
0.6262601522200862	0.2505712253953934	0.4108778675988796	T	T	T
0.6250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6251061066290335	0.9999998760957319	0.1649615560718824	T	T	T
0.6256410893216311	0.0000003630549778	0.3302474541944969	T	T	T
0.6250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.6250526304889875	0.7500265779105416	0.2472636001208882	T	T	T
0.6262604108948675	0.7494291257079926	0.4108778549692324	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.6252045901461727	0.4999999638593614	0.1648986836611462	T	T	T
0.6259643165687089	0.4999997639517800	0.3298768051544630	T	T	T
0.0124609439461539	0.2506549935834613	0.4982813983276221	T	T	T
0.0124604974761172	0.7493458511421480	0.4982814277358141	T	T	T
0.1272819523158548	0.0000006415568728	0.4954005411103113	T	T	T
0.1291333116041010	0.5000000840655282	0.4953643524285378	T	T	T

0.2531088175742317	0.2527264166257349	0.4958126267011141	T	T	T
0.2531084678588349	0.7472756332426224	0.4958130557977892	T	T	T
0.3657433532715419	0.0000019769092197	0.4953693111853015	T	T	T
0.3721026530862970	0.5000040918597628	0.4991622513811248	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7502437407297281	0.2499811334667097	0.1650111410539729	T	T	T
0.7497432055968133	0.2499207896873498	0.3302738313222267	T	T	T
0.7500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.7503232981770136	0.9999998021989100	0.2474138045900544	T	T	T
0.7487092345738934	0.0000004723792891	0.4110892197072323	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7502437137364534	0.7500185714103151	0.1650111794166792	T	T	T
0.7497434098306202	0.7500789693410953	0.3302739631512668	T	T	T
0.7500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.7504486198988081	0.4999998190642220	0.2473601621026537	T	T	T
0.7486375622169820	0.4999994581849307	0.4110125397732712	T	T	T
0.8750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.8752470301624885	0.2500144106513253	0.2478120886813933	T	T	T
0.8704993294958103	0.2501550640789750	0.4107657554675383	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.8754863651386552	0.9999998209216808	0.1653436150824382	T	T	T
0.8752203895089919	0.9999997859561706	0.3315130382799626	T	T	T
0.8750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.8752469896034325	0.7499851618150734	0.2478121371988825	T	T	T
0.8704994800322611	0.7498447499293291	0.4107658116276590	T	T	T
0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8755389363528048	0.4999998731323318	0.1653360800539018	T	T	T
0.8753306131223691	0.4999998864887578	0.3315652377022656	T	T	T
0.4721946484555413	0.6190602455874704	0.5067881490090419	T	T	T
0.4721952375377585	0.3809360111332948	0.5067874975100437	T	T	T
0.4423688023367722	0.5000115326395937	0.5048830873023433	T	T	T

MS1-pbc-2CO2 (-1371.0560 eV)

1.0000000000000000

19.2439999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 9.6219999999999999 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.2439999999999998

Ca O C

104 108 2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0003510044603014	-0.0000001783931659	0.1655865726499607	T	T	T
0.9994152163489501	0.0000002643249550	0.3326190412218129	T	T	T
0.0000000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.0004209699971071	0.2499543376012257	0.2490667123450144	T	T	T
0.9930055325760732	0.2500322816849028	0.4201323643149029	T	T	T
0.1250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.1252191921656995	0.0000003182777117	0.2492208420567047	T	T	T
0.1246148765172568	0.0000002641010369	0.4139979579192408	T	T	T
0.1250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.1251629432184005	0.2499414718406335	0.1657236843191480	T	T	T
0.1243195225222439	0.2498140000779423	0.3328940839290462	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0003190598913507	0.5000000249168178	0.1655447476217192	T	T	T
0.9994375666109041	0.4999999093925167	0.3325827478921274	T	T	T
0.0000000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.0004208902860287	0.7500454510198427	0.2490665625360518	T	T	T
0.9930056429304133	0.7499679912164990	0.4201322402443604	T	T	T

0.1250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.1250389551337811	0.5000000544285506	0.2490525540582206	T	T	T
0.1248285375052955	0.4999996972236275	0.4137766513603043	T	T	T
0.1250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.1251627150141461	0.7500585005177141	0.1657234868233032	T	T	T
0.1243194832298555	0.7501861597102906	0.3328938671511404	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2499816606081693	0.0000001398330079	0.1656467829853508	T	T	T
0.2514560754856748	0.0000001161560215	0.3322571086853661	T	T	T
0.2500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.2502186555886813	0.2497678448986805	0.2490814581062771	T	T	T
0.2534481172611047	0.2493258836203353	0.4143024401509407	T	T	T
0.3750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.3755606986286030	-0.0000001119632326	0.2484461487541163	T	T	T
0.3836939744857277	0.0000001287702098	0.4149867916027012	T	T	T
0.3750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.3749621727870786	0.2499487583989133	0.1653499495722956	T	T	T
0.3777677357149625	0.2487157326283621	0.3314436392435551	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2498899512771215	0.5000000077255443	0.1655800932661496	T	T	T
0.2507787864846418	0.4999995201249972	0.3315181550525537	T	T	T
0.2500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.2502187628323027	0.7502317180714030	0.2490814506342671	T	T	T
0.2534477073994713	0.7506744612677301	0.4143026662603494	T	T	T
0.3750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.3752094516582268	0.4999998988034908	0.2481454003507958	T	T	T
0.3812924908270059	0.4999999648778810	0.4108341006342296	T	T	T
0.3750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.3749619526414948	0.7500508896156599	0.1653499878976343	T	T	T
0.3777677288927170	0.7512846941618636	0.3314436916137213	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5000119151064830	0.0000001248003570	0.1650548220601225	T	T	T
0.5018653048305629	-0.0000004481402262	0.3317279298109005	T	T	T
0.5000000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.5004095293846734	0.2492832425788760	0.2478397757432718	T	T	T
0.5061274993019801	0.2571769166813512	0.4171511770899461	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000001151662659	0.4999996747056111	0.1650070094396910	T	T	T
0.5021547493701189	0.5000002246631466	0.3289929958504130	T	T	T
0.5000000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.5004093834545223	0.7507164359280468	0.2478396426468185	T	T	T
0.5061276679169522	0.7428231180007908	0.4171515509940534	T	T	T
0.6250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.6250454329090041	-0.0000001502404712	0.2476228252740157	T	T	T
0.6256945517398624	0.0000000535530879	0.4127151125151056	T	T	T
0.6250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.6250917265733849	0.2499154290937867	0.1649305480703419	T	T	T
0.6247303652665736	0.2502170125578688	0.3304313424339795	T	T	T
0.6250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.6254632529332925	0.4999999665257881	0.2472110141104792	T	T	T
0.6258852138682851	0.5000000224807650	0.4126592913105006	T	T	T
0.6250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.6250917873692386	0.7500843427760069	0.1649304181577420	T	T	T
0.6247303466165153	0.7497830221909917	0.3304313870654341	T	T	T
0.0118853088187147	0.0000005891340841	0.4998628914350322	T	T	T
0.0122327207614107	0.4999998198837334	0.4996992105849427	T	T	T
0.1292407893409646	0.2505604858671437	0.4958269884804529	T	T	T
0.1292406364217258	0.7494401818600844	0.4958267984182876	T	T	T
0.2459380953835385	0.0000008976702616	0.4961711392128187	T	T	T
0.2474001831954953	0.4999995384319372	0.4951599272530293	T	T	T

0.3724024045781076	0.2506966516553764	0.5013813070981212	T	T	T
0.3724013926686866	0.7493029237334033	0.5013808971558311	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7502418169353654	-0.0000001591614861	0.1650325974315955	T	T	T
0.7491427800761493	-0.0000002853737898	0.3300383298133503	T	T	T
0.7500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.7501967710755875	0.2499249436675566	0.2477399449418340	T	T	T
0.7485074194829932	0.2500374297076650	0.4121335568909404	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7503461421010033	0.4999999044783775	0.1649564988808533	T	T	T
0.7491861196706545	0.4999999558207753	0.3298825604976841	T	T	T
0.7500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.7501967392959550	0.7500745822715212	0.2477399355320092	T	T	T
0.7485074549194015	0.7499624086057755	0.4121335134941796	T	T	T
0.8750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.8753844836625352	-0.0000002435955149	0.2481220766751409	T	T	T
0.8692665691633782	0.0000000641695092	0.4117711179374436	T	T	T
0.8750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.8753704184778892	0.2499594324482918	0.1652862274878609	T	T	T
0.8750648791441384	0.2499980176660457	0.3309648387922329	T	T	T
0.8750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.8754157899074543	0.4999998351519787	0.2480803073580254	T	T	T
0.8692587990173689	0.4999998315705526	0.4117099831952207	T	T	T
0.8750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.8753704207458076	0.7500402211136086	0.1652862956372362	T	T	T
0.8750648818429267	0.7500014563215577	0.3309646921840454	T	T	T
0.1250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.1253306234810200	0.2499431904871435	0.2492547351486002	T	T	T
0.1274436851942559	0.2500752946851578	0.4152062973474558	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1251236416530851	0.0000000859441840	0.1660319633781011	T	T	T
0.1249120200289518	0.0000005564006865	0.3329024908999468	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0004723367995842	0.2499639831724826	0.1658510724993826	T	T	T
0.0004685116596738	0.2499555345311284	0.3327070419176727	T	T	T
0.0000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.0003169514862849	-0.0000001587421261	0.2496173459312115	T	T	T
0.9958862973844173	0.0000002288036870	0.4207576586521704	T	T	T
0.1250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.1253301645770732	0.7500571578056914	0.2492546055243712	T	T	T
0.1274430187044067	0.7499246209424554	0.4152066617845112	T	T	T
0.1250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1250380581535446	0.5000000036145446	0.1659653642053274	T	T	T
0.1248392993271260	0.4999999064124686	0.3327523820566758	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0004720061998423	0.7500355383736036	0.1658510920660478	T	T	T
0.0004686390165467	0.7500445769088901	0.3327068361132788	T	T	T
0.0000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.0002998681477912	0.4999999613115183	0.2495579197374882	T	T	T
0.9960710534881562	0.4999999971742876	0.4206254739863036	T	T	T
0.3750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.3752025242110227	0.2496922799350547	0.2489570640170282	T	T	T
0.3794780079765606	0.2492695981997752	0.4185696730902698	T	T	T
0.3750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3746657886827766	0.0000000043677049	0.1657759895426545	T	T	T
0.3754573365791068	-0.0000003722509172	0.3330551715316884	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2499987259504046	0.2499007524786944	0.1658866136299711	T	T	T
0.2515162396893263	0.2497875592323885	0.3323689752463476	T	T	T
0.2500000000000000	0.0000000000000000	0.0822561893037914	F	F	F

0.2502946239546637	0.0000002497584732	0.2494388555646732	T	T	T
0.2523319811247680	0.0000003120174928	0.4170003342409392	T	T	T
0.3750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.3752024364918064	0.7503074564702470	0.2489571101595093	T	T	T
0.3794778286969154	0.7507310080466850	0.4185701049279868	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3745391828778222	0.4999997993948541	0.1656198703181543	T	T	T
0.3744916788192164	0.5000002534907262	0.3315013968188840	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2499985775094173	0.7500991296265265	0.1658865163555513	T	T	T
0.2515165506337937	0.7502121780376249	0.3323687794876234	T	T	T
0.2500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.2499873907512379	0.4999996979618997	0.2491142847698387	T	T	T
0.2532984319598164	0.4999995689365910	0.4160792679422388	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4997489351651799	0.2497510555103371	0.1650895040179961	T	T	T
0.5001367575055203	0.2491723478404368	0.3304899825990559	T	T	T
0.5000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.5000816610060926	0.0000002515991498	0.2475953767339278	T	T	T
0.5037902685916592	-0.0000005107819429	0.4116537088950796	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.4997487167025775	0.7502488203832420	0.1650893084563353	T	T	T
0.5001365064621371	0.7508274377552306	0.3304897279312019	T	T	T
0.5000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.5000879329033067	0.4999995289535435	0.2466524486044328	T	T	T
0.5030339576716008	0.5000007141768082	0.4053532733184961	T	T	T
0.6250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.6252310534919067	0.2498709395736436	0.2473285177302686	T	T	T
0.6266089156394861	0.2505459101003097	0.4109854333585222	T	T	T
0.6250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6251480194914762	0.0000001268438108	0.1651074185525513	T	T	T
0.6257690025061163	0.0000000815768868	0.3306261589358566	T	T	T
0.6250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.6252311709861702	0.7501287211696858	0.2473284963176408	T	T	T
0.6266088064872769	0.7494539869197276	0.4109854521439640	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.6252878406530523	0.4999997382776100	0.1649520637113400	T	T	T
0.6264425513020068	0.4999997790084710	0.3297881981793678	T	T	T
0.0129044942848051	0.2504377474273999	0.4983479720042286	T	T	T
0.0129048079072500	0.7495628426722675	0.4983480679925352	T	T	T
0.1284529406833839	-0.0000001705922093	0.4958700295560450	T	T	T
0.1294230100130973	0.5000005285602432	0.4954989733967507	T	T	T
0.2535202260239907	0.2528719669161087	0.4958405804955193	T	T	T
0.2535208923637440	0.7471282804257297	0.4958401381495893	T	T	T
0.3711547505076583	0.0000032572021983	0.5003453768762633	T	T	T
0.3780841544770089	0.4999989024593920	0.4988277808193444	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7503662210670244	0.2499544173972916	0.1651181180631465	T	T	T
0.7500468704450084	0.2498641972116472	0.3304283065203352	T	T	T
0.7500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.7504959199863713	-0.0000003864398874	0.2476032257553019	T	T	T
0.7490159751376908	-0.0000002847533814	0.4112237539008209	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7503662488842981	0.7500453868071416	0.1651182008939563	T	T	T
0.7500470071143366	0.7501356057130110	0.3304284656700558	T	T	T
0.7500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.7506822546066551	0.4999998345004543	0.2474194957137474	T	T	T
0.7489608052853748	0.5000000915201828	0.4110153750006327	T	T	T
0.8750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.8755210147649676	0.2499512488981783	0.2479964326767905	T	T	T

0.8709353811863375	0.2500897334039129	0.4109521213094966	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.8756331912654163	-0.0000004528879517	0.1655109544610642	T	T	T
0.8756731310798782	-0.0000000855661762	0.3317813739782720	T	T	T
0.8750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.8755209046005695	0.7500483078455426	0.2479962323204123	T	T	T
0.8709351166175814	0.7499101315246482	0.4109519491856655	T	T	T
0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8756594514323749	0.5000000490743393	0.1654610844091772	T	T	T
0.8757375191542989	0.4999997352934452	0.3317359946342304	T	T	T
0.4793601663880120	0.6188146472794769	0.4983146452834745	T	T	T
0.4793594365652684	0.3811848788615510	0.4983140063479158	T	T	T
0.3964420683840159	0.1182453065876718	0.5653343910432278	T	T	T
0.3964416952742311	0.8817508617507419	0.5653353943031472	T	T	T
0.4498576308970775	0.4999998863233112	0.4989551066928917	T	T	T
0.3899038475366399	0.0000099442881605	0.5467456704101753	T	T	T

MS2-pbc-0CO2 (-1985.4688 eV)

1.0000000000000000

19.2439999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4329999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.2439999999999998

Ca O

156 156

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0004470667898562	0.00000000009189262	0.1654241321950489	T	T	T
-0.0006303246689386	0.0000000167986128	0.3323520496557899	T	T	T
0.0000000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.0004708420146049	0.1666665466731968	0.2487791180139498	T	T	T
-0.0077040079710367	0.1666665858495983	0.4196859858075101	T	T	T
0.1250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.1251511361729464	0.0000000451090206	0.2491462599951747	T	T	T
0.1243305549182919	0.0000000656821639	0.4140770878679520	T	T	T
0.1250000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.1251088307233424	0.1666665585266030	0.1656785328077134	T	T	T
0.1237239233627423	0.1666666927618196	0.3326592227208878	T	T	T
0.0000000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.0004472477417617	0.3333332551791208	0.1654241071779849	T	T	T
-0.0006302355352547	0.3333332512238801	0.3323521057721176	T	T	T
0.0000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.0004708750027611	0.4999999322372755	0.2487791456038900	T	T	T
-0.0077039128664381	0.4999999783488323	0.4196858665714338	T	T	T
0.1250000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.1251512180271917	0.3333332908832071	0.2491462728341259	T	T	T
0.1243305431329080	0.333333293532103	0.4140771061786382	T	T	T
0.1250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1251088919535628	0.4999999349366246	0.1656785302650735	T	T	T
0.1237239538434460	0.4999999618150497	0.3326592188810871	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2498950764542323	-0.0000000155088758	0.1656727193471546	T	T	T
0.2512875727535834	-0.0000000732397794	0.3326582878221068	T	T	T
0.2500000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.2498493334382590	0.1666666840938200	0.2491489815566025	T	T	T
0.2506956633137197	0.1666666924224332	0.4140807099002272	T	T	T
0.3750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.3745352460990600	0.0000000363755863	0.2487721483850554	T	T	T
0.3826950287351935	0.0000000083082612	0.4196888386724654	T	T	T

0.3750000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.3745550612273716	0.1666666556010394	0.1654201811306826	T	T	T
0.3756319876591068	0.1666666816744913	0.3323471824159262	T	T	T
0.2500000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.2498951368210322	0.3333333054894511	0.1656726785245173	T	T	T
0.2512875306083273	0.3333333980909433	0.3326582647115543	T	T	T
0.2500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.2498492616275047	0.4999999853842493	0.2491488892335013	T	T	T
0.2506957648913767	0.5000001205763908	0.4140806601831081	T	T	T
0.3750000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.3745352447543722	0.3333333265649854	0.2487720869039608	T	T	T
0.3826948961157396	0.3333333586328608	0.4196889236448619	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3745550591926090	0.4999999763370571	0.1654201826012893	T	T	T
0.3756320435675358	0.5000000748907243	0.3323470838929181	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.4995315333027370	-0.0000000193598080	0.1650814617764157	T	T	T
0.4999601382141252	-0.0000000004192609	0.3302473208372074	T	T	T
0.5000000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.4995390488547143	0.1666666849764664	0.2476422567502519	T	T	T
0.5059267097880524	0.1666667490722137	0.4109634314528789	T	T	T
0.5000000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.4995315947359241	0.3333332658159820	0.1650814782928620	T	T	T
0.4999600632980583	0.3333333101686551	0.3302473412535804	T	T	T
0.5000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.4995390444000080	0.4999999811393815	0.2476421975721766	T	T	T
0.5059266735757578	0.4999999783965793	0.4109633205702974	T	T	T
0.6250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.6246378475278970	0.0000000011932943	0.2469491437310966	T	T	T
0.6263773037307407	0.0000000081419146	0.4109886018223834	T	T	T
0.6250000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.6248626031865316	0.1666667868187337	0.1647310608427196	T	T	T
0.6255427124907392	0.1666666593020225	0.3289874580630937	T	T	T
0.6250000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.6246379255083884	0.3333333290883048	0.2469491529946004	T	T	T
0.6263772227531952	0.3333332954378346	0.4109886075133269	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.6248626617799731	0.5000000029587209	0.1647310547195769	T	T	T
0.6255427704335602	0.5000000142077707	0.3289874904551254	T	T	T
0.0000000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.0004472450888324	0.6666667424104706	0.1654240990108418	T	T	T
-0.0006302051165155	0.6666667458378743	0.3323520298237769	T	T	T
0.1250000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.1251511928397717	0.6666666674365548	0.2491462629274360	T	T	T
0.1243306421518528	0.6666667474907841	0.4140771517566545	T	T	T
0.2500000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.2498950907476355	0.6666666943885261	0.1656726435654454	T	T	T
0.2512875619314470	0.6666666784002371	0.3326582463865653	T	T	T
0.3750000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.3745352248011175	0.6666666745515478	0.2487719333758994	T	T	T
0.3826950069084203	0.6666666547799953	0.4196889453706641	T	T	T
0.5000000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.4995316366639037	0.6666666394903638	0.1650814678116220	T	T	T
0.4999600334366569	0.6666666866627456	0.3302472677629101	T	T	T
0.6250000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.6246379042443019	0.6666666822039431	0.2469491278455488	T	T	T
0.6263772445073170	0.6666666935263222	0.4109885418530906	T	T	T
0.0000000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.0004708662114823	0.8333333895601110	0.2487790979657855	T	T	T
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0.1237239933454415	0.8333332820058029	0.3326592451032301	T	T	T
0.2500000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.2498492720414936	0.8333333626166098	0.2491488852896170	T	T	T
0.2506957958047726	0.8333331875189541	0.4140806272081691	T	T	T
0.3750000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.3745550718474995	0.8333334187909748	0.1654201901061978	T	T	T
0.3756320114282521	0.8333331754925545	0.3323472140792325	T	T	T
0.5000000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.4995390035107737	0.8333333819818924	0.2476422208109581	T	T	T
0.5059267445156257	0.8333333775477476	0.4109634140011629	T	T	T
0.6250000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.6248625724984973	0.8333332095954812	0.1647310593650071	T	T	T
0.6255427275627041	0.8333332800155995	0.3289874827476602	T	T	T
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0.0100189153769222	0.6666666555075473	0.4990231316071546	T	T	T
0.1269779858165084	0.1666665475555860	0.4958329058372856	T	T	T
0.1269782306105594	0.5000000473201873	0.4958329503689907	T	T	T
0.1269783301748073	0.8333333369702763	0.4958329553728079	T	T	T
0.2480461961107842	0.0000001312997161	0.4958351185899521	T	T	T
0.2480460233633134	0.3333332916461310	0.4958352137243053	T	T	T
0.2480464980535199	0.6666665702623493	0.4958353196082841	T	T	T
0.3650038462246795	0.1666666309679179	0.4990354768578488	T	T	T
0.3650038624597229	0.4999997650138575	0.4990355982232675	T	T	T
0.3650039499257735	0.8333336226681747	0.4990355349423247	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
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0.7494649237057056	-0.0000000143404656	0.3289877227827134	T	T	T
0.7500000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.7503653934633877	0.1666666779626315	0.2469474115900662	T	T	T
0.7486200487479815	0.1666666806241168	0.4109911861470985	T	T	T
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0.7494649940251741	0.3333332599472691	0.3289876798853826	T	T	T
0.7500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
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0.7486200209173020	0.5000000332902370	0.4109912201518475	T	T	T
0.7500000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.7501429498526312	0.6666666040372664	0.1647310766998026	T	T	T
0.7494649887421604	0.6666666775804880	0.3289876930563866	T	T	T
0.7500000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.7503654107770820	0.833333386222190	0.2469474363160916	T	T	T
0.7486201496045757	0.8333332554575354	0.4109912559418862	T	T	T
0.8750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.8754545355168730	-0.0000000401463124	0.2476362687029237	T	T	T
0.8690735741164384	-0.0000001197041923	0.4109616605248247	T	T	T
0.8750000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.8754689103340567	0.1666666388519742	0.1650759425635458	T	T	T
0.8750481196724802	0.1666666312153761	0.3302441815046209	T	T	T
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0.8754546906975872	0.3333332686229507	0.2476362809224443	T	T	T
0.8690735947115840	0.3333333732825809	0.4109616327387668	T	T	T
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0.8750481219468701	0.4999999584502656	0.3302441728245049	T	T	T
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0.8754546643264894	0.6666666867389862	0.2476362866826904	T	T	T
0.8690736708259763	0.6666666534314957	0.4109615624255121	T	T	T

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0.1250000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.1251436090505549	0.1666666780502285	0.2488618302416804	T	T	T
0.1254511241725009	0.1666666941924238	0.4147052258557693	T	T	T
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0.1239522216218508	0.0000000054695271	0.3322310997560770	T	T	T
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0.0002849175509289	0.1666665449725465	0.1655027229639375	T	T	T
-0.0003348593945842	0.1666665878589112	0.3319384493462305	T	T	T
0.0000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.0000563278096463	-0.0000000439641945	0.2489885579007452	T	T	T
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0.1251435583458990	0.4999999325961255	0.2488618262990858	T	T	T
0.1254512245768885	0.50000000212157433	0.4147051861977378	T	T	T
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0.1250137687440175	0.3333333190395785	0.1656605578040537	T	T	T
0.1239522749144056	0.333333320949102	0.3322311204440826	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0002850800832662	0.4999999638195881	0.1655027156045141	T	T	T
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0.0000565109421981	0.3333332683536048	0.2489886350859230	T	T	T
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0.3750000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.3749501828725559	0.1666666486665309	0.2489902799438257	T	T	T
0.3810124423305550	0.1666667266530849	0.4195980657153304	T	T	T
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0.3747199021299460	0.0000000269634686	0.1655082524561901	T	T	T
0.3753329290760292	0.0000000253350564	0.3319403826718753	T	T	T
0.2500000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.2499873251799059	0.1666666202296691	0.1656603723392235	T	T	T
0.2510409729368103	0.1666666915600813	0.3322260158887293	T	T	T
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0.2498543749049661	0.0000000394500887	0.2488632634103693	T	T	T
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0.3749501936991256	0.50000000371083575	0.2489901772511920	T	T	T
0.3810124478546388	0.4999999351655866	0.4195980590634903	T	T	T
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0.3747199540032065	0.3333332853610325	0.1655082545729019	T	T	T
0.3753329204700426	0.3333333837049648	0.3319403597520633	T	T	T
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0.2499873099835643	0.4999999548327326	0.1656603266246797	T	T	T
0.2510409734432512	0.5000000874384612	0.3322260083339855	T	T	T
0.2500000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.2498543844030623	0.3333332746407317	0.2488632148073517	T	T	T
0.2495574848821327	0.3333334272189157	0.4147135039754562	T	T	T
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0.4996043392212690	0.1666666691305576	0.1651701632919116	T	T	T
0.5000727556563769	0.1666667125667438	0.3308417920914303	T	T	T
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0.4998401007635163	0.0000000470575110	0.2474229214365241	T	T	T
0.5052047392936733	0.0000000160920798	0.4101436682658643	T	T	T
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0.4996043494370789	0.4999999686897399	0.1651701198823210	T	T	T
0.5000727338011328	0.5000000125912226	0.3308416859419278	T	T	T

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0.5052047345291544	0.3333333736279392	0.4101436709908634	T	T	T
0.6250000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.6247957426620557	0.1666666626768586	0.2469153182335500	T	T	T
0.6263856511139738	0.1666666722830154	0.4103940548542651	T	T	T
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0.6249374842682424	-0.0000000219711247	0.1648152284633208	T	T	T
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0.6250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
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0.6249375767669823	0.3333333555746866	0.1648152540102579	T	T	T
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0.0000565014833729	0.6666666454691391	0.2489885786814621	T	T	T
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0.2495497074658574	0.1666666947394296	0.4955895682747836	T	T	T
0.2495498420618227	0.4999999886191950	0.4955896181046405	T	T	T
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0.3652647388627424	-0.0000000074149988	0.4980236043370128	T	T	T
0.3652646778065443	0.3333333601659803	0.4980236483648490	T	T	T
0.3652647000953193	0.6666667204190665	0.4980237590281475	T	T	T
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0.7500629493075444	0.1666667776723844	0.1648119539343665	T	T	T
0.7495644925049829	0.1666666468296175	0.3294838393562668	T	T	T
0.7500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.7502072494403470	-0.0000000174151276	0.2469121499803547	T	T	T
0.7486074016777240	0.0000000127269112	0.4104029599886833	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7500630587190709	0.4999999921945064	0.1648119362392106	T	T	T
0.7495645202128440	0.5000000101918264	0.3294838369793486	T	T	T
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0.7500000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.7502073685121791	0.6666666990411653	0.2469121034551285	T	T	T
0.7486074274004403	0.6666666389217258	0.4104029156364129	T	T	T
0.7500000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.7500629188992524	0.8333332224062505	0.1648119627332559	T	T	T
0.7495645616877532	0.8333333301764320	0.3294839046314077	T	T	T
0.8750000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.8751621181500857	0.1666666196811344	0.2474240685676016	T	T	T
0.8697948881924192	0.1666665861068116	0.4101393593432768	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.8753860930595292	-0.0000000044988009	0.1651668230776094	T	T	T
0.8749250636540370	0.0000000368726836	0.3308504287309720	T	T	T
0.8750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.8751622320794028	0.4999999730979917	0.2474240432620667	T	T	T
0.8697950280224775	0.4999999500314375	0.4101392782634691	T	T	T
0.8750000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.8753857554793437	0.3333332697426024	0.1651667454875972	T	T	T
0.8749250854804845	0.3333333218148592	0.3308504045898285	T	T	T
0.8750000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.8753857502278063	0.6666666492498394	0.1651667542158632	T	T	T
0.8749250882874147	0.6666666378158524	0.3308503854916390	T	T	T
0.8750000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.8751621704812022	0.8333333252845008	0.2474240659058952	T	T	T
0.8697949389203942	0.8333332988971384	0.4101393134618642	T	T	T

MS2-pbc-1CO2 (-2011.0694 eV)

1.0000000000000000

19.2439999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4329999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.2439999999999998

Ca O C

156 158 1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0003785037091089	0.0000177124141295	0.1655411181663175	T	T	T
-0.0007318500923201	0.0000892056792252	0.3325514146530241	T	T	T
0.0000000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.0002811737583603	0.1666755464947123	0.2489976628276106	T	T	T
-0.0070370910628599	0.1668421742409667	0.4202282699961796	T	T	T
0.1250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.1250163727858275	0.0000380529819015	0.2491534142768522	T	T	T
0.1243300462404149	0.0001054556247871	0.4139737969152637	T	T	T
0.1250000000000000	0.1666666666666643	0.0000000000000000	F	F	F

0.1251043475096975	0.1666317970201043	0.1657226223679341	T	T	T
0.1239583037104268	0.1665897650188746	0.3328112256146722	T	T	T
0.0000000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.0003138896518616	0.3333332129072313	0.1655508312360346	T	T	T
-0.0005823569114095	0.3333331102819447	0.3326230515747540	T	T	T
0.0000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.0002815831602472	0.4999910274246087	0.2489976377676321	T	T	T
-0.0070367779210412	0.4998242454864479	0.4202282206228574	T	T	T
0.1250000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.1249706961979001	0.3333333579015255	0.2490974234938025	T	T	T
0.1249230572503131	0.3333339231425999	0.4140863009447096	T	T	T
0.1250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1251044892303859	0.5000347233767015	0.1657226202842462	T	T	T
0.1239581301262738	0.5000768193594536	0.3328117516896906	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2498713643504953	-0.0000233737247456	0.1656567928640439	T	T	T
0.2510769409471461	0.0000340357536797	0.3322600384390830	T	T	T
0.2500000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.2499641696429274	0.1665438851661258	0.2490630785188819	T	T	T
0.2522375270950582	0.1658041130628789	0.4142281362525517	T	T	T
0.3750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.3749779790525997	-0.0001346402495699	0.2485350882665725	T	T	T
0.3823995407254204	-0.0016986415977024	0.4173862190251095	T	T	T
0.3750000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.3747331582985748	0.1666138540075808	0.1654112415944792	T	T	T
0.3765313184316127	0.1654636646901661	0.3318569431065258	T	T	T
0.2500000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.2498325711562693	0.3333332906169227	0.1656459117077611	T	T	T
0.2507292175550425	0.3333335241088924	0.3318901023873737	T	T	T
0.2500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.2499642563788243	0.5001231999575664	0.2490630727528970	T	T	T
0.2522370178356752	0.5008627805658067	0.4142271114965881	T	T	T
0.3750000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.3748797702402546	0.3333333700519615	0.2485015730007651	T	T	T
0.3809501598346113	0.3333326945056973	0.4130178975948472	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3747333197012321	0.5000528531374213	0.1654114958294039	T	T	T
0.3765309499400289	0.5012026664497746	0.3318569304761546	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.4997512582056952	-0.0000362348187302	0.1651097959341165	T	T	T
0.5006068381966116	0.0010414032930785	0.3307450981618226	T	T	T
0.5000000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.4999598116940083	0.1665699052635324	0.2477554691774063	T	T	T
0.5055938555660771	0.1695412148607786	0.4146762112974590	T	T	T
0.5000000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.4997421372325668	0.3333334617984968	0.1650552459166379	T	T	T
0.5011187677191311	0.3333337415323595	0.3297329750269766	T	T	T
0.5000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.4999596286644921	0.5000972994402992	0.2477552729871933	T	T	T
0.5055930701513488	0.4971272921690335	0.4146737800329371	T	T	T
0.6250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.6249300587862552	0.0001539098152751	0.2473867653196978	T	T	T
0.6259485933658175	0.0005942709757246	0.4118841236583282	T	T	T
0.6250000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.6249987456998621	0.1666738035270677	0.1649122971733469	T	T	T
0.6250078531874862	0.1669821011339152	0.3300322661596168	T	T	T
0.6250000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.6251251174357327	0.3333332241985320	0.2472569600252770	T	T	T
0.6256055890970581	0.3333327381584689	0.4125974213522762	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F

0.6249987794804569	0.4999930753119720	0.1649125563079436	T	T	T
0.6250078887265886	0.4996852857358434	0.3300318138530778	T	T	T
0.0000000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.0003785347528772	0.6666493412447310	0.1655409839640245	T	T	T
-0.0007322394202576	0.6665771830364112	0.3325514599070612	T	T	T
0.1250000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.1250166608823900	0.6666283889644651	0.2491535153287557	T	T	T
0.1243306274613606	0.6665616259435435	0.4139736559035894	T	T	T
0.2500000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.2498715676097793	0.6666900953073734	0.1656569551998547	T	T	T
0.2510766967847694	0.6666329719706082	0.3322603715177102	T	T	T
0.3750000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.3749777769676490	0.6668011231412633	0.2485351172606201	T	T	T
0.3823983906746423	0.6683651687898176	0.4173850472555031	T	T	T
0.5000000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.4997514628007304	0.6667027472619420	0.1651100478563784	T	T	T
0.5006067065158593	0.6656259912431151	0.3307444840892311	T	T	T
0.6250000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.6249297633014017	0.6665128854742119	0.2473868138322698	T	T	T
0.6259490626370376	0.6660737001306699	0.4118843383439383	T	T	T
0.0000000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.0002394580192295	0.8333335157743733	0.2489054726466212	T	T	T
-0.0074084694723390	0.8333337363823773	0.4201381239587501	T	T	T
0.1250000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.1251339159465496	0.8333336744933247	0.1657090676696039	T	T	T
0.1234902976234079	0.8333334218902434	0.3325919884308340	T	T	T
0.2500000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.2498276659960095	0.8333331287243176	0.2490081748231808	T	T	T
0.2505998233327119	0.8333325051900304	0.4134566214012512	T	T	T
0.3750000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.3747487271869816	0.8333333303990682	0.1654236311889022	T	T	T
0.3759935639041774	0.8333329373387325	0.3316455441528641	T	T	T
0.5000000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.4999843350464958	0.8333331226483714	0.2478641694904113	T	T	T
0.5060247117514363	0.8333333388581448	0.4109174281882657	T	T	T
0.6250000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.6249907413718470	0.8333332486071866	0.1649426229282323	T	T	T
0.6256807362169061	0.8333329265378985	0.3295991377718427	T	T	T
0.0109664466158097	0.0003749736780185	0.4995249845724366	T	T	T
0.0124083746264110	0.3333327937967897	0.4996267207981062	T	T	T
0.0109675369677943	0.6662928831655217	0.4995245771310468	T	T	T
0.1291561731239927	0.1661980267549309	0.4959665925177254	T	T	T
0.1291563781559884	0.5004685521580783	0.4959663584529731	T	T	T
0.1274108208143514	0.8333324347237074	0.4956938906502200	T	T	T
0.2482455242057843	-0.0013117524695714	0.4953331102165278	T	T	T
0.2486764883028021	0.3333335840056018	0.4953557506700840	T	T	T
0.2482444045851635	0.6679773817770110	0.4953327754837727	T	T	T
0.3715031115775290	0.1525646860188639	0.4987165049779883	T	T	T
0.3714962802982456	0.5141062895213114	0.4987157689636920	T	T	T
0.3658558192403560	0.8333324544978624	0.4978920453645528	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7502150796231585	0.0000513378379273	0.1649598197898814	T	T	T
0.7493150753069252	0.0001826315379193	0.3297431682105862	T	T	T
0.7500000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.7502126416690320	0.1667085117722316	0.2475305103668899	T	T	T
0.7484825650973611	0.1668530088325246	0.4119128622002867	T	T	T
0.7500000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.7502625975702231	0.3333335214366885	0.1649420378380416	T	T	T
0.7491783782309558	0.3333335757587124	0.3298281783426147	T	T	T
0.7500000000000000	0.5000000000000000	0.0822561893037914	F	F	F

0.7502124157239999	0.4999578690827929	0.2475305584069679	T	T	T
0.7484832131204788	0.4998139114496960	0.4119128542268332	T	T	T
0.7500000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.7502148904127593	0.6666152407040693	0.1649598717259906	T	T	T
0.7493143275203223	0.6664837816796926	0.3297426949384969	T	T	T
0.7500000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.7502976978350926	0.8333337172402585	0.2474109419359834	T	T	T
0.7485135926682579	0.8333330719863719	0.4117824037048030	T	T	T
0.8750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.8753634236898153	0.0000544007216788	0.2479566590441183	T	T	T
0.8692748412930048	0.0000898083299848	0.4114920893459739	T	T	T
0.8750000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.8754140663980265	0.1666772847187471	0.1652381015314807	T	T	T
0.8750664703650876	0.1667713961551360	0.3308712515973157	T	T	T
0.8750000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.8753467761101716	0.3333331149500123	0.2480228674300777	T	T	T
0.8692757221363012	0.3333330055727577	0.4116224501373705	T	T	T
0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8754138378925019	0.4999893624483016	0.1652380691403741	T	T	T
0.8750660526867506	0.4998950981449842	0.3308710951811037	T	T	T
0.8750000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.8753634259196410	0.6666126551810724	0.2479565952994341	T	T	T
0.8692752352833532	0.6665769517366230	0.4114920049531505	T	T	T
0.8750000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.8754505626237421	0.8333335570859084	0.1652041414027120	T	T	T
0.8750518360561211	0.8333334505408755	0.3307732543699519	T	T	T
0.1250000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.1251046448946747	0.1667524593341232	0.2490496446912036	T	T	T
0.1265393903896047	0.1670026469864528	0.4150369360445487	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1250109981086003	0.0000338447921162	0.1657804617948382	T	T	T
0.1239660561744090	0.0000962195305036	0.3323015900152381	T	T	T
0.0000000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.0003559940850096	0.1666952338832240	0.1656581463325367	T	T	T
-0.0000357072192995	0.1667707722693963	0.3324072288076138	T	T	T
0.0000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
-0.0000065644901098	0.0000472864527594	0.2492240525195439	T	T	T
-0.0054061943001611	0.0002885050268196	0.4202286383268017	T	T	T
0.1250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.1251050194044140	0.4999140875347660	0.2490496779343590	T	T	T
0.1265387875396606	0.4996644204700109	0.4150367308040012	T	T	T
0.1250000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.1249957306137715	0.3333332105039872	0.1658124704632075	T	T	T
0.1244979303468978	0.3333331568595284	0.3325943273079114	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0003561643654146	0.4999712591467689	0.1656579654550220	T	T	T
-0.0000358870821100	0.4998955002646894	0.3324074004724905	T	T	T
0.0000000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.0000660640410420	0.3333332363627220	0.2493176199018063	T	T	T
-0.0045342129515096	0.3333334106798869	0.4203291457080500	T	T	T
0.3750000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.3751037116641478	0.1666653926746984	0.2488967725442247	T	T	T
0.3795656769904339	0.1663939709524838	0.4185152122887766	T	T	T
0.3750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3747255685164984	0.0000192622307229	0.1655054846478327	T	T	T
0.3752732080511156	-0.0002811746524168	0.3317448983734589	T	T	T
0.2500000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.2499554980134811	0.1667001165286375	0.1657333144896127	T	T	T
0.2511824138395371	0.1668560447751901	0.3321808356922289	T	T	T
0.2500000000000000	0.0000000000000000	0.0822561893037914	F	F	F

0.2499208479117939	0.0000382164622249	0.2488748584605832	T	T	T
0.2496350016097934	-0.0002555011359141	0.4144520985879867	T	T	T
0.3750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.3751035246490193	0.5000013364542149	0.2488964513972403	T	T	T
0.3795643911473897	0.5002728513804042	0.4185125551028213	T	T	T
0.3750000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.3746027360439119	0.3333334229582718	0.1655496584599928	T	T	T
0.3747261831475704	0.3333322554396131	0.3320774508486075	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2499556627626413	0.4999665725152954	0.1657334283058145	T	T	T
0.2511813153230696	0.4998109741886782	0.3321803526268921	T	T	T
0.2500000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.2499381463706522	0.3333334078508110	0.2489962375454632	T	T	T
0.2526098630547153	0.3333326263583634	0.4156955483763287	T	T	T
0.5000000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.4996954364837908	0.1666010277009529	0.1651254057386034	T	T	T
0.4999871840104636	0.1665462621026464	0.3309870820011563	T	T	T
0.5000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.5000483464435310	-0.0000013565401109	0.2475335260710717	T	T	T
0.5046174606223316	0.0000014651440472	0.4105243408406361	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4996953388871980	0.5000658068189812	0.1651256961388902	T	T	T
0.4999874829428786	0.5001209553760989	0.3309859603982331	T	T	T
0.5000000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.4999310277796494	0.3333331962334866	0.2470921607182169	T	T	T
0.5029099966936809	0.3333311860737365	0.4075565832848692	T	T	T
0.6250000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.6249822130610706	0.1667159665811710	0.2472588302966099	T	T	T
0.6262958099271458	0.1670578026480979	0.4109128968627034	T	T	T
0.6250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6250531399769527	0.0000279419738259	0.1649556454424990	T	T	T
0.6255710406449321	0.0000133514042377	0.3301097811196916	T	T	T
0.6250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.6249825613091063	0.4999511935022787	0.2472584306854620	T	T	T
0.6262968963003489	0.4996099010213110	0.4109114090572542	T	T	T
0.6250000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.6251022751018560	0.3333332784739133	0.1648966112894943	T	T	T
0.6258209246147322	0.3333331248140929	0.3299262798745276	T	T	T
0.0000000000000000	0.6666666666666643	0.0822561893037914	F	F	F
-0.0000064083927570	0.6666195092081486	0.2492243885071511	T	T	T
-0.0054066797920422	0.6663779465524817	0.4202295264580198	T	T	T
0.1250000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.1250113412920207	0.6666331773740651	0.1657804479475933	T	T	T
0.1239655823081630	0.6665700204302969	0.3323016066924465	T	T	T
0.2500000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.2499208099546100	0.6666282653001188	0.2488750145566979	T	T	T
0.2496340347942586	0.6669237008218788	0.4144518926403947	T	T	T
0.3750000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.3747257532463316	0.6666475147454450	0.1655055961663205	T	T	T
0.3752726335558415	0.6669489315770131	0.3317443898756141	T	T	T
0.5000000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.5000482245523934	0.6666681561963077	0.2475335489227396	T	T	T
0.5046182706502911	0.6666665817483971	0.4105235097584366	T	T	T
0.6250000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.6250528895799584	0.6666388876888367	0.1649559304504495	T	T	T
0.6255704643752554	0.6666534563406790	0.3301094845659260	T	T	T
0.0000000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.0003881936639154	0.8333337268100375	0.1656327498630325	T	T	T
-0.0003046792178932	0.8333331667561418	0.3321903140978913	T	T	T
0.1250000000000000	0.8333333333333357	0.0822561893037914	F	F	F

0.1250326445300348	0.8333333420752773	0.2489567860027313	T	T	T
0.1253557630303870	0.8333338611936165	0.4146616926876525	T	T	T
0.2500000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.2499832333656085	0.8333332787522285	0.1657013280045971	T	T	T
0.2508290635549958	0.8333336099429197	0.3319148212654881	T	T	T
0.3750000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.3751233747755336	0.8333331752657341	0.2488067985007194	T	T	T
0.3804350717693516	0.8333347249770197	0.4180560437535329	T	T	T
0.5000000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.4997537965329317	0.8333331218160108	0.1651851365032351	T	T	T
0.5002345961314990	0.8333333907860905	0.3309628279583318	T	T	T
0.6250000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.6250292994759423	0.8333335333299936	0.2472815501560944	T	T	T
0.6262509927041237	0.8333332166585480	0.4109675389989566	T	T	T
0.0120508529670030	0.1673983346195749	0.4986244285237630	T	T	T
0.0120511669366542	0.4992685708008660	0.4986242879555833	T	T	T
0.0104727658519247	0.8333330318047463	0.4984880473538178	T	T	T
0.1265784575032979	0.0001301310508371	0.4955407176177503	T	T	T
0.1292225411722932	0.3333329897932695	0.4957335515954434	T	T	T
0.1265785382186275	0.6665371333389336	0.4955403354684448	T	T	T
0.2530255874545888	0.1678286492272488	0.4961464739606786	T	T	T
0.2530234713965676	0.4988379319809060	0.4961458718803312	T	T	T
0.2496479964255165	0.8333313429783435	0.4951280919768110	T	T	T
0.3657839134289066	-0.0042176706932089	0.4965576795800036	T	T	T
0.3711292448792706	0.3333192807528728	0.4996243997802269	T	T	T
0.3657841624661396	0.6708895773010016	0.4965572165554179	T	T	T
0.7500000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.7501995307776040	0.1666845459558227	0.1649948837465154	T	T	T
0.7497339947893714	0.1666567821692446	0.3302184087262986	T	T	T
0.7500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.7503087046907235	0.0000260706743868	0.2473883828493898	T	T	T
0.7487502422074163	0.0000823894012138	0.4111336401442051	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7501993547457440	0.4999819675518333	0.1649950150123401	T	T	T
0.7497339782193213	0.5000099606103440	0.3302181652019829	T	T	T
0.7500000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.7503747387113209	0.3333332845319791	0.2473618398241718	T	T	T
0.7486287784978954	0.3333334244331038	0.4111381241091427	T	T	T
0.7500000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.7503088498145177	0.6666408534043095	0.2473884318899909	T	T	T
0.7487501316582863	0.6665843554138580	0.4111329022135530	T	T	T
0.7500000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.7502003100612287	0.8333336111760881	0.1649977958189606	T	T	T
0.7496756248214778	0.8333332640358223	0.3301457666966921	T	T	T
0.8750000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.8752481823509797	0.1667010115804732	0.2478235050145231	T	T	T
0.8704127162228579	0.1668695948833506	0.4108756245554034	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.8754708577970454	0.0000383109126468	0.1653210063991496	T	T	T
0.8751473405538573	0.0000936789710671	0.3314226460964734	T	T	T
0.8750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.8752481358833363	0.4999656738904095	0.2478237207362723	T	T	T
0.8704130311302188	0.4997973245239618	0.4108757367140316	T	T	T
0.8750000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.8754799009947857	0.3333330947012024	0.1653254260323807	T	T	T
0.8752679018398017	0.3333335846316836	0.3315264293751602	T	T	T
0.8750000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.8754708208756109	0.6666288481828342	0.1653209279354352	T	T	T
0.8751473175496933	0.6665726128557544	0.3314228653218266	T	T	T
0.8750000000000000	0.8333333333333357	0.0822561893037914	F	F	F

0.8752035535249719	0.8333335133480751	0.2477394170265668	T	T	T
0.8702184568437713	0.8333329047101643	0.4106774374943471	T	T	T
0.4708981128153688	0.4127542882710916	0.5090490139089581	T	T	T
0.4708800009363687	0.2539328756039179	0.5090478537166684	T	T	T
0.4412774368174693	0.3333104726717306	0.5065300816467441	T	T	T

MS2-pbc-2CO2 (-2036.0349 eV)

1.000000000000000

19.243999999999998	0.000000000000000	0.000000000000000
0.000000000000000	14.432999999999998	0.000000000000000
0.000000000000000	0.000000000000000	29.243999999999998

Ca O C

156 160 2

Selective dynamics

Direct

0.000000000000000	0.000000000000000	0.000000000000000	F	F	F
0.0002052600361734	-0.0000140327452895	0.1655803486575097	T	T	T
0.9989250322948384	-0.0000192991965689	0.3325181800517206	T	T	T
0.000000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.0001230324589589	0.1666831190660221	0.2490128709554455	T	T	T
0.9926355494122658	0.1669812338921187	0.4201688909263570	T	T	T
0.125000000000000	0.000000000000000	0.0822561893037914	F	F	F
0.1248376365197158	-0.0000159322260534	0.2491375736609507	T	T	T
0.1236248000442946	0.0000296990181296	0.4138406913092231	T	T	T
0.125000000000000	0.1666666666666643	0.000000000000000	F	F	F
0.1250462719225839	0.1666447846260151	0.1657202165001160	T	T	T
0.1236066965214994	0.1666158444049404	0.3327241984900015	T	T	T
0.000000000000000	0.3333333333333357	0.000000000000000	F	F	F
0.0002476757061061	0.3333496276104145	0.1655840189433745	T	T	T
0.9992961172110466	0.3334182400581289	0.3326808655468587	T	T	T
0.000000000000000	0.500000000000000	0.0822561893037914	F	F	F
0.0002953455556516	0.5000111603774108	0.2491374718272791	T	T	T
0.9929750593201925	0.4999748960469806	0.4203419018279391	T	T	T
0.125000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.1249055589423763	0.3333954771692106	0.2490959990919443	T	T	T
0.1248158350182980	0.3336013768354562	0.4141075977290307	T	T	T
0.125000000000000	0.500000000000000	0.000000000000000	F	F	F
0.1251029641430026	0.5000405671318905	0.1657533870292818	T	T	T
0.1242056968144708	0.5001265517941926	0.3330718909606030	T	T	T
0.250000000000000	0.000000000000000	0.000000000000000	F	F	F
0.2498488198605353	-0.0000378524455134	0.1656791634784378	T	T	T
0.2506488262572348	-0.0000269394148529	0.3321933775259866	T	T	T
0.250000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.2498883183001934	0.1665245807138538	0.2490600675459688	T	T	T
0.2514704551515820	0.1660700864990218	0.4138154608197227	T	T	T
0.375000000000000	0.000000000000000	0.0822561893037914	F	F	F
0.3750633832659773	-0.0001085281717735	0.2486232996581425	T	T	T
0.3818714944378493	0.0002968053171098	0.4159758869096800	T	T	T
0.375000000000000	0.1666666666666643	0.000000000000000	F	F	F
0.3747984664813657	0.1665482084344828	0.1654309138971765	T	T	T
0.3767881336861740	0.1655911267600090	0.3317152789154948	T	T	T
0.250000000000000	0.3333333333333357	0.000000000000000	F	F	F
0.2498507427965007	0.3333285767667856	0.1656315269617610	T	T	T
0.2505614299294230	0.3334857404625824	0.3317528983912884	T	T	T
0.250000000000000	0.500000000000000	0.0822561893037914	F	F	F
0.2500290158027850	0.5001338487006604	0.2491105971445621	T	T	T
0.2534082245696282	0.5003563573488597	0.4150129861230184	T	T	T
0.375000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.3749937343359070	0.3331532241084966	0.2483489561187178	T	T	T

0.3810189373282728	0.3324363634808904	0.4119427087828322	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3748470515118726	0.5000521495302759	0.1654475312369815	T	T	T
0.3771641309401401	0.5004030360766754	0.3314866423955545	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.4998233565625215	0.9998671894191289	0.1651889615402868	T	T	T
0.5009000229000328	0.0006483084404529	0.3314355916302521	T	T	T
0.5000000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.5000261617239168	0.1662590932955153	0.2479078773571511	T	T	T
0.5055374279759415	0.1700761539586131	0.4164876069252884	T	T	T
0.5000000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.4998670873931774	0.3332394090929713	0.1650704517037183	T	T	T
0.5015467538496253	0.3330302915741631	0.3295734066211049	T	T	T
0.5000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.5001782194839002	0.5000554243850740	0.2478367797939098	T	T	T
0.5060721460084205	0.4961694493842799	0.4164564940160000	T	T	T
0.6250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.6247951477366722	-0.0000629351737748	0.2476769145995161	T	T	T
0.6256098746734099	0.0003153159300685	0.4124867995667321	T	T	T
0.6250000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.6249598400663522	0.1665548122727211	0.1649949465516730	T	T	T
0.6245692886984419	0.1667627454157073	0.3304187725006737	T	T	T
0.6250000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.6251773593754379	0.3332140464590654	0.2473679446005524	T	T	T
0.6254819046944418	0.3330808539209330	0.4128434440501860	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.6250126836059119	0.4999882688155786	0.1649840173095271	T	T	T
0.6247541896325602	0.4996228643034915	0.3304389753815636	T	T	T
0.0000000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.0002539652899821	0.6666453980854572	0.1656142419215082	T	T	T
0.9992215736580443	0.6665984663403778	0.3327159489651893	T	T	T
0.1250000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.1249723797681112	0.6666576460250472	0.2492143951560714	T	T	T
0.1245618937882597	0.6666252307249663	0.4142094783733180	T	T	T
0.2500000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.2498971640524472	0.6667104178591987	0.1656909914944847	T	T	T
0.2509239590936913	0.6666657077874591	0.3322355515022419	T	T	T
0.3750000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.3751722872349785	0.6669135705108955	0.2486162625137098	T	T	T
0.3821725415415476	0.6678889889143356	0.4142325608151537	T	T	T
0.5000000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.4998617469052183	0.6667507560000689	0.1651862963215329	T	T	T
0.5013962674860508	0.6656294425719995	0.3310521469296970	T	T	T
0.6250000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.6249562603375408	0.6665353027065889	0.2476298379871391	T	T	T
0.6254914901072671	0.6657719232183019	0.4131218100681074	T	T	T
0.0000000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.0001100167348417	0.8332828275199176	0.2490437830952949	T	T	T
0.9924478262550838	0.8331378441450001	0.4202523839267031	T	T	T
0.1250000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.1250511122171003	0.8333287527733011	0.1657447260914756	T	T	T
0.1235898245816690	0.8333533862252799	0.3328157415169836	T	T	T
0.2500000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.2498825752158006	0.8333633547006892	0.2491489646634798	T	T	T
0.2514214826947556	0.8340002472409913	0.4141147987481371	T	T	T
0.3750000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.3748227761038297	0.8333588924057794	0.1654944876592782	T	T	T
0.3765583404758578	0.8340610800841010	0.3319248807662074	T	T	T
0.5000000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.5000504933014180	0.8333490595281040	0.2482337002228412	T	T	T

0.5058086247014164	0.8323018809026375	0.4141595908004292	T	T	T
0.6250000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.6249322418349396	0.8333025550273172	0.1650637019911761	T	T	T
0.6250540913963207	0.8330827996319076	0.3303679305954942	T	T	T
0.0101955939686789	0.0003021231718052	0.4995965549824403	T	T	T
0.0122316091984370	0.3337529387210770	0.4997028685860683	T	T	T
0.0117947382627729	0.6663065823745309	0.4997716523406003	T	T	T
0.1281171257623681	0.1665869434313760	0.4958876430550050	T	T	T
0.1298675126219663	0.4999617174317441	0.4962802095701594	T	T	T
0.1277450541144286	0.8339851869490502	0.4960024832304336	T	T	T
0.2462156386203220	0.0005296358661392	0.4950461758057595	T	T	T
0.2484611330598918	0.3322414185469092	0.4955354681218934	T	T	T
0.2473860042010499	0.6682706250338413	0.4958629547576124	T	T	T
0.3697488907245485	0.1534776745392913	0.4980592139745079	T	T	T
0.3765353302796358	0.5002994166309604	0.5006590726580044	T	T	T
0.3688187794665544	0.8481108997761214	0.4986378742969554	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7500986556522938	-0.0000527568474715	0.1650616117602162	T	T	T
0.7489435332749858	-0.0000237727635173	0.3299984040612474	T	T	T
0.7500000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.7500089154276874	0.1665770028480154	0.2477435486407326	T	T	T
0.7482795399123684	0.1667236179390115	0.4121126672539627	T	T	T
0.7500000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.7502269707252995	0.3332889957595145	0.1650141038584992	T	T	T
0.7489864554350720	0.3332431323063332	0.3299982517885239	T	T	T
0.7500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.7500994166257158	0.4999361921924674	0.2477835747459615	T	T	T
0.7483325031675062	0.4996673731259470	0.4122569339906807	T	T	T
0.7500000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.7501580610907662	0.6666184624511790	0.1650684700633308	T	T	T
0.7489284708330339	0.6663990165120608	0.3301423458858006	T	T	T
0.7500000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.7500530192776397	0.8332182788411739	0.2477472948265892	T	T	T
0.7481744081785301	0.8331214134286938	0.4122149613765351	T	T	T
0.8750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.8751252546823506	-0.0000461946736817	0.2480757238493694	T	T	T
0.8689572262055407	-0.0000219992550175	0.4115573365265234	T	T	T
0.8750000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.8752671817140062	0.1666357196840455	0.1652867950772094	T	T	T
0.8748168620999465	0.1667188986532735	0.3309406407349810	T	T	T
0.8750000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.8752548055563883	0.3333288478592920	0.2481213187337639	T	T	T
0.8691452612394615	0.3332650765564713	0.4117433693126576	T	T	T
0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8753232920706510	0.4999870047167169	0.1653195124073299	T	T	T
0.8749368721392065	0.4999062217395912	0.3310831249953914	T	T	T
0.8750000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.8752111701493782	0.6665628475023442	0.2481656005384567	T	T	T
0.8690511684086428	0.6665199158478611	0.4117830915753422	T	T	T
0.8750000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.8752686522183354	0.8332845496530117	0.1652913324065138	T	T	T
0.8747572414181918	0.8331741209110809	0.3309806202374166	T	T	T
0.1250000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.1249742535505396	0.1667845759898703	0.2490786456994216	T	T	T
0.1259310550004028	0.1672624200654861	0.4149953256083466	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1249350479708782	-0.0000205022148877	0.1658399681576025	T	T	T
0.1236846538401951	-0.0000177206089867	0.3323511316819537	T	T	T
0.0000000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.0003004005638308	0.1666959438198544	0.1657244978155967	T	T	T

-0.0001802951006762	0.1667984960205425	0.3324905471159101	T	T	T
0.0000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
-0.0001167309084335	-0.0000152020599012	0.2493388379229679	T	T	T
0.9944247861437235	0.0000892062796914	0.4204104149973044	T	T	T
0.1250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.1252343467636758	0.5000481095255596	0.2492794109165077	T	T	T
0.1275689070663769	0.5000547181206134	0.4155075127935877	T	T	T
0.1250000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.1249973690433124	0.3334036497191254	0.1658884523308554	T	T	T
0.1245263561044925	0.3335616305239207	0.3327781418665080	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0003882582935950	0.5000154454492153	0.1657902093557375	T	T	T
0.0002252643822665	0.5000066610107500	0.3327570736377506	T	T	T
0.0000000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.0001269054443548	0.3334133805699319	0.2494585700533003	T	T	T
0.9956125620487370	0.3336708362322315	0.4205493507053999	T	T	T
0.3750000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.3749496899563689	0.1666471568325205	0.2488031715195812	T	T	T
0.3780787120932767	0.1669167651461449	0.4172774677852841	T	T	T
0.3750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3746377149816856	-0.0000854115518992	0.1656103256488643	T	T	T
0.3749274157423872	0.9998598414157582	0.3318512226483644	T	T	T
0.2500000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.2499009529130345	0.1666919560858850	0.1657648077619656	T	T	T
0.2506893627386979	0.1670110952923858	0.3320822167966141	T	T	T
0.2500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.2497940505084495	-0.0000841348053162	0.2489957871253770	T	T	T
0.2485806726297784	0.0000371607970300	0.4144384202995586	T	T	T
0.3750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.3750758414005468	0.5001359742177665	0.2490568521762917	T	T	T
0.3800520936973352	0.5001321621933972	0.4198205810796177	T	T	T
0.3750000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.3745590627276087	0.3333778751932150	0.1655855307582039	T	T	T
0.3744542598885691	0.3336162705880885	0.3318480334824829	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2499737266363904	0.5000541659368173	0.1658594663423475	T	T	T
0.2515270776327869	0.5001272448392727	0.3326798847059392	T	T	T
0.2500000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.2498810029322743	0.3334967944293982	0.2491062771060322	T	T	T
0.2528648932107307	0.3336596436236991	0.4160669609285137	T	T	T
0.5000000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.4996804302743828	0.1664673281423493	0.1651375544984714	T	T	T
0.4998349259309922	0.1661633133367107	0.3307721437987866	T	T	T
0.5000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.4999155250451472	-0.0002866273960636	0.2477043903097704	T	T	T
0.5040486467996063	0.0000587150662451	0.4111447807046862	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4996906740036112	0.5001047149898290	0.1651588374149665	T	T	T
0.4998742003434484	0.4999615409303216	0.3308406703585507	T	T	T
0.5000000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.4998898645740637	0.3332415393874614	0.2469613668338474	T	T	T
0.5028029534604939	0.3326170904957604	0.4066373032857672	T	T	T
0.6250000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.6249410133695220	0.1665381476493174	0.2473782618920932	T	T	T
0.6262230422134770	0.1669284959475173	0.4111748388704070	T	T	T
0.6250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6249965116881656	-0.0000998986973439	0.1650800814486610	T	T	T
0.6254226769262832	-0.0001380878825375	0.3304667872835307	T	T	T
0.6250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.6249997163173850	0.4999612847552370	0.2473809380669650	T	T	T

0.6263805815296566	0.4993584570433858	0.4110368390497788	T	T	T
0.6250000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.6251317789811862	0.3332949313633473	0.1649618140716384	T	T	T
0.6259666729327533	0.3331787026947846	0.3299796722896788	T	T	T
0.0000000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.0001027346976931	0.6665848406472529	0.2494878540250722	T	T	T
0.9953679716903093	0.6663455815028930	0.4205961106935209	T	T	T
0.1250000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.1250260526803124	0.6666342901948986	0.1659322064444297	T	T	T
0.1244945731310391	0.6665462011907077	0.3328521147599416	T	T	T
0.2500000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.2500226543757197	0.6666087535864861	0.2492965508185135	T	T	T
0.2522471699937584	0.6667062738382660	0.4163531373042860	T	T	T
0.3750000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.3746472073677058	0.6666747196374697	0.1657163451042304	T	T	T
0.3750805607883232	0.6666262939389891	0.3326212267932950	T	T	T
0.5000000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.4998965528581055	0.6666954769085238	0.2476930507232502	T	T	T
0.5030603631904675	0.6655026045103377	0.4104423278641280	T	T	T
0.6250000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.6250320583838433	0.6666533599527936	0.1650913517896078	T	T	T
0.6254900061422501	0.6664253841722374	0.3305363743716377	T	T	T
0.0000000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.0002980757486750	0.8332753042937086	0.1657407000607081	T	T	T
0.9997698751937181	0.8331926454674029	0.3325118792226341	T	T	T
0.1250000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.1250073345773626	0.8332015306537986	0.2491376198561890	T	T	T
0.1258132282626103	0.8329474817735001	0.4150510872971079	T	T	T
0.2500000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.2499300239451671	0.8332527394295633	0.1658291850452555	T	T	T
0.2508626568251472	0.8329803190380445	0.3323085282954222	T	T	T
0.3750000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.3750503326221700	0.8331924460855971	0.2490466972371977	T	T	T
0.3794536112552239	0.8337367029522471	0.4179733474661471	T	T	T
0.5000000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.4996794540863890	0.8332797986783785	0.1653099637338759	T	T	T
0.4999996096841285	0.8330720539566089	0.3317038662837599	T	T	T
0.6250000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.6248908933343572	0.8331815945625219	0.2475500880436921	T	T	T
0.6261106473357605	0.8329206283109079	0.4111662847411617	T	T	T
0.0113822921668431	0.1678189484403611	0.4986204368782467	T	T	T
0.0130430742835791	0.4998392692566661	0.4987583477273382	T	T	T
0.0109997823203710	0.8327016900785025	0.4986397643513742	T	T	T
0.1257127627475950	0.0004013305095650	0.4955984873214456	T	T	T
0.1293710348667682	0.3337320845332174	0.4958405933453819	T	T	T
0.1285510241575751	0.6663589445975518	0.4959981404497158	T	T	T
0.2512613281848129	0.1687221787718215	0.4960097729213643	T	T	T
0.2555181195538344	0.4992689868663822	0.4973698395175912	T	T	T
0.2503065415545582	0.8326841616512278	0.4960954921688048	T	T	T
0.3633969640723092	0.0012234685132236	0.4951516115393683	T	T	T
0.3743080926958722	0.3277646664868631	0.5002360758407196	T	T	T
0.3697092885738225	0.6725268560379450	0.4987310100601841	T	T	T
0.7500000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.7501900779962604	0.1665992137085917	0.1650850550942526	T	T	T
0.7496225563010601	0.1665237902173968	0.3303837532965246	T	T	T
0.7500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.7501964836449315	-0.0001202212754511	0.2475641012132512	T	T	T
0.7485905578482290	-0.0000639222575520	0.4113187527460943	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7502405805315119	0.4999941305485187	0.1651070976633443	T	T	T

0.7497858853858543	0.4999069896833750	0.3304436356943649	T	T	T
0.7500000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.7504090270781943	0.3332810755880292	0.2474781176451288	T	T	T
0.7486520740841313	0.3332022833878912	0.4112369302511639	T	T	T
0.7500000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.7502724301687930	0.6665716344975239	0.2476091240442035	T	T	T
0.7486056812123666	0.6663511393832350	0.4113889390268357	T	T	T
0.7500000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.7501626517095121	0.8332598849229472	0.1651190737069449	T	T	T
0.7495821441707079	0.8331730347017730	0.3304281976887161	T	T	T
0.8750000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.8752086014092252	0.1666656089923768	0.2479183498368520	T	T	T
0.8703709041083011	0.1668078846820860	0.4109245439075084	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.8754056783342511	-0.0000524885322095	0.1654020884639034	T	T	T
0.8750365302070363	-0.0000478095047941	0.3315378894357972	T	T	T
0.8750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.8753413555048599	0.4999645852834356	0.2480076968111842	T	T	T
0.8706372110644539	0.4998396484506522	0.4111530866011801	T	T	T
0.8750000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.8755094305897925	0.3333360895232638	0.1654151237555923	T	T	T
0.8753720437278250	0.3333570799547289	0.3316736051965736	T	T	T
0.8750000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.8754688035804802	0.6666158830559857	0.1654493271564743	T	T	T
0.8752626298196551	0.6664917931704362	0.3317141761123547	T	T	T
0.8750000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.8751786912454292	0.8332116022545971	0.2479325654035233	T	T	T
0.8702422405186611	0.8331014861231846	0.4109312374015210	T	T	T
0.4774591393606383	0.4012365902273128	0.5023700613366199	T	T	T
0.4733015034861187	0.2430331913949024	0.5024054993738423	T	T	T
0.4614030926429032	0.7575114068645324	0.5233115680267548	T	T	T
0.4580865517448049	0.6013565898001958	0.5348255812328291	T	T	T
0.4456915332863791	0.3240807477240392	0.5022166787121052	T	T	T
0.4335636572926781	0.6772837579671299	0.5203545802734965	T	T	T

MS2-pbc-3CO2 (-2060.5144 eV)

1.0000000000000000

19.243999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.432999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.243999999999998

Ca O C

156 162 3

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0001331919557343	0.9999992078297952	0.1655926694121994	T	T	T
0.9991280774989160	0.0000252310594611	0.3326781308354337	T	T	T
0.0000000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.0001153134498056	0.1666855451863322	0.2491242257920114	T	T	T
0.9929272976889152	0.1666739968517086	0.4202442383752161	T	T	T
0.1250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.1247880314876855	0.9999831972527485	0.2490389073497237	T	T	T
0.1247925488489262	0.0001278771313694	0.4139450984935645	T	T	T
0.1250000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.1250010477593546	0.1666764188474818	0.1657069067194747	T	T	T
0.1241010394379038	0.1666736651260358	0.3328493589035944	T	T	T
0.0000000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.0001314608710527	0.3333596603427433	0.1655937750607281	T	T	T
0.9991270588052669	0.3333469052721057	0.3326754103248690	T	T	T

0.0000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.0000204885699331	0.5000367231267747	0.2491143837031284	T	T	T
0.9925625400374567	0.4997663855642669	0.4203316424423314	T	T	T
0.1250000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.1247941638735309	0.3333815829143303	0.2490374581762004	T	T	T
0.1247840800453720	0.3332047245961011	0.4139347943468555	T	T	T
0.1250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1249927227391271	0.5000616828551218	0.1657393873405205	T	T	T
0.1237410856273081	0.5000625403743983	0.3328408555887744	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2498163891825026	0.9999430455160963	0.1655734357611488	T	T	T
0.2505919728948178	-0.0000118938812489	0.3315154132193936	T	T	T
0.2500000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.2500307770913869	0.1666737010028524	0.2489190256630916	T	T	T
0.2534196273854724	0.1666530024295017	0.4142625251509558	T	T	T
0.3750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.3751727268508120	0.9997568808716503	0.2481713473288152	T	T	T
0.3814832217990687	-0.0006247522518702	0.4112565738488256	T	T	T
0.3750000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.3748529108971870	0.1666711975634046	0.1652965577259380	T	T	T
0.3780022829585193	0.1666611517728052	0.3309509257181983	T	T	T
0.2500000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.2498231915461307	0.3334030420863514	0.1655730788994896	T	T	T
0.2505946211033933	0.3333424865323399	0.3315108929138925	T	T	T
0.2500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.2499512189121892	0.5001785260321826	0.2490659960925521	T	T	T
0.2523694348435426	0.5003805713381552	0.4141558486631469	T	T	T
0.3750000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.3751823155536828	0.3335904057245739	0.2481730754315406	T	T	T
0.3814790652797442	0.3339328737436578	0.4112540811708423	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3748814367124834	0.5001189859275100	0.1654024861973727	T	T	T
0.3772277258923435	0.5008309716071252	0.3316636084193183	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.4999284894878001	0.9998408617406215	0.1649975525597780	T	T	T
0.5018460270846467	0.0009755084895505	0.3297962112434042	T	T	T
0.5000000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.5003074710920207	0.1666762260300976	0.2474670848719389	T	T	T
0.5067008494850405	0.1666412490920383	0.4203198269344405	T	T	T
0.5000000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.4999339382896366	0.3335072082966180	0.1650005407685129	T	T	T
0.5018441589057384	0.3323655816113967	0.3298086651024849	T	T	T
0.5000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.5001619894579588	0.5002809849239888	0.2481043285271361	T	T	T
0.5054158710159655	0.4955424318003833	0.4172919526033522	T	T	T
0.6250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.6251072244191530	0.0000240029957026	0.2474280533967288	T	T	T
0.6250873821020687	0.0005704070082387	0.4129489918126876	T	T	T
0.6250000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.6250509855041437	0.1666775148700467	0.1649075141411459	T	T	T
0.6239669550050708	0.1666782156790218	0.3306103086138093	T	T	T
0.6250000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.6251051156881512	0.3333395329657133	0.2474281398217769	T	T	T
0.6250878283531884	0.3327726388476501	0.4129485765677889	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.6249547723059701	0.5000859016269067	0.1650379405652337	T	T	T
0.6242911097978130	0.4997249865816152	0.3307178744624887	T	T	T
0.0000000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.0001358368891567	0.6666845173330743	0.1656288951798275	T	T	T
0.9989085783013359	0.6666845184222481	0.3326453314188597	T	T	T

0.1250000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.1248672819706667	0.6666837814989057	0.2491911368214032	T	T	T
0.1237732499698339	0.6666659396197538	0.4139958968881217	T	T	T
0.2500000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.2498811888790930	0.6666790905629399	0.1656612509277221	T	T	T
0.2508933596087723	0.6666787734484568	0.3322115087659347	T	T	T
0.3750000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.3753375340760405	0.6666772631669644	0.2485660435666791	T	T	T
0.3827448355410546	0.6666724595922350	0.4148973574017725	T	T	T
0.5000000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.4999084560132808	0.6666743344757593	0.1651806914211720	T	T	T
0.5013555882644423	0.6666718902444455	0.3319457030441734	T	T	T
0.6250000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.6247237896113373	0.6666782925557101	0.2478339619072955	T	T	T
0.6251066131106925	0.6666736514199716	0.4129653275116220	T	T	T
0.0000000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.0000233124492954	0.8333422490216608	0.2491139274498602	T	T	T
0.9925710200482468	0.8335876984407957	0.4203329951247151	T	T	T
0.1250000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.1249925457323767	0.8332980715736341	0.1657378544990920	T	T	T
0.1237475499969643	0.8332957047997733	0.3328463655492582	T	T	T
0.2500000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.2499434473409957	0.8331779123747326	0.2490685555242565	T	T	T
0.2523855381131040	0.8329430359188323	0.4141800433260628	T	T	T
0.3750000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.3748748173416589	0.8332310710714722	0.1654027171133756	T	T	T
0.3772241321908723	0.8325144672329713	0.3316638646150298	T	T	T
0.5000000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.5001597810898251	0.8330715163549366	0.2481043825507564	T	T	T
0.5054163744223352	0.8377947159521155	0.4172898507615198	T	T	T
0.6250000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.6249515644345206	0.8332678695137311	0.1650394619504275	T	T	T
0.6242877235319562	0.8336322546290964	0.3307181776460431	T	T	T
0.0123615383277221	0.0006440457513839	0.4997852195228937	T	T	T
0.0123456859960508	0.3326879434309972	0.4997753881903454	T	T	T
0.0109641827257151	0.6666646365661760	0.4998868225787544	T	T	T
0.1300621914611934	0.1666708752564899	0.4960520521881248	T	T	T
0.1283987860987375	0.4991878673511465	0.4959283406441100	T	T	T
0.1284106916664743	0.8341169769763559	0.4959368248964934	T	T	T
0.2482871888045309	0.0002851987500982	0.4953281080612436	T	T	T
0.2482784386244119	0.3330340787380756	0.4953080818268782	T	T	T
0.2442052036508477	0.6666343038502702	0.4960897163966324	T	T	T
0.3781934175526323	0.1666682028342343	0.4986734663482080	T	T	T
0.3697984324150402	0.5019916150699747	0.5011865958525512	T	T	T
0.3698295775822149	0.8312848718193158	0.5012382410813084	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7501677012379027	0.9999892498791458	0.1650456405923831	T	T	T
0.7487235519357744	0.0001340549066091	0.3301276876589083	T	T	T
0.7500000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.7499036500928836	0.1666836450950198	0.2478699137462314	T	T	T
0.7481206699268107	0.1666822989726988	0.4122807509083775	T	T	T
0.7500000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.7501680628433262	0.3333682503351902	0.1650441213628785	T	T	T
0.7487246006611281	0.3332333047301544	0.3301240608241477	T	T	T
0.7500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.7498616137633584	0.5000517646606584	0.2479080523624339	T	T	T
0.7479142255157590	0.4998004366925489	0.4123418282688608	T	T	T
0.7500000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.7500445901265822	0.6666813512192348	0.1651266090644040	T	T	T
0.7486442055144990	0.6666854095578316	0.3302648696208541	T	T	T

0.7500000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.7498603710009923	0.8333222988251647	0.2479079090244222	T	T	T
0.7479142566575893	0.8335601672806778	0.4123442409716673	T	T	T
0.8750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.8750757595439379	0.0000238014654949	0.2482017225392329	T	T	T
0.8688936027030474	0.0000546863843057	0.4118673107123860	T	T	T
0.8750000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.8752138612480832	0.1666796114910095	0.1653443112466011	T	T	T
0.8747349451656499	0.1666835604633609	0.3311481283051054	T	T	T
0.8750000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.8750765353786263	0.3333485252956684	0.2482033742246624	T	T	T
0.8688916115253551	0.3333088704074983	0.4118568056916742	T	T	T
0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8751737304879703	0.5000413071631701	0.1653480464648650	T	T	T
0.8746090987945652	0.4999688589792397	0.3311457287590847	T	T	T
0.8750000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.8749848815150559	0.6666954079027055	0.2482315722647187	T	T	T
0.8687589042722409	0.6666887235750018	0.4118306619036965	T	T	T
0.8750000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.8751768966732826	0.8333229312800688	0.1653486689199624	T	T	T
0.8746095757029216	0.8334122800982696	0.3311451261024907	T	T	T
0.1250000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.1250899217505620	0.1666831827887270	0.2493019980354492	T	T	T
0.1278387355772945	0.1666623772968591	0.4154454304755790	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1249124914654609	0.0000055277271553	0.1659585160433601	T	T	T
0.1245558150503926	0.0001125244741511	0.3328543353681603	T	T	T
0.0000000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.0003377567756442	0.1666805357957166	0.1658696999566511	T	T	T
0.0002405805669800	0.1666811134482064	0.3329237406987588	T	T	T
0.0000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.0000702117761481	0.0000447308967393	0.2496049977123890	T	T	T
0.9957887162223342	0.0003167721198978	0.4208086589435447	T	T	T
0.1250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.1249719154068826	0.5000332382394693	0.2492536925195385	T	T	T
0.1263027879673329	0.4997659755900274	0.4151726658689755	T	T	T
0.1250000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.1249185803876968	0.3333570245832121	0.1659585972733011	T	T	T
0.1245586871059908	0.3332407592100385	0.3328492791331080	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0002893486207744	0.5000344413790732	0.1658554867278015	T	T	T
-0.0000922318535446	0.5000023956419696	0.3327566228507585	T	T	T
0.0000000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.0000715818959726	0.3333274175545668	0.2496002509481913	T	T	T
0.9957929735606019	0.3330271436478368	0.4208033637198662	T	T	T
0.3750000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.3748227748865716	0.1666697909996044	0.2486885739494520	T	T	T
0.3793939280034654	0.1666547979688809	0.4190175501672803	T	T	T
0.3750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3744610776937777	0.9999163793269072	0.1655681797885751	T	T	T
0.3743666889818041	0.0000134099084163	0.3316643127393949	T	T	T
0.2500000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.2498234291523702	0.1666718754980495	0.1658187620979725	T	T	T
0.2513968437837070	0.1666604035495305	0.3324334998201153	T	T	T
0.2500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.2497764053227250	0.9999836708712695	0.2491348380818726	T	T	T
0.2530251800061298	0.0003923997940141	0.4162033549680155	T	T	T
0.3750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.3749024674091315	0.5002503936012088	0.2489413162061848	T	T	T
0.3781727759528791	0.5010637477117034	0.4178922855487950	T	T	T

0.3750000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.3744704983292344	0.3334310088056571	0.1655654420973611	T	T	T
0.3743677491886604	0.3333203772319703	0.3316592285796732	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2498503126400556	0.5000836060134145	0.1658664307215387	T	T	T
0.2508415336521186	0.5000676971969344	0.3323186212289025	T	T	T
0.2500000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.2497870385071766	0.3333634983607060	0.2491302345594243	T	T	T
0.2530090215330683	0.3329224121096537	0.4161824076217310	T	T	T
0.5000000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.4996635275098089	0.1666764293501678	0.1648907099105273	T	T	T
0.4998091211746902	0.1666779979702463	0.3292066635288535	T	T	T
0.5000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.4998562876491035	0.9996954879593425	0.2468408209698286	T	T	T
0.5025874451857658	0.0013184278689315	0.4068917417260414	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4996571094733443	0.5002361241372351	0.1651664058681309	T	T	T
0.4997512243116613	0.5003160071826155	0.3310324684856145	T	T	T
0.5000000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.4998639154303491	0.3336555292886419	0.2468470077734078	T	T	T
0.5025740261932530	0.3319888910862298	0.4069186130244509	T	T	T
0.6250000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.6251502272932515	0.1666804789854403	0.2471985843179263	T	T	T
0.6263910581665798	0.1666789828045054	0.4112165751251921	T	T	T
0.6250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6251495897335350	0.9999337385545003	0.1649856502794178	T	T	T
0.6259104154062979	0.0000556642435161	0.3301210939664133	T	T	T
0.6250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.6249402804020052	0.5001125260058682	0.2475156797499772	T	T	T
0.6259709511357995	0.4995556048394997	0.4113511918252536	T	T	T
0.6250000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.6251524865554163	0.3334250851600102	0.1649850176534713	T	T	T
0.6259013889440351	0.3333041237480004	0.3301237746499369	T	T	T
0.0000000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.0000041438754272	0.6666930613707509	0.2496221297294085	T	T	T
0.9951205066498805	0.6666817632298363	0.4208709859618236	T	T	T
0.1250000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.1249659576943221	0.6666783373979730	0.1660149328934703	T	T	T
0.1243495862448167	0.6666787891134554	0.3329214117209252	T	T	T
0.2500000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.2499576388081159	0.6666808629297707	0.2494305356235830	T	T	T
0.2513958996712355	0.6666614040569453	0.4168779197685759	T	T	T
0.3750000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.3745789582009226	0.6666722909147703	0.1657527521882615	T	T	T
0.3750526355016994	0.6666732612776326	0.3329475312112795	T	T	T
0.5000000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.4997956379675766	0.6666765870966593	0.2478751264988239	T	T	T
0.5029943868158413	0.6666593738683405	0.4122699161256335	T	T	T
0.6250000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.6249904378738582	0.6666697781870333	0.1651777131525460	T	T	T
0.6251806467755795	0.6666766606066458	0.3308742786965129	T	T	T
0.0000000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.0002931119093061	0.8333295722156308	0.1658570545290469	T	T	T
0.9999113743788962	0.8333767679553560	0.3327618280721531	T	T	T
0.1250000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.1249738716427156	0.8333330383255897	0.2492586384481128	T	T	T
0.1263157969776140	0.8335687208703024	0.4151847346517636	T	T	T
0.2500000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.2498486716817725	0.8332676320940225	0.1658642187929648	T	T	T
0.2508376561550697	0.8332781728668371	0.3323254161578241	T	T	T

0.3750000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.3748970075054849	0.8331068374928295	0.2489427086461457	T	T	T
0.3781735341824768	0.8322623975905480	0.4179117120108012	T	T	T
0.5000000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.4996491238897394	0.8331098912734410	0.1651671441565692	T	T	T
0.4997483753686695	0.8330148664214662	0.3310302308782224	T	T	T
0.6250000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.6249364739459242	0.8332513607062235	0.2475109667077650	T	T	T
0.6259686885540880	0.8337832450661836	0.4113439434340854	T	T	T
0.0135638206315806	0.1666698797764495	0.4987599872069095	T	T	T
0.0119831303695556	0.4991352211467409	0.4987612581742877	T	T	T
0.0119865400820605	0.8341925623643982	0.4987645324280894	T	T	T
0.1298109522319341	0.0007764113106551	0.4957880181796266	T	T	T
0.1298020977189783	0.3325482647813793	0.4957799826614395	T	T	T
0.1271644369129599	0.6666519385751531	0.4958992489178509	T	T	T
0.2566866415546247	0.1666590100667266	0.4970615500325943	T	T	T
0.2513994610473279	0.4982906473640854	0.4955976847265006	T	T	T
0.2514232420817006	0.8350009728677423	0.4956350615853503	T	T	T
0.3764158484082515	-0.0029408678387781	0.4991616091890134	T	T	T
0.3764039698122106	0.3362539880273230	0.4991031352470661	T	T	T
0.3691707771740154	0.6666418469168712	0.5010969074659943	T	T	T
0.7500000000000000	0.1666666666666643	0.0000000000000000	F	F	F
0.7502995179318127	0.1666829635936899	0.1651192406349942	T	T	T
0.7497552525165870	0.1666826299021531	0.3305190882321706	T	T	T
0.7500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.7503838025753264	0.9999739489801992	0.2475678686463988	T	T	T
0.7485606771390497	0.0001265422774983	0.4113297756826849	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7502079272191218	0.5000718115390818	0.1651735656198597	T	T	T
0.7495671383088403	0.5000899531842191	0.3305858361424441	T	T	T
0.7500000000000000	0.3333333333333357	0.0822561893037914	F	F	F
0.7503854992739331	0.3333920979579694	0.2475655633719873	T	T	T
0.7485573008337021	0.3332351035630648	0.4113280042506425	T	T	T
0.7500000000000000	0.6666666666666643	0.0822561893037914	F	F	F
0.7501564992215265	0.6666904008031013	0.2477493806143890	T	T	T
0.7484464522847138	0.6666835319320426	0.4115422751990604	T	T	T
0.7500000000000000	0.8333333333333357	0.0000000000000000	F	F	F
0.7502089134251697	0.8332848998897325	0.1651761157205328	T	T	T
0.7495722581393133	0.8332788537372920	0.3305901065964136	T	T	T
0.8750000000000000	0.1666666666666643	0.0822561893037914	F	F	F
0.8753381874588299	0.1666844366875858	0.2481124097259934	T	T	T
0.8707403607751311	0.1666806795570696	0.4112934619938567	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.8755120415506740	0.0000003605083799	0.1655003299504026	T	T	T
0.8753873395207975	0.0000718266468326	0.3318568909906956	T	T	T
0.8750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.8752089922370260	0.5000382067561935	0.2480962194364776	T	T	T
0.8704133751988663	0.4998856576738832	0.4111889661762945	T	T	T
0.8750000000000000	0.3333333333333357	0.0000000000000000	F	F	F
0.8755084740422777	0.3333625945106624	0.1654984277035209	T	T	T
0.8753833317251363	0.3333017901789226	0.3318469781487503	T	T	T
0.8750000000000000	0.6666666666666643	0.0000000000000000	F	F	F
0.8754365909531133	0.6666810537834270	0.1655358508136595	T	T	T
0.8751618367670800	0.6666927820583786	0.3318415117439298	T	T	T
0.8750000000000000	0.8333333333333357	0.0822561893037914	F	F	F
0.8752069197152998	0.8333431493020165	0.2480986827049676	T	T	T
0.8704148379521687	0.8334866741917324	0.4111892166089177	T	T	T
0.4759248824062441	0.4207232719682083	0.4988989995931112	T	T	T
0.4795404967374960	0.2631317781076938	0.5037588234311444	T	T	T
0.3901043221323190	0.7454603204009859	0.5668693211983691	T	T	T

0.3898927457444180	0.5877389408646527	0.5668730057893233	T	T	T
0.4795530118354995	0.0702053478870005	0.5036233202468603	T	T	T
0.4759267191462148	0.9126068235415630	0.4988721534266715	T	T	T
0.4483773528149300	0.3402251165926976	0.5011066734982330	T	T	T
0.3848669421894020	0.6666013042220775	0.5481904235345518	T	T	T
0.4483773377528413	-0.0068997800480167	0.5010578147674780	T	T	T

MS3-pbc-0CO2 (-2647.5191 eV)

1.0000000000000000		
19.2439999999999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	19.2439999999999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.2439999999999998

Ca O
208 208

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0004502748086789	-0.0000000037310199	0.1655252562902942	T	T	T
-0.0006910978451978	-0.0000000109842579	0.3324901163084655	T	T	T
0.0000000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.0004684953688910	0.1249993663672235	0.2488832679162713	T	T	T
-0.0076012268224210	0.1250039304113274	0.4198735921611869	T	T	T
0.1250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.1251803556573672	-0.0000000217796055	0.2492745156263463	T	T	T
0.1242661931014118	-0.0000000135469033	0.4142927981272742	T	T	T
0.1250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.1251792026899668	0.1250000344768090	0.1657470862113378	T	T	T
0.1236696775176353	0.1249988171601270	0.3328685002432889	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0004522902105300	0.2499999987891151	0.1655217806870718	T	T	T
-0.0006862943931929	0.2499999950849219	0.3324895346550185	T	T	T
0.0000000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.0004685014923945	0.3750006059333943	0.2488832847521368	T	T	T
-0.0076012519985404	0.3749960730488145	0.4198735947486092	T	T	T
0.1250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.1251838427103013	0.2499999877664704	0.2492788805781931	T	T	T
0.1242702530439672	0.2500000021733334	0.4142927959950471	T	T	T
0.1250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.1251791994438024	0.3749999826728684	0.1657470919234170	T	T	T
0.1236696755207583	0.3750011638001653	0.3328684980189550	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2498185736848435	0.0000000090040868	0.1657435001502241	T	T	T
0.2513420061114505	-0.0000000077275692	0.3328693432489814	T	T	T
0.2500000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.2498120976042071	0.1249979092710149	0.2492767559363001	T	T	T
0.2507602191420116	0.1250002943993975	0.4142984820747027	T	T	T
0.3750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.3745220998564018	0.0000000152939408	0.2488816276940066	T	T	T
0.3826052208991569	-0.0000000173243435	0.4198786148497513	T	T	T
0.3750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.3745446162169854	0.1250019788148578	0.1655218716944509	T	T	T
0.3756861606113804	0.1250015050604107	0.3324908052165463	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2498154539977012	0.2500000140705472	0.1657475118064221	T	T	T
0.2513479612366273	0.2500000245844864	0.3328678076327643	T	T	T
0.2500000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.2498121381219243	0.3750021472264789	0.2492767547134410	T	T	T
0.2507602087581678	0.3749997342256425	0.4142984798062215	T	T	T
0.3750000000000000	0.2500000000000000	0.0822561893037914	F	F	F

0.3745247716814620	0.25000000416338517	0.2488872697013382	T	T	T
0.3826065106868856	0.2499999896396905	0.4198779809164783	T	T	T
0.3750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.3745446508117274	0.3749980470154924	0.1655218531033308	T	T	T
0.3756861370773448	0.3749985341075657	0.3324908016831519	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.4994893487375124	0.0000000003031617	0.1650977423804293	T	T	T
0.4998777446527824	0.0000000088063302	0.3303350875815023	T	T	T
0.5000000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.4994141471960461	0.1250015583655018	0.2476503040981179	T	T	T
0.5058223911174153	0.1250028544546171	0.4110118491186139	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4994879656520561	0.2499999912810670	0.1650972953719669	T	T	T
0.4998803070738126	0.2500000015903149	0.3303347719796282	T	T	T
0.5000000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.4994141109883842	0.3749984702186307	0.2476503106549675	T	T	T
0.5058223735340588	0.3749971565742740	0.4110118456573942	T	T	T
0.6250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.6246932105371104	-0.0000000117930575	0.2470279927836715	T	T	T
0.6263851309084102	-0.0000000244701634	0.4111106728185293	T	T	T
0.6250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.6248597772761577	0.1250020116701691	0.1648177957708592	T	T	T
0.6255679766298395	0.1249996134150057	0.3290838177222102	T	T	T
0.6250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.6246996172431958	0.2500000010519492	0.2470269897070439	T	T	T
0.6263883358234712	0.2500000213620452	0.4111065328450323	T	T	T
0.6250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.6248597771627536	0.3749979832211355	0.1648177985418829	T	T	T
0.6255679485175849	0.3750003842077767	0.3290838047521177	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0004502800252913	0.4999999892087588	0.1655252627331244	T	T	T
-0.0006911379399901	0.4999999769690296	0.3324901241222539	T	T	T
0.1250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.1251804056955956	0.4999999666459362	0.2492745156500442	T	T	T
0.1242660805335013	0.5000000371213446	0.4142927778457683	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2498186261067055	0.4999999924614554	0.1657435021813886	T	T	T
0.2513419951291468	0.4999999949279339	0.3328693473902655	T	T	T
0.3750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.3745221282468250	0.4999999776075290	0.2488815903984492	T	T	T
0.3826051766623886	0.5000000089832239	0.4198786366754274	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4994893796484640	0.4999999996206147	0.1650977157503628	T	T	T
0.4998777042858873	0.5000000069299755	0.3303350688915557	T	T	T
0.6250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.6246931609888751	0.4999999881269555	0.2470280120343288	T	T	T
0.6263851157096454	0.5000000121510864	0.4111106445381409	T	T	T
0.0000000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.0004685029034120	0.6249993545811898	0.2488832631087804	T	T	T
-0.0076012195005077	0.6250039447864855	0.4198735843317649	T	T	T
0.1250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.1251791900121090	0.6250000001453804	0.1657471060695798	T	T	T
0.1236696686456808	0.6249988159758869	0.3328684941655388	T	T	T
0.2500000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.2498121187576129	0.6249978068916162	0.2492767446916306	T	T	T
0.2507601589074025	0.6250002703127443	0.4142985088421395	T	T	T
0.3750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.3745446473946718	0.6250019450864516	0.1655218543155732	T	T	T
0.3756861215017032	0.6250014360583708	0.3324907923268693	T	T	T
0.5000000000000000	0.6250000000000000	0.0822561893037914	F	F	F

0.4994140927683278	0.6250015304587537	0.2476503008076165	T	T	T
0.5058223725356161	0.6250028531325020	0.4110118361097802	T	T	T
0.6250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.6248597746538457	0.6250020342423109	0.1648177975353014	T	T	T
0.6255679584444744	0.6249996134617716	0.3290837998732754	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0004522893997553	0.7499999947372987	0.1655217810910127	T	T	T
-0.0006863027055116	0.7499999824135370	0.3324895254963082	T	T	T
0.1250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.1251838256721822	0.7499999740187111	0.2492788812885664	T	T	T
0.1242702807584323	0.7499999836464764	0.4142927836703295	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2498154468996019	0.7499999650691742	0.1657475085108588	T	T	T
0.2513480015348248	0.7499999601308222	0.3328677865813146	T	T	T
0.3750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.3745247803622530	0.7499999483822185	0.2488872588171376	T	T	T
0.3826065055159137	0.7499999754138614	0.4198779508629287	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.4994879565264691	0.7500000060241581	0.1650972876319710	T	T	T
0.4998802955101946	0.7499999750837426	0.3303347421494064	T	T	T
0.6250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.6246996061665415	0.7500000325768793	0.2470269795012534	T	T	T
0.6263883103230470	0.749999952905050	0.4111064900965916	T	T	T
0.0000000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.0004684876917991	0.8750006099042459	0.2488832629997599	T	T	T
-0.0076012121069576	0.8749960854666979	0.4198735600631263	T	T	T
0.1250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.1251791841967269	0.8749999603890464	0.1657470716233841	T	T	T
0.1236696938926824	0.8750011488767488	0.3328684978387766	T	T	T
0.2500000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.2498121125057608	0.8750020966699024	0.2492767534396639	T	T	T
0.2507602444649474	0.8749996898587623	0.4142984531850994	T	T	T
0.3750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.3745446164281284	0.8749980353567612	0.1655218660071433	T	T	T
0.3756861545278616	0.8749984765487193	0.3324908141931694	T	T	T
0.5000000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.4994141407097832	0.8749984508678091	0.2476503049663859	T	T	T
0.5058223737382528	0.8749971066719389	0.4110118298693767	T	T	T
0.6250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.6248597572114400	0.8749979839329993	0.1648177969472956	T	T	T
0.6255679724028869	0.8750003754224763	0.3290838057990416	T	T	T
0.0099554533682825	-0.0000000215597693	0.4992713114582077	T	T	T
0.0099610840694516	0.2500000213450219	0.4992749889439636	T	T	T
0.0099553614706216	0.5000000464618296	0.4992713116080498	T	T	T
0.0099610701460706	0.7500000505957163	0.4992749557215849	T	T	T
0.1270699611083826	0.1249970858985898	0.4960451497105206	T	T	T
0.1270699166887912	0.3750030158364208	0.4960451384897720	T	T	T
0.1270698983968328	0.6249970988829590	0.4960452338859820	T	T	T
0.1270699804421374	0.8750029309406447	0.4960451748403375	T	T	T
0.2479576426824303	-0.0000000273302210	0.4960559310429665	T	T	T
0.2479560171091122	0.2500000156657214	0.4960558876577483	T	T	T
0.2479575766059788	0.5000000183967079	0.4960559816691884	T	T	T
0.2479560893554989	0.7500000064839738	0.4960559001996709	T	T	T
0.3650760112991578	0.1249972872661840	0.4992809127811493	T	T	T
0.3650759434045409	0.3750027372232947	0.4992809294523446	T	T	T
0.3650759920972548	0.6249972619218646	0.4992809578555932	T	T	T
0.3650760229380324	0.8750027319654018	0.4992809097918013	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7501358003592611	0.0000000035768730	0.1648202409376641	T	T	T
0.7494283058051877	0.0000000001524549	0.3290838237201512	T	T	T

0.7500000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.7503009451341058	0.1250039039999251	0.2470274813232649	T	T	T
0.7486089851552625	0.1249988541390084	0.4111092067650864	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7501456337164376	0.2499999939391538	0.1648222631076805	T	T	T
0.7494325448725795	0.2500000064727181	0.3290859006276824	T	T	T
0.7500000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.7503009356951377	0.3749961055337320	0.2470274625553285	T	T	T
0.7486089755350619	0.3750011749713327	0.4111091779515516	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7501358110501904	0.4999999935510779	0.1648202429520348	T	T	T
0.7494282986559990	0.5000000071221717	0.3290838214677488	T	T	T
0.7500000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.7503009182027776	0.6250038925330477	0.2470274773100410	T	T	T
0.7486089441544711	0.6249988745293931	0.4111092059400064	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7501456121368516	0.7500000018543923	0.1648222702723244	T	T	T
0.7494325464784164	0.7500000113579944	0.3290858821937533	T	T	T
0.7500000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.7503009379423731	0.8749961097064500	0.2470274731838930	T	T	T
0.7486089702216651	0.8750011278624795	0.4111092017588435	T	T	T
0.8750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.8755730437376942	0.0000000073016160	0.2476519880380421	T	T	T
0.8691847763848313	-0.0000000291975521	0.4110105372979285	T	T	T
0.8750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.8755059324459160	0.1249989754315350	0.1650975561011440	T	T	T
0.8751174283097024	0.1250010658744279	0.3303369848639283	T	T	T
0.8750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.8755845805655323	0.2500000063915289	0.2476525610044563	T	T	T
0.8691824960464437	0.2500000156724019	0.4110067181339776	T	T	T
0.8750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.8755059433774237	0.3750010175833274	0.1650975588174453	T	T	T
0.8751174295703277	0.3749989229325478	0.3303369717664986	T	T	T
0.8750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.8755730275403885	0.4999999907896528	0.2476519889287148	T	T	T
0.8691847609046530	0.5000000234949880	0.4110105330660240	T	T	T
0.8750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.8755059316712345	0.6249989791727937	0.1650975550394336	T	T	T
0.8751174150653417	0.6250010696810439	0.3303369645289523	T	T	T
0.8750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.8755845805201564	0.7499999921169721	0.2476525718583228	T	T	T
0.8691824974993200	0.7500000012409347	0.4110066903230700	T	T	T
0.8750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.8755059393124107	0.8750010137015654	0.1650975648030168	T	T	T
0.8751174330437446	0.8749989306962588	0.3303369662648599	T	T	T
0.1250000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.1251471853351288	0.1249962873189756	0.2490317705071457	T	T	T
0.1254157965624820	0.1249978497709705	0.4149134209618647	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1249998603136179	-0.0000000142432979	0.1657304575697205	T	T	T
0.1239159216437821	-0.0000000263811154	0.3323788395958536	T	T	T
0.0000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.0003206671809222	0.1249943443632431	0.1655791740419062	T	T	T
-0.0003671265734076	0.1249943204296901	0.3321239210737237	T	T	T
0.0000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.0000890182450301	-0.0000000090726691	0.2491036756909297	T	T	T
-0.0059183470546459	-0.0000000195777717	0.4198131846385488	T	T	T
0.1250000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.1251471543807529	0.3750036866537294	0.2490317898877914	T	T	T
0.1254157537872868	0.3750021483250173	0.4149134313798956	T	T	T

0.1250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.1250154964843037	0.2499999978915710	0.1657288624119274	T	T	T
0.1239125439138386	0.2499999843987058	0.3323796614532673	T	T	T
0.0000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.0003206752987085	0.3750056559653070	0.1655791776165832	T	T	T
-0.0003671551079541	0.3750056498792741	0.3321239362914981	T	T	T
0.0000000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.0000985615877652	0.2500000124553962	0.2491055148002428	T	T	T
-0.0059112597221893	0.2500000020053252	0.4198114698899106	T	T	T
0.3750000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.3748977205276995	0.1249962408369122	0.2491065142056363	T	T	T
0.3809246694463108	0.1249954608706489	0.4198152221197722	T	T	T
0.3750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3746844683087506	-0.0000000028595057	0.1655719126118271	T	T	T
0.3753637454385437	-0.0000000043127412	0.3321268297066376	T	T	T
0.2500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.2499864916662850	0.1250007576461884	0.1657293038215900	T	T	T
0.2510878604295786	0.1250005961113103	0.3323839885609744	T	T	T
0.2500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.2498453888513428	-0.0000000179389764	0.2490332080089533	T	T	T
0.2496037189766631	-0.0000000012196742	0.4149124121478203	T	T	T
0.3750000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.3748977645661415	0.3750037504551834	0.2491064881590683	T	T	T
0.3809246362604870	0.3750045404894802	0.4198152278471917	T	T	T
0.3750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.3746891668560340	0.2499999792180001	0.1655776669141888	T	T	T
0.3753707229279276	0.2499999682588760	0.3321218235928961	T	T	T
0.2500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.2499865277526599	0.3749992618673485	0.1657292873473828	T	T	T
0.2510878365815483	0.3749993509497405	0.3323840032242257	T	T	T
0.2500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.2498439261030657	0.2499999749479025	0.2490338187899190	T	T	T
0.2496140006898890	0.2499999967986311	0.4149176671362373	T	T	T
0.5000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.4996327394992078	0.1249959470151392	0.1651597344932321	T	T	T
0.5001118827304875	0.1249945398239234	0.3309484631546418	T	T	T
0.5000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.4997460241633791	0.0000000039682015	0.2474838116430185	T	T	T
0.5051372071349850	-0.0000000087753333	0.4102423367082558	T	T	T
0.5000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.4996327969204953	0.3750039746276072	0.1651597198090426	T	T	T
0.5001118692800949	0.3750054487781397	0.3309484861058733	T	T	T
0.5000000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.4997486739677753	0.2499999949833478	0.2474815391764768	T	T	T
0.5051250476693760	0.2499999933900638	0.4102385513446166	T	T	T
0.6250000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.6247703130630626	0.1250035906198045	0.2470204509827531	T	T	T
0.6263301791845933	0.1250016415308717	0.4105075469691561	T	T	T
0.6250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6249143950210910	0.0000000004387377	0.1648312717640598	T	T	T
0.6254671739879792	-0.0000000024412390	0.3296042879809993	T	T	T
0.6250000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.6247703161583065	0.3749964252046629	0.2470204354026291	T	T	T
0.6263301745517610	0.3749983690093018	0.4105075207939433	T	T	T
0.6250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.6249191757220747	0.2499999867932577	0.1648273461957779	T	T	T
0.6254744626755240	0.2499999944014848	0.3295985198413879	T	T	T
0.0000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.0000889925430737	0.4999999827922758	0.2491036982441419	T	T	T
-0.0059184072060929	0.5000000062067623	0.4198131693289519	T	T	T

0.1250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1249998713798379	0.4999999828633473	0.1657304469733082	T	T	T
0.1239158566958253	0.4999999850249163	0.3323788475222189	T	T	T
0.2500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.2498453953148731	0.4999999827339164	0.2490331625353597	T	T	T
0.2496036152581469	0.4999999983612785	0.4149124756872101	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3746845578275597	0.4999999945311566	0.1655720006266328	T	T	T
0.3753637157547933	0.4999999870071724	0.3321268204627371	T	T	T
0.5000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.4997460119044648	0.5000000005003351	0.2474837957505933	T	T	T
0.5051371747468042	0.5000000116039641	0.4102423433808589	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.6249144641484601	0.4999999901083003	0.1648312730367051	T	T	T
0.6254671719192743	0.5000000150787383	0.3296042749518112	T	T	T
0.0000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.0003206504919554	0.6249943175646213	0.1655791757364041	T	T	T
-0.0003671677700655	0.6249943284016419	0.3321239140991671	T	T	T
0.1250000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.1251471316794393	0.6249962987626150	0.2490317938443335	T	T	T
0.1254157392501268	0.6249978976559720	0.4149134780929474	T	T	T
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0.2499865106141110	0.6250007152786791	0.1657292868011919	T	T	T
0.2510878098937496	0.6250006208980349	0.3323840257749652	T	T	T
0.3750000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.3748977339782478	0.6249962493461390	0.2491064817060805	T	T	T
0.3809246323148122	0.6249954522850006	0.4198152285070378	T	T	T
0.5000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.4996328033929897	0.6249960082743244	0.1651597213936808	T	T	T
0.5001118666958827	0.6249945618665921	0.3309484711931552	T	T	T
0.6250000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.6247702997125757	0.6250035672970330	0.2470204375441533	T	T	T
0.6263301676166096	0.6250016612469966	0.4105075177642089	T	T	T
0.0000000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.0000985809890257	0.7500000385634004	0.2491055035376119	T	T	T
-0.0059112597806400	0.7500000143590061	0.4198114309167469	T	T	T
0.1250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.1250154873976596	0.749999969238319	0.1657288591927278	T	T	T
0.1239125518246850	0.7499999881154236	0.3323796597934836	T	T	T
0.2500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.2498439134618399	0.7499999944521585	0.2490337969693996	T	T	T
0.2496140525975681	0.7500000014176648	0.4149176616925246	T	T	T
0.3750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.3746891674283966	0.7500000087050868	0.1655776562367397	T	T	T
0.3753707417243667	0.7500000100953673	0.3321217838831615	T	T	T
0.5000000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.4997486742062150	0.7500000035581611	0.2474815237596293	T	T	T
0.5051250295117606	0.7499999934979703	0.4102385131671489	T	T	T
0.6250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.6249191724545494	0.7499999962727714	0.1648273415516048	T	T	T
0.6254744689436259	0.7499999921186582	0.3295984842699334	T	T	T
0.0000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.0003206705433042	0.8750056642029960	0.1655791760883438	T	T	T
-0.0003671113469627	0.8750056675362919	0.3321239260182591	T	T	T
0.1250000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.1251471948602361	0.8750037214299440	0.2490317686338001	T	T	T
0.1254157924545418	0.8750020869921148	0.4149134409913089	T	T	T
0.2500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.2499865032010477	0.8749992317872447	0.1657293051091975	T	T	T
0.2510878647004468	0.8749993388943732	0.3323839727834371	T	T	T

0.3750000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.3748977464485356	0.8750037456828490	0.2491065211752158	T	T	T
0.3809246575379248	0.8750045352621366	0.4198151948065225	T	T	T
0.5000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.4996327253024549	0.8750040467660741	0.1651597294036758	T	T	T
0.5001118787577542	0.8750054557067810	0.3309484568688223	T	T	T
0.6250000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.6247702996945325	0.8749964234860439	0.2470204355373569	T	T	T
0.6263301683843743	0.8749983308067355	0.4105075222646896	T	T	T
0.0097323223205174	0.1249945327512642	0.4982774189931327	T	T	T
0.0097322662930238	0.3750055311529232	0.4982774271347469	T	T	T
0.0097322392943957	0.6249945609336078	0.4982774268454559	T	T	T
0.0097323362207095	0.8750054945712331	0.4982774021755066	T	T	T
0.1255404207578855	-0.0000000010058703	0.4958018985757810	T	T	T
0.1255421339708190	0.2500000229845721	0.4957979544420085	T	T	T
0.1255403223500312	0.5000000284818201	0.4958018815836860	T	T	T
0.1255421618764397	0.7500000055971485	0.4957979612761694	T	T	T
0.2494916994830977	0.1249979017772639	0.4958059913993680	T	T	T
0.2494916266341160	0.3750020853267385	0.4958060149927043	T	T	T
0.2494916665755988	0.6249979300023830	0.4958060531465364	T	T	T
0.2494917263645975	0.8750020567400845	0.4958059727800698	T	T	T
0.3652938729600451	-0.0000000359167796	0.4982737198961915	T	T	T
0.3652974812261600	0.2499999975189687	0.4982795860047445	T	T	T
0.3652938231202045	0.4999999829595606	0.4982737449590192	T	T	T
0.3652975317011362	0.7499999636332150	0.4982795590831938	T	T	T
0.7500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.7500778455739108	0.1249962012053933	0.1648274099670364	T	T	T
0.7495346850331969	0.1250009887540962	0.3295979272551227	T	T	T
0.7500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.7502234652519345	0.0000000108066779	0.2470269461448317	T	T	T
0.7486720632049233	-0.0000000190673935	0.4105052834109312	T	T	T
0.7500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.7500778270695253	0.3750038003182781	0.1648274026042468	T	T	T
0.7495346756737773	0.3749990192395980	0.3295979056985452	T	T	T
0.7500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.7502293312662459	0.2500000097073094	0.2470230491747668	T	T	T
0.7486777791523276	0.2500000036258888	0.4105149296474342	T	T	T
0.7500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.7502234526897321	0.5000000172613348	0.2470269468073292	T	T	T
0.7486720528853943	0.50000000215490746	0.4105052886612078	T	T	T
0.7500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.7500778297424123	0.6249961997802812	0.1648274087836412	T	T	T
0.7495346699984030	0.6250010019086357	0.3295979233382953	T	T	T
0.7500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.7502293313427927	0.7500000094118551	0.2470230422139161	T	T	T
0.7486777822103539	0.7499999978185137	0.4105149123564804	T	T	T
0.7500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.7500778297292685	0.8750038075325076	0.1648274077417719	T	T	T
0.7495346803262192	0.8749990292563439	0.3295979180081577	T	T	T
0.8750000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.8752453872244049	0.1249972866589189	0.2474806642537052	T	T	T
0.8698637952195831	0.1250018270580645	0.4102403414085976	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.8753632161687450	-0.0000000030359265	0.1651641506057243	T	T	T
0.8748830402994775	-0.0000000282623463	0.3309506882743898	T	T	T
0.8750000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.8752453594690872	0.3750027031351919	0.2474806512224529	T	T	T
0.8698637652038942	0.3749981432993591	0.4102403310318610	T	T	T
0.8750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.8753721771964382	0.2500000029089147	0.1651604148761966	T	T	T

0.8748956335528855	0.2500000056536203	0.3309478578793267	T	T	T
0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8753632173299857	0.5000000008527369	0.1651641529974857	T	T	T
0.8748829887763141	0.5000000145604704	0.3309506758521329	T	T	T
0.8750000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.8752453759526327	0.6249973265120663	0.2474806457241074	T	T	T
0.8698637853766509	0.6250018553898788	0.4102403348639999	T	T	T
0.8750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.8753721751834583	0.7499999991937494	0.1651604014927502	T	T	T
0.8748956434447551	0.7500000080883070	0.3309478454699715	T	T	T
0.8750000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.8752453747972384	0.8750027127293977	0.2474806482031203	T	T	T
0.8698637898266971	0.8749981524511614	0.4102403225044067	T	T	T

MS3-pbc-1CO2 (-2673.1204 eV)

1.0000000000000000

19.2439999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.2439999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.2439999999999998

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Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0003464179142064	0.0000421120866274	0.1655906887601391	T	T	T
0.9993256499425737	0.0000869750185305	0.3326144986825830	T	T	T
0.0000000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.0003877748481342	0.1250283762434024	0.2490742703538275	T	T	T
0.9930488737234316	0.1251356249055443	0.4202668177774672	T	T	T
0.1250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.1250452351477493	0.0000074982718236	0.2492418594454676	T	T	T
0.1244073429354224	-0.0000912933118872	0.4141533889069248	T	T	T
0.1250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.1251409157933675	0.1249871139307209	0.1657743175347466	T	T	T
0.1240538267178282	0.1248723690021177	0.3329734475591925	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0003611368322281	0.2500000557588724	0.1656057698083813	T	T	T
0.9995577134493635	0.2500000973514097	0.3327362587402031	T	T	T
0.0000000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.0003875791411785	0.3749714930745831	0.2490743089113413	T	T	T
0.9930486182710389	0.3748649504235915	0.4202668605615051	T	T	T
0.1250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.1250655769295838	0.2500000117610507	0.2492100204760493	T	T	T
0.1250662531348511	0.2500003993408104	0.4142307628609811	T	T	T
0.1250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.1251409484690425	0.3750130389897942	0.1657742782146155	T	T	T
0.1240541476325991	0.3751279078529455	0.3329733548707670	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2498383491671358	-0.0000096718942557	0.1657210166502722	T	T	T
0.2511362741453539	0.9998744997523836	0.3325404414275172	T	T	T
0.2500000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.2499848040156862	0.1248714802140483	0.2492255753825523	T	T	T
0.2523026676827426	0.1242083555237357	0.4145563961036250	T	T	T
0.3750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.3748661336911163	0.9998154344509326	0.2487640712827765	T	T	T
0.3823899101645943	0.9982715197610815	0.4179632660664508	T	T	T
0.3750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.3746923858699888	0.1249599490311089	0.1655192409418434	T	T	T
0.3764587756650505	0.1240101036941783	0.3321743466144832	T	T	T

0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2498548177182081	0.2500000427023037	0.1657146605089491	T	T	T
0.2508086111021657	0.2500006051150912	0.3321423137116707	T	T	T
0.2500000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.2499848129421378	0.3751285901226640	0.2492259064151111	T	T	T
0.2523039618828855	0.3757928765978238	0.4145576619531936	T	T	T
0.3750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.3748326945126840	0.2500000977339444	0.2486924101367663	T	T	T
0.3809523602343926	0.2500014009660319	0.4135182231438689	T	T	T
0.3750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.3746922929167770	0.3750401449976777	0.1655192484562059	T	T	T
0.3764589129192233	0.3759907650424437	0.3321743247784790	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.4997022144251620	0.0000069618835977	0.1651619051895874	T	T	T
0.5004469783436649	0.0007485141853149	0.3309540397395623	T	T	T
0.5000000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.4998316211580084	0.1249303272020572	0.2478996874703917	T	T	T
0.5055234564912516	0.1270325485958332	0.4148374815254031	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4997260789365319	0.2499999550578424	0.1651300294607946	T	T	T
0.5009775229124034	0.2500009992011529	0.3299764256367843	T	T	T
0.5000000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.4998316624361718	0.3750699620372918	0.2478999847222229	T	T	T
0.5055230799079435	0.3729690616572695	0.4148384159338641	T	T	T
0.6250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.6248471898024172	0.0001630313929335	0.2474925946854378	T	T	T
0.6259880930527576	0.0004816344363124	0.4120098690685322	T	T	T
0.6250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.6249233774525625	0.1250094469783402	0.1649814453752070	T	T	T
0.6249614037107576	0.1252605542646420	0.3301707031161326	T	T	T
0.6250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.6250298630931630	0.2500002814628705	0.2473939080026614	T	T	T
0.6256035055372672	0.2500008872580320	0.4127581873064132	T	T	T
0.6250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.6249233322385384	0.3749905739770931	0.1649814584328153	T	T	T
0.6249602551784540	0.3747400005621958	0.3301712358311535	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0003464542794513	0.4999578468876011	0.1655906924007592	T	T	T
0.9993255779874867	0.4999132203284664	0.3326143502403317	T	T	T
0.1250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.1250451334270822	0.4999926439871263	0.2492418519071763	T	T	T
0.1244079190049803	0.5000913358440328	0.4141533205520675	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2498383743762170	0.5000098459493136	0.1657210466608036	T	T	T
0.2511361682438822	0.5001251085442266	0.3325404411149283	T	T	T
0.3750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.3748661141859454	0.5001846073966414	0.2487643122291867	T	T	T
0.3823897154439902	0.5017266678473022	0.4179643060574462	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4997021388210852	0.4999932665797294	0.1651619440763456	T	T	T
0.5004461689825366	0.4992508423616265	0.3309544962037205	T	T	T
0.6250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.6248468950622177	0.4998370137019147	0.2474925561986986	T	T	T
0.6259869191473811	0.4995183034168358	0.4120102882185442	T	T	T
0.0000000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.0002437664060048	0.6249667388111595	0.2489514321801417	T	T	T
0.9925194921495828	0.6248997413282789	0.4200484762666704	T	T	T
0.1250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.1250729690907317	0.6249924276271868	0.1657370226373603	T	T	T
0.1235269124868088	0.6250501144807878	0.3327018035279763	T	T	T

0.2500000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.2498077500554040	0.6250451585565310	0.2491305497322980	T	T	T
0.2505834586959159	0.6254438802117923	0.4138401668053043	T	T	T
0.3750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.3746484204750810	0.6250216336979574	0.1654925812669727	T	T	T
0.3758597466961627	0.6253709516195926	0.3320592395351275	T	T	T
0.5000000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.4998013920425980	0.6248541774809601	0.2478883543350667	T	T	T
0.5059477268969638	0.6250669356515066	0.4110990548985266	T	T	T
0.6250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.6249054110997941	0.6249588098571880	0.1649701465404437	T	T	T
0.6257146373951882	0.6248199715175689	0.3296227006983931	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0003292998128537	0.7500000665051927	0.1655630217532363	T	T	T
0.9991911798099704	0.7500000044145398	0.3325275418126316	T	T	T
0.1250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.1249878376556890	0.7500002414078016	0.2491975070458890	T	T	T
0.1239727413128885	0.7499997197196250	0.4141034790365729	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2497842208394191	0.7500000510146027	0.1656948948582491	T	T	T
0.2511548684394381	0.7499997389374106	0.3324727791175656	T	T	T
0.3750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.3747591651268204	0.7500000232003708	0.2486777987969805	T	T	T
0.3824701544854419	0.7499992256971288	0.4189775567114469	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.4996896127688140	0.7500000157038226	0.1651707767122398	T	T	T
0.5002448377845513	0.7499995460310329	0.3304182511473936	T	T	T
0.6250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.6248903508208965	0.7499999405108949	0.2473714763602796	T	T	T
0.6264175675716509	0.7499994184248723	0.4116740611393229	T	T	T
0.0000000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.0002438802847774	0.8750333853330525	0.2489514870406329	T	T	T
0.9925194254742630	0.8750998928512964	0.4200486684530081	T	T	T
0.1250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.1250728155568853	0.8750075757777036	0.1657369876448315	T	T	T
0.1235272278124993	0.8749499394225672	0.3327016711962824	T	T	T
0.2500000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.2498078757314555	0.8749550027500257	0.2491306242811288	T	T	T
0.2505833157689194	0.8745552524616957	0.4138406044664902	T	T	T
0.3750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.3746483939630991	0.8749783400249740	0.1654925498338597	T	T	T
0.3758600043013842	0.8746283767052893	0.3320592046794963	T	T	T
0.5000000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.4998016005421630	0.8751456952900163	0.2478883500606347	T	T	T
0.5059486095040793	0.8749317670338348	0.4110989582705775	T	T	T
0.6250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.6249054148758112	0.8750412428820337	0.1649700403636988	T	T	T
0.6257151577420718	0.8751797131822151	0.3296226293367548	T	T	T
0.0107981742950583	0.0001647829115940	0.4995396398518867	T	T	T
0.0123741232256259	0.2500005838842084	0.4996416461292543	T	T	T
0.0107983769364210	0.4998351347181647	0.4995398245460139	T	T	T
0.0099442263124867	0.7499996313320995	0.4994183371552403	T	T	T
0.1290731383885632	0.1244823344096331	0.4961036061819614	T	T	T
0.1290745808500955	0.3755189897213050	0.4961036225988546	T	T	T
0.1271151292102695	0.6253315622259956	0.4959191101217696	T	T	T
0.1271144016847496	0.8746676156575319	0.4959193300505173	T	T	T
0.2481432780958947	0.9985854802089065	0.4956217341422240	T	T	T
0.2484855404240635	0.2500016724114940	0.4956425598592734	T	T	T
0.2481461504689222	0.5014122695643426	0.4956220875635483	T	T	T
0.2478560554327115	0.7499991258790671	0.4956772591222284	T	T	T

0.3713608199329158	0.1140695541232873	0.4991648569356298	T	T	T
0.3713613787687366	0.3859309915157133	0.4991658210243097	T	T	T
0.3654032445637128	0.6263902032421915	0.4985394776934579	T	T	T
0.3654024706544113	0.8736070256321675	0.4985396532895290	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7501837597173637	0.0000679064726896	0.1650136997277149	T	T	T
0.7493262804789762	0.0002658260883306	0.3297974980869015	T	T	T
0.7500000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.7501866695015770	0.1250792471798023	0.2476454496648941	T	T	T
0.7485390286945899	0.1252074886048972	0.4120210933921308	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7502473221446394	0.2499998913524383	0.1650107055484114	T	T	T
0.7491672391924319	0.2500001973836934	0.3299364042025228	T	T	T
0.7500000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.7501863769070259	0.3749208159369296	0.2476454441608223	T	T	T
0.7485384318825337	0.3747932674403116	0.4120213211672144	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7501836438863058	0.4999322937281325	0.1650137796892542	T	T	T
0.7493258485903956	0.4997341675362117	0.3297972486213179	T	T	T
0.7500000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.7502957901639035	0.6249123865747506	0.2474570318264645	T	T	T
0.7486648815671159	0.6248013881785952	0.4117943349018059	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7501928405841508	0.7500000649783277	0.1649768506974055	T	T	T
0.7494481492330471	0.7499999148454156	0.3296512330760016	T	T	T
0.7500000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.7502962328563337	0.8750875435570572	0.2474571863096230	T	T	T
0.7486651416697597	0.8751981524559400	0.4117944977155683	T	T	T
0.8750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.8753822918087032	0.0001126118941782	0.2480091630008166	T	T	T
0.8693552915409556	0.0001496401129571	0.4114882048733383	T	T	T
0.8750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.8753982996248317	0.1250295396074604	0.1652794807323233	T	T	T
0.8751500522628475	0.1251262944733924	0.3309132485973320	T	T	T
0.8750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.8754148039593286	0.2500000475448138	0.2480890374973024	T	T	T
0.8694215993668807	0.2500004063358052	0.4116849814429556	T	T	T
0.8750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.8753983687413118	0.3749705844671059	0.1652795119177644	T	T	T
0.8751499385652348	0.3748736555079455	0.3309131790908743	T	T	T
0.8750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.8753819252389805	0.4998872726181906	0.2480090246199452	T	T	T
0.8693549311401956	0.4998503860738744	0.4114882210137471	T	T	T
0.8750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.8753874858136853	0.6249552447791296	0.1652147426155695	T	T	T
0.8750596504134692	0.6248839034024198	0.3307297819272552	T	T	T
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0.8753630181311275	0.7500001747418567	0.2479270412672192	T	T	T
0.8692717512658655	0.7499998774960723	0.4113455381538111	T	T	T
0.8750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.8753875932065561	0.8750448213106148	0.1652147776880041	T	T	T
0.8750597013812357	0.8751160568855300	0.3307300251030494	T	T	T
0.1250000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.1251718948263711	0.1250519677178353	0.2491391803875369	T	T	T
0.1265818209794409	0.1251927553034756	0.4151818632468873	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1249732587819360	0.0000337883849972	0.1658019796964975	T	T	T
0.1239995545587648	0.0000240657954660	0.3324133017866232	T	T	T
0.0000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.0003589320455826	0.1250293754772089	0.1657028778772386	T	T	T

0.0000461706005090	0.1250809418713370	0.3324743285359325	T	T	T
0.0000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.0000026305339315	0.0000667666912182	0.2492772409277575	T	T	T
0.9946007396307367	0.0002236830372389	0.4202067785653356	T	T	T
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0.1251715514430890	0.3749480458748622	0.2491390508605848	T	T	T
0.1265819388746344	0.37480738544446659	0.4151817703328568	T	T	T
0.1250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.1250385440665469	0.2500000155620630	0.1658715734938912	T	T	T
0.1245875253085088	0.2499998718988117	0.3327428966175257	T	T	T
0.0000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.0003588898771561	0.3749706192900734	0.1657030823240727	T	T	T
0.0000457996570258	0.3749192204576868	0.3324742908485205	T	T	T
0.0000000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.0001620708100526	0.2500000207227410	0.2493973467668839	T	T	T
0.9955261393130578	0.2500001400163242	0.4203847279077639	T	T	T
0.3750000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.3750674589013371	0.1249755278968513	0.2490853369512879	T	T	T
0.3796422607499104	0.1246149389619013	0.4189355901050311	T	T	T
0.3750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3746761331648029	-0.0000125266037101	0.1655932995445801	T	T	T
0.3752849228076341	0.9996055378741481	0.3320677263348084	T	T	T
0.2500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.2499749173588202	0.1250193798221339	0.1658024131173871	T	T	T
0.2512211316738785	0.1250899820952210	0.3324025301126788	T	T	T
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0.2499218915649454	-0.0000031938884079	0.2490099464874747	T	T	T
0.2497254127215285	0.9996263627938486	0.4147506915316584	T	T	T
0.3750000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.3750674666955482	0.3750242092479028	0.2490851588687266	T	T	T
0.3796432940715643	0.3753846426590371	0.4189361391066029	T	T	T
0.3750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.3746179687687720	0.2499999369391340	0.1656483115550252	T	T	T
0.3747600600077037	0.2500000847322494	0.3324258328225414	T	T	T
0.2500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.2499748991184299	0.3749806010825168	0.1658024865492089	T	T	T
0.2512212789988227	0.3749098917659077	0.3324023891997703	T	T	T
0.2500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.2499917907738984	0.2499998433059817	0.2491653360807320	T	T	T
0.2527274262174735	0.2499998609829777	0.4159593699461654	T	T	T
0.5000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.4996593939607870	0.1249409585058105	0.1652029483599527	T	T	T
0.4999147497095052	0.1249001386297629	0.3312129750092554	T	T	T
0.5000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.4999419097390777	0.0000056284494736	0.2476574641812701	T	T	T
0.5046398180988919	-0.0001151714836756	0.4107511837870660	T	T	T
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0.4996594626496481	0.3750590497358935	0.1652028371766444	T	T	T
0.4999145771715313	0.3750999695681435	0.3312128499736048	T	T	T
0.5000000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.4998344076051759	0.2500000281827792	0.2472766598659870	T	T	T
0.5029105315120110	0.2500001159475028	0.4079164980723602	T	T	T
0.6250000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.6249053104951207	0.1250371623545359	0.2473912411614078	T	T	T
0.6263036683781105	0.1252803371554663	0.4110575509520271	T	T	T
0.6250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6249842913258826	0.0000115399650283	0.1650219966944584	T	T	T
0.6255668900996174	0.0000405202582731	0.3302379452089953	T	T	T
0.6250000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.6249054269509972	0.3749629002689269	0.2473912920469780	T	T	T

0.6263043940490587	0.3747198630455572	0.4110583128993801	T	T	T
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0.6250610020408023	0.2500000131051198	0.1649783864330623	T	T	T
0.6257568508773260	0.2500002063972281	0.3300931986715908	T	T	T
0.0000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.0000023409011526	0.4999331513050377	0.2492772948086961	T	T	T
0.9946003750653749	0.4997767451069813	0.4202062091718435	T	T	T
0.1250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1249732462124044	0.4999662481583305	0.1658021094880999	T	T	T
0.1239987098336295	0.4999764198027142	0.3324129543468219	T	T	T
0.2500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.2499214860886995	0.5000035799138347	0.2490096650779338	T	T	T
0.2497255255125095	0.5003737057566069	0.4147497414869744	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3746760075567518	0.5000124508384444	0.1655931762757124	T	T	T
0.3752843534908522	0.5003942577763377	0.3320674229223133	T	T	T
0.5000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.4999418988332219	0.4999944752545759	0.2476572034049958	T	T	T
0.5046397318328313	0.5001154946412630	0.4107512543331430	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.6249843226803686	0.4999885819314809	0.1650219028201043	T	T	T
0.6255668268605435	0.4999597001056450	0.3302376923590110	T	T	T
0.0000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.0002827645171756	0.6249647675258476	0.1656450807394465	T	T	T
0.9996478959204124	0.6249363893651072	0.3322343192084474	T	T	T
0.1250000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.1249856164489545	0.6249721121062943	0.2490020601173532	T	T	T
0.1252588036395870	0.6250064065968616	0.4148080146364803	T	T	T
0.2500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.2499243194316768	0.6249884732801470	0.1657347399545763	T	T	T
0.2509162127133686	0.6250500519701853	0.3321322683923000	T	T	T
0.3750000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.3750430426848144	0.6250322779671763	0.2489644947366982	T	T	T
0.3805603372315789	0.6256626623049357	0.4188139940568842	T	T	T
0.5000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.4996707797772418	0.6249919979736132	0.1652464972884623	T	T	T
0.5001966641125953	0.6249748271670206	0.3311060003416348	T	T	T
0.6250000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.6249683226641378	0.6249493805370272	0.2473778472517383	T	T	T
0.6263504597962590	0.6249617964794839	0.4110532430424689	T	T	T
0.0000000000000000	0.7500000000000000	0.0822561893037914	F	F	F
-0.0000862226419479	0.7500000881589612	0.2492032587041640	T	T	T
0.9942431227055463	0.7499999494685546	0.4200277916378851	T	T	T
0.1250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.1249318223110918	0.7500001304627818	0.1657602967921465	T	T	T
0.1237887812477561	0.7500002474782420	0.3323014722504912	T	T	T
0.2500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.2498342573198032	0.7500001901479187	0.2489049524060087	T	T	T
0.2493181327374548	0.7499997059803147	0.4145314464861935	T	T	T
0.3750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.3746789416354515	0.7500001366992647	0.1655352556834710	T	T	T
0.3753456358512135	0.7500001773371420	0.3317896939634715	T	T	T
0.5000000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.4999903882577298	0.7500001372062692	0.2476164216077431	T	T	T
0.5050525048021046	0.7499999274487810	0.4103482949597574	T	T	T
0.6250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.6249887455624645	0.7499999915706780	0.1649987392321005	T	T	T
0.6256274819018262	0.7499997803384029	0.3300645906803902	T	T	T
0.0000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.0002827439227845	0.8750350474123330	0.1656450315265044	T	T	T

0.9996483144430186	0.8750633838178772	0.3322344535862654	T	T	T
0.1250000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.1249858140330575	0.8750281864440286	0.2490021344627273	T	T	T
0.1252589348415538	0.8749937123105841	0.4148084948846159	T	T	T
0.2500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.2499243104038902	0.8750118258359372	0.1657346720267321	T	T	T
0.2509169259595340	0.8749503163073117	0.3321325200748489	T	T	T
0.3750000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.375043336323727	0.8749680540891868	0.2489647697730176	T	T	T
0.3805608981201303	0.8743372442755412	0.4188144400551660	T	T	T
0.5000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.4996706151730119	0.8750081710599915	0.1652465927203916	T	T	T
0.5001967084878682	0.8750253017669815	0.3311062293877559	T	T	T
0.6250000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.6249684281174434	0.8750507519550703	0.2473779573372291	T	T	T
0.6263504107776117	0.8750382592320807	0.4110531958200251	T	T	T
0.0119451566957059	0.1255302628591467	0.4986774155241225	T	T	T
0.0119454548772057	0.3744700697566368	0.4986770983204922	T	T	T
0.0100181836820760	0.6247784998150031	0.4984856002217269	T	T	T
0.0100186292973969	0.8752215952579369	0.4984857347308383	T	T	T
0.1264378779983552	-0.0000566971738836	0.4957420386570961	T	T	T
0.1291614416155817	0.2500001060798349	0.4958459800606140	T	T	T
0.1264373311556869	0.5000566265710870	0.4957414500730147	T	T	T
0.1254867188530862	0.7499998435622819	0.4956583132731933	T	T	T
0.2529471635695806	0.1256331447571247	0.4964307260713683	T	T	T
0.2529461828495682	0.3743662755097907	0.4964307253375924	T	T	T
0.2494188110591931	0.6254765019074828	0.4954397395014447	T	T	T
0.2494186625948654	0.8745239874301117	0.4954401244878162	T	T	T
0.3657023432611915	0.9961384564328893	0.4970777605855768	T	T	T
0.3707214970748339	0.2499947331112499	0.5001057968338897	T	T	T
0.3657035901113383	0.5038613402391359	0.4970781328109979	T	T	T
0.3652729244135460	0.7499995857740048	0.4975944709481945	T	T	T
0.7500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.7501759927933631	0.1250104701894386	0.1650685772363366	T	T	T
0.7497030589523955	0.1250378597202166	0.3303159188310278	T	T	T
0.7500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.7502613589116126	0.0000604338435705	0.2474780803755626	T	T	T
0.7487985922496289	0.0001100226628074	0.4112271458535002	T	T	T
0.7500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.7501759531433400	0.3749895446421049	0.1650685846508098	T	T	T
0.7497029105018261	0.3749623979571726	0.3303160678624452	T	T	T
0.7500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.7503527502381405	0.2499999345771044	0.2474736896891970	T	T	T
0.7487072117603079	0.2500005218914269	0.4112442593233695	T	T	T
0.7500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.7502611015599012	0.4999395965301517	0.2474778299408378	T	T	T
0.7487988625597799	0.4998897550539239	0.4112270185544952	T	T	T
0.7500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.7501447317869003	0.6249759900259840	0.1650342609832395	T	T	T
0.7496402951247206	0.6249282166603831	0.3301694170722917	T	T	T
0.7500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.7502587159508600	0.7500000744856141	0.2474184312503626	T	T	T
0.7488241941698488	0.7499997618656913	0.4111381054739209	T	T	T
0.7500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.7501448205751626	0.8750241693735531	0.1650342304598388	T	T	T
0.7496405107523042	0.8750716443545417	0.3301698350622553	T	T	T
0.8750000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.8752779702149930	0.1250569179283720	0.2478850849764610	T	T	T
0.8704781989175414	0.1251603760306737	0.4109124745004272	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F

0.8754158125841230	0.0000467226975639	0.1653479513439534	T	T	T
0.8751497562811704	0.0001275312806526	0.3314265849453417	T	T	T
0.8750000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.8752778956326325	0.3749430625581681	0.2478849906149718	T	T	T
0.8704778153095859	0.3748398582232962	0.4109123292411967	T	T	T
0.8750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.8754935003909617	0.2500001212078425	0.1653777559948876	T	T	T
0.8753484714515344	0.2499999694701306	0.3315790726347040	T	T	T
0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8754156654925757	0.4999532839976057	0.1653480874204118	T	T	T
0.8751495925343972	0.4998726183219512	0.3314261451379912	T	T	T
0.8750000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.8751636747300126	0.6249426049984175	0.2477616539439113	T	T	T
0.8701623623099451	0.6249117149105611	0.4106333831912463	T	T	T
0.8750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.8753882719678834	0.7500001163778373	0.1653036539945609	T	T	T
0.8750285208836419	0.7499997437531564	0.3313048086456751	T	T	T
0.8750000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.8751638240253566	0.8750575001284069	0.2477616875229979	T	T	T
0.8701620530441740	0.8750882026091787	0.4106335091196022	T	T	T
0.4703375379060924	0.3095576586421340	0.5100537076561220	T	T	T
0.4703235659024141	0.1904451896826055	0.5100516338016907	T	T	T
0.4407019067595129	0.2500023406082966	0.5074605259068695	T	T	T

MS3-pbc-2CO2 (1,2 S) (-2698.1516 eV)

1.0000000000000000

19.2439999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.2439999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.2439999999999998

Ca O C

208 212 2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0002529872428082	0.0000467585434702	0.1655676589010783	T	T	T
0.9989978167016816	0.0001378185346759	0.3324983031998193	T	T	T
0.0000000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.0002206594262383	0.1251020554249230	0.2490500024572559	T	T	T
0.9928349935175560	0.1253540903228323	0.4202066005846932	T	T	T
0.1250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.1248488111492834	0.0000522563483764	0.2491385095694859	T	T	T
0.1236729739161246	0.0000625075125525	0.4139300029317409	T	T	T
0.1250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.1250640890861079	0.1250271719577704	0.1657461499883886	T	T	T
0.1237849853994753	0.1249660607649091	0.3328489040699608	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0003037850575603	0.2500578160371482	0.1656155469953809	T	T	T
0.9994860712122429	0.2501301718822109	0.3328068052686733	T	T	T
0.0000000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.0004073071588402	0.3750274871205113	0.2492309601866999	T	T	T
0.9932310565578338	0.3749333236289282	0.4205345415578922	T	T	T
0.1250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.1249798070511392	0.2500886822672863	0.2492138720435493	T	T	T
0.1251951910788569	0.2500438768529806	0.4143193437149915	T	T	T
0.1250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.1251286570456685	0.3750504421303287	0.1658181548443619	T	T	T
0.1243987249169978	0.3751106869688202	0.3332989865986815	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2497910506364650	0.9999987800834157	0.1656658284214256	T	T	T

0.2507465835413735	0.9999834044408117	0.3322430079506182	T	T	T
0.2500000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.2498934434916045	0.1249191047137788	0.2491339155317871	T	T	T
0.2518784106208068	0.1239577500624974	0.4141496977645095	T	T	T
0.3750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.3748559382298181	0.9998745764742299	0.2485963842076726	T	T	T
0.3819572240034426	0.9984318499897247	0.4171404453016616	T	T	T
0.3750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.3746943918125490	0.1249489320675590	0.1654488380164420	T	T	T
0.3766330480852068	0.1237920956308030	0.3319941275879767	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2498169815337893	0.2500358017023540	0.1656868271539912	T	T	T
0.2506980354284055	0.2500093822673600	0.3320112622261752	T	T	T
0.2500000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.2500441340410192	0.3751356993758062	0.2493011350378382	T	T	T
0.2536864829714375	0.3752655832403547	0.4153614219522190	T	T	T
0.3750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.3748736761420663	0.2498556686766203	0.2485149019666971	T	T	T
0.3810356341084913	0.2489778222444221	0.4124211274675340	T	T	T
0.3750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.3747540067080484	0.3750460099381296	0.1655186649697003	T	T	T
0.3769830687479564	0.3753801349811340	0.3318770410898806	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.4997171410926510	0.9999747293744371	0.1651167629719784	T	T	T
0.5005110492635751	0.0010176348972441	0.3309806932168315	T	T	T
0.5000000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.4998706513907774	0.1248279106199583	0.2477987581740468	T	T	T
0.5054238239699883	0.1272961703368868	0.4162695321925012	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4997678280505525	0.2499870322372204	0.1650714996722766	T	T	T
0.5013465826268870	0.2496491975891784	0.3295637411789869	T	T	T
0.5000000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.5000331269044579	0.3750383924392627	0.2478997774634740	T	T	T
0.5058089497250410	0.3717437091396111	0.4159448388216710	T	T	T
0.6250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.6247965276277172	0.0001482423767912	0.2474826594509869	T	T	T
0.6258265058148287	0.0005377036793799	0.4120550610895997	T	T	T
0.6250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.6249315257121481	0.1250042766376738	0.1649492030255816	T	T	T
0.6246224984604904	0.1252236127498698	0.3302799846107787	T	T	T
0.6250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.6251443370096720	0.2499745994455640	0.2473401872919249	T	T	T
0.6254569288426844	0.2497356172365870	0.4128017612422702	T	T	T
0.6250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.6249772179018721	0.3749949160917374	0.1649843567582649	T	T	T
0.6248199406715399	0.3746693017541843	0.3303954328773474	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0003329075401710	0.4999680254694269	0.1656570724200144	T	T	T
0.9994221918270806	0.4998951882346659	0.3328615103898288	T	T	T
0.1250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.1250953323102732	0.4999915174232109	0.2493746966836454	T	T	T
0.1248565002905928	0.5000809454711537	0.4144473869474340	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2498851932029848	0.5000254010043490	0.1657649983716256	T	T	T
0.2511586545294116	0.5001263119392350	0.3326370435872951	T	T	T
0.3750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.3750792484041782	0.5002156286801154	0.2488081326312747	T	T	T
0.3826038896077134	0.5013062571012282	0.4153181946090082	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4997697426986370	0.5000028010298205	0.1651866670951461	T	T	T

0.5011694621724576	0.4991655692224111	0.3311459502427326	T	T	T
0.6250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.6249268775326059	0.4998313376083023	0.2476049890501804	T	T	T
0.6255797193945823	0.4993597264970211	0.4128819319292311	T	T	T
0.0000000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.0002409163531675	0.6248993279273539	0.2491052881609729	T	T	T
0.9925845791659551	0.6247345996301757	0.4203159180774646	T	T	T
0.1250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.1250847292442741	0.6249636466196190	0.1657896200494178	T	T	T
0.1237984670017761	0.6250540601382686	0.3330227577279161	T	T	T
0.2500000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.2498948530070555	0.6250427785546525	0.2492671158496974	T	T	T
0.2518627454522562	0.6260602363048667	0.4146418355248427	T	T	T
0.3750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.3747254497689205	0.6250307314075728	0.1655249333110174	T	T	T
0.3762408358414803	0.6259044929988397	0.3322013525603419	T	T	T
0.5000000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.4999111787660640	0.6248383215401470	0.2480660307595549	T	T	T
0.5057867627467297	0.6249815160277157	0.4128446709862129	T	T	T
0.6250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.6249246815994635	0.6249367746640658	0.1650141150542055	T	T	T
0.6254089059363125	0.6247228024583644	0.3300652976257257	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0002657198336111	0.7499443702389197	0.1655808631125512	T	T	T
0.9989742180559248	0.7498934825142637	0.3325403006901236	T	T	T
0.1250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.1248650192134594	0.7499305807385218	0.2491979454892819	T	T	T
0.1235632215303607	0.7500733971513367	0.4139910032207613	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2497870341205108	0.7499653778371322	0.1656918571909465	T	T	T
0.2507914893936131	0.7500610003482424	0.3323929359629891	T	T	T
0.3750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.3748198307291613	0.7500761952237048	0.2486632626452898	T	T	T
0.3819356395308940	0.7518518999875742	0.4175226392703728	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.4997217846630879	0.7499724876493877	0.1651920163847404	T	T	T
0.5004980228352306	0.7498226446800028	0.3306239861239291	T	T	T
0.6250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.6248634718335012	0.7499056714488329	0.2474646549224663	T	T	T
0.6261668660316688	0.7499533509004294	0.4119986799882444	T	T	T
0.0000000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.0000537692257964	0.8749992315590801	0.2489183160180737	T	T	T
0.9921025744988192	0.8751140023802804	0.4199831007789026	T	T	T
0.1250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.1250036363828812	0.8749850333746066	0.1657077723018807	T	T	T
0.1231592503194488	0.8750125345304747	0.3325694739307916	T	T	T
0.2500000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.2496664290909316	0.8749752494309190	0.2490303237717934	T	T	T
0.2499401857102671	0.8751117378481874	0.4134845129550799	T	T	T
0.3750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.3746715319001953	0.8749725473430370	0.1654525851103713	T	T	T
0.3757715241513133	0.8750505599576109	0.3317497665958020	T	T	T
0.5000000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.4998332501071625	0.8751376035496968	0.2479219094660825	T	T	T
0.5058408618989924	0.8752240982634917	0.4110761153731576	T	T	T
0.6250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.6249020240580646	0.8750026265658641	0.1649687591540528	T	T	T
0.6256007257140863	0.8751333307242674	0.3296739077929257	T	T	T
0.0099226001322666	0.0004479315479182	0.4994912248026545	T	T	T
0.0126620470062865	0.2500824101869318	0.4998190997868751	T	T	T

0.0120678897962818	0.4997491376035571	0.4999114823299086	T	T	T
0.0095904082342418	0.7500411141671772	0.4995041583415369	T	T	T
0.1285849082302520	0.1243089119650702	0.4960402921472337	T	T	T
0.1301983325427873	0.3747984648150480	0.4964854058874515	T	T	T
0.1279055375100904	0.6260875325498525	0.4962134758625252	T	T	T
0.1261489330302067	0.8752648963798351	0.4957787146308021	T	T	T
0.2469934033719662	0.9986279135068699	0.4952891191514726	T	T	T
0.2488835358536721	0.2484173431943985	0.4957866660948185	T	T	T
0.2473073919817422	0.5017340782284090	0.4961644527873890	T	T	T
0.2464916281454380	0.7521262874813957	0.4954037277197423	T	T	T
0.3704908583473862	0.1124233300765494	0.4985497904187081	T	T	T
0.3757029151128184	0.3750385298299611	0.5016122139107957	T	T	T
0.3689197320734664	0.6386852616683589	0.4999259110020765	T	T	T
0.3648136316024823	0.8753297018991542	0.4980374283880394	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7501347034323477	0.0000526556010605	0.1649993084156791	T	T	T
0.7491398504460562	0.0002554534212485	0.3297991003806455	T	T	T
0.7500000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.7500735972289793	0.1250823206085025	0.2476705416065307	T	T	T
0.7483920178537028	0.1251946118128574	0.4120286556635848	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7502531074825742	0.2500244564567273	0.1650036893724418	T	T	T
0.7490690732397594	0.2500056188764699	0.3299873343124775	T	T	T
0.7500000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.7501598724366063	0.3749563600340396	0.2477704041870111	T	T	T
0.7483587957682983	0.3747279760457563	0.4122486736112451	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7501925380783080	0.4999403702270535	0.1650615681253470	T	T	T
0.7491003496231978	0.4997166951436511	0.3301055248995376	T	T	T
0.7500000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.7501945223446779	0.6248538551016825	0.2476376523680166	T	T	T
0.7483800497350951	0.6247066718562256	0.4121090074892302	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7501498960361419	0.7499442530958829	0.1649961267315475	T	T	T
0.7492319339970500	0.7498661512148384	0.3297887992265866	T	T	T
0.7500000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.7501922652442670	0.8750193941492951	0.2474790790334737	T	T	T
0.7484352090347971	0.8751546768411061	0.4118424754173883	T	T	T
0.8750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.8752192099825046	0.0001095017761349	0.2479914696124693	T	T	T
0.8690781346492568	0.0001804479083165	0.4114383996411497	T	T	T
0.8750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.8753343514561113	0.1250586278112020	0.1652755331064136	T	T	T
0.8749634423146164	0.1251990751963372	0.3309271464912094	T	T	T
0.8750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.8753536345445089	0.2500794629939906	0.2481512986073794	T	T	T
0.8692850234943929	0.2500268273556894	0.4118097311728383	T	T	T
0.8750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.8753918658484841	0.3750116559311492	0.1653345378932025	T	T	T
0.8750935578442171	0.3749390819362484	0.3311510940727300	T	T	T
0.8750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.8753392056021030	0.4998898956557020	0.2481887129387042	T	T	T
0.8692136244910916	0.4997984081322465	0.4118517127757692	T	T	T
0.8750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.8753618869368118	0.6249250912971815	0.1652808266462119	T	T	T
0.8749457095393468	0.6247682281836925	0.3309721233308201	T	T	T
0.8750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.8752390292737751	0.7498985785488992	0.2479987997804766	T	T	T
0.8690158911835534	0.7499266095877122	0.4114326430375810	T	T	T
0.8750000000000000	0.8750000000000000	0.0000000000000000	F	F	F

0.8753205278775742	0.8749983382208057	0.1652106528305978	T	T	T
0.8748151909064974	0.8750418318826555	0.3307329916544677	T	T	T
0.1250000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.1250171989448212	0.1251669596755691	0.2491093179439056	T	T	T
0.1261713658519322	0.1253916904058102	0.4150956920110874	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1249036326968184	0.0000425753856902	0.1657979890950040	T	T	T
0.1236444130065411	0.0001092102326552	0.3322901481378962	T	T	T
0.0000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.0003101929559898	0.1250800764161593	0.1657187705227037	T	T	T
0.9998842678586575	0.1252112360853932	0.3324912031768576	T	T	T
0.0000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.9998586391774107	0.0000925131794775	0.2492615280108330	T	T	T
0.9942495376501911	0.0003736495968214	0.4201944880153213	T	T	T
0.1250000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.1252950121474889	0.3750621389092353	0.2493806172875168	T	T	T
0.1277498767071961	0.3750029758712042	0.4156672372243386	T	T	T
0.1250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.1250082179158024	0.2500975726044006	0.1659267110936826	T	T	T
0.1246731696953207	0.2501806292039996	0.3329127625467472	T	T	T
0.0000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.0004032495728249	0.3750335997060816	0.1658078247009108	T	T	T
0.0003169946037355	0.3750244556730729	0.3328246578629745	T	T	T
0.0000000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.0001707170411182	0.2501193901235745	0.2495018775661348	T	T	T
0.9957481808775871	0.2502586775120872	0.4205959623548314	T	T	T
0.3750000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.3749289662372021	0.1249933406936022	0.2488692554533330	T	T	T
0.3784526213823597	0.1242057522403980	0.4179132693989605	T	T	T
0.3750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3746266010338377	0.9999738508907317	0.1655436700630745	T	T	T
0.3750083751628052	0.9996601800653508	0.3317741226292045	T	T	T
0.2500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.2498937301651905	0.1250844512378712	0.1657763559281964	T	T	T
0.2508573669828453	0.1252196940768812	0.3322065923843395	T	T	T
0.2500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.2497529550733680	0.0000285902302411	0.2489063817826175	T	T	T
0.2488333676582222	0.9997561223034053	0.4144167681097355	T	T	T
0.3750000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.3750801886764021	0.3751407407991077	0.2492212639584029	T	T	T
0.3802500178424774	0.3750525719988838	0.4199423664033735	T	T	T
0.3750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.3745337137045832	0.2500786351899802	0.1656345019068179	T	T	T
0.3745214227617226	0.2500449532517568	0.3321192577182588	T	T	T
0.2500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.2499838951872863	0.3750718944524402	0.1659265151229248	T	T	T
0.2516384563584969	0.3751323100418712	0.3328802396837335	T	T	T
0.2500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.2499164646832559	0.2501561955521347	0.2492217213005025	T	T	T
0.2532155223207730	0.2499343790757549	0.4162794723894872	T	T	T
0.5000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.4996429615453276	0.1249167559343389	0.1651105196503076	T	T	T
0.4998125301919990	0.1246523105067905	0.3307368111305272	T	T	T
0.5000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.4998914256592413	0.9999123490414460	0.2475666396873866	T	T	T
0.5043731517152562	0.9998989560592327	0.4108161899965835	T	T	T
0.5000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.4996425104654733	0.3751230941102583	0.1652013589346772	T	T	T
0.4998664620830177	0.3750360338375077	0.3310521320801237	T	T	T
0.5000000000000000	0.2500000000000000	0.0822561893037914	F	F	F

0.4998395926799966	0.2500001131132250	0.2469911787497026	T	T	T
0.5028395504612496	0.2492157198360221	0.4066450093806753	T	T	T
0.6250000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.6249130041010377	0.1250081958905342	0.2473151817063153	T	T	T
0.6262758965550248	0.1251810130121194	0.4110808175292059	T	T	T
0.6250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6249768096942704	0.9999789533213075	0.1650083971629271	T	T	T
0.6254623075256392	0.9999848450816249	0.3302343342764134	T	T	T
0.6250000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.6249451378515801	0.3750012576050483	0.2473993661078090	T	T	T
0.6263059010240036	0.3745237467502612	0.4110364976952618	T	T	T
0.6250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.6250921628248239	0.2500272558080274	0.1649485244819906	T	T	T
0.6259388726886015	0.2499248386388927	0.3299475429800245	T	T	T
0.0000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.0001725678356732	0.4999175076859506	0.2495372774355592	T	T	T
0.9954643604809441	0.4996808180851920	0.4206615796646992	T	T	T
0.1250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1250634895756718	0.4999651024918453	0.1659749556878687	T	T	T
0.1246558454348446	0.4999357101103467	0.3330181624224789	T	T	T
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0.2501163757955557	0.4999905992801397	0.2494572915743878	T	T	T
0.2524742821192615	0.5002957847618904	0.4166639897071484	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3746633150807628	0.5000227635366935	0.1657882979154938	T	T	T
0.3753127724156484	0.5002440680874177	0.3329837499597845	T	T	T
0.5000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.4998678247555829	0.5000168467883593	0.2478066786945771	T	T	T
0.5033920406672381	0.4995928792941203	0.4109462687593706	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.6249792447961019	0.4999912249762590	0.1650945111664882	T	T	T
0.6254424992809324	0.4998675214330024	0.3305249208439426	T	T	T
0.0000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.0003233252349116	0.6249108834999083	0.1657452540276073	T	T	T
0.9998452439783027	0.6247863803507305	0.3325325736067753	T	T	T
0.1250000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.1250965294226560	0.6248476005219179	0.2492096360758962	T	T	T
0.1260269662128610	0.6247667443998116	0.4152103740415140	T	T	T
0.2500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.2499633416213253	0.6249063566788260	0.1658730116011178	T	T	T
0.2511317849678258	0.6248215468296026	0.3325447803380590	T	T	T
0.3750000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.3750850255642695	0.6249505731032714	0.2491792319225245	T	T	T
0.3804262030946790	0.6261999651501159	0.4189838797866570	T	T	T
0.5000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.4996529424078802	0.6249511057381185	0.1653290167639535	T	T	T
0.5000524996905911	0.6248725762054974	0.3315346072607621	T	T	T
0.6250000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.6248868069929345	0.6248760030962580	0.2474889486372886	T	T	T
0.6262117236533045	0.6248316878224016	0.4110146694810958	T	T	T
0.0000000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.9998585748990652	0.7498997377622258	0.2492836803581674	T	T	T
0.9941073580381355	0.7498169614171915	0.4202006752632318	T	T	T
0.1250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.1249283418879388	0.7499240176052916	0.1658271980395786	T	T	T
0.1236397172268593	0.7499133130120051	0.3323393078708313	T	T	T
0.2500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.2497831854591003	0.7498960647826043	0.2489788643997560	T	T	T
0.2488148485956706	0.7503721457734041	0.4144749547695056	T	T	T
0.3750000000000000	0.7500000000000000	0.0000000000000000	F	F	F

0.3746556909473985	0.7499308715691531	0.1656028781871747	T	T	T
0.3751230899639449	0.7502242487542188	0.3318628530399568	T	T	T
0.5000000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.4999227498175584	0.7499017300173454	0.2477057724400908	T	T	T
0.5045986288960618	0.7502960503873433	0.4104564630475475	T	T	T
0.6250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.6249614248614244	0.7499413060087504	0.1650452130898160	T	T	T
0.6254889495963928	0.7499788037544777	0.3301951665450675	T	T	T
0.0000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.0002399347431368	0.8749954739886480	0.1656599113775848	T	T	T
0.9994238796110457	0.8750217760618256	0.3322190226792228	T	T	T
0.1250000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.1248336442463003	0.8749863312028557	0.2489664640175673	T	T	T
0.1246036662939342	0.8750959549017138	0.4146676879428975	T	T	T
0.2500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.2498710259709281	0.8749618239348952	0.1657334272246317	T	T	T
0.2505376830546422	0.8750115021170445	0.3319436032558191	T	T	T
0.3750000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.3749510526984466	0.8749482743922267	0.2488374065760160	T	T	T
0.3799523262503959	0.8752097500522711	0.4178164594248099	T	T	T
0.5000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.4996639366838239	0.8749449760264274	0.1652411155243513	T	T	T
0.5001137431886632	0.8750415073011740	0.3310572382156731	T	T	T
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0.6249104582980890	0.8749762345925274	0.2473743132945746	T	T	T
0.6261759263821185	0.8750646020191938	0.4110319398714218	T	T	T
0.0116190991506651	0.1259456503392790	0.4986625160617821	T	T	T
0.0132859612492202	0.3747128590272025	0.4989045160063998	T	T	T
0.0109871192283979	0.6243115686097215	0.4986964547299545	T	T	T
0.0092798206341718	0.8752858589461134	0.4984404565531658	T	T	T
0.1255179953493488	0.0001921041736072	0.4955988848405433	T	T	T
0.1298070524947230	0.2499019538609646	0.4959900432271217	T	T	T
0.1286372353484593	0.4999108911025441	0.4961884460088039	T	T	T
0.1250794100969550	0.7503657206348719	0.4956096492461217	T	T	T
0.2521864989246503	0.1254329844427565	0.4962244941356226	T	T	T
0.2553253292624889	0.3740414537467665	0.4974727930759915	T	T	T
0.2507879289495741	0.6254507626670096	0.4963712950543273	T	T	T
0.2481493911876668	0.8754688214778072	0.4951320912665886	T	T	T
0.3645811343940689	0.9961102752369759	0.4963605851296268	T	T	T
0.3741292960673549	0.2451524178826662	0.5006594057201691	T	T	T
0.3693148901572794	0.5041852123183640	0.4985111971300877	T	T	T
0.3638998854042723	0.7554151064454995	0.4963267771715273	T	T	T
0.7500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.7501842124237424	0.1250236891742545	0.1650583784675510	T	T	T
0.7496498931108888	0.1250107185954003	0.3303121329362318	T	T	T
0.7500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.7502041671134713	0.0000244733050536	0.2474631689227890	T	T	T
0.7486482465342386	0.0000903029916236	0.4111998424306176	T	T	T
0.7500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.7502252247922825	0.3750268217741079	0.1651136749297574	T	T	T
0.7497887758566527	0.3749660254988443	0.3304427648206969	T	T	T
0.7500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.7504109962794582	0.2500373626231995	0.2474665138970848	T	T	T
0.7486684361181700	0.2499519212685928	0.4112340033930270	T	T	T
0.7500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.7502672644270908	0.4999355829844873	0.2476135917343971	T	T	T
0.7486617115679466	0.4997890647978070	0.4113743113315743	T	T	T
0.7500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.7501524395841422	0.6249357749911663	0.1651018495273429	T	T	T
0.7496322295747501	0.6248575107859603	0.3303481564465322	T	T	T

0.7500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.7502004286913043	0.7499174051772901	0.2474763072928218	T	T	T
0.7486333072327223	0.7499516554843285	0.4111840529576865	T	T	T
0.7500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.7501296054387337	0.8749769661464017	0.1650381471555215	T	T	T
0.7495252717421026	0.8750077119464178	0.3301768857576043	T	T	T
0.8750000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.8752175036531012	0.1251151031583879	0.2478988417690242	T	T	T
0.8703917739624054	0.1252437714676826	0.4109227156656220	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.8753908978434888	0.0000352473657693	0.1653529312493400	T	T	T
0.8749975362024295	0.0001331886870209	0.3314096446954660	T	T	T
0.8750000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.8753626460084241	0.3750080356829255	0.2480416490719222	T	T	T
0.8706616080824859	0.3748930936568763	0.4112279052034457	T	T	T
0.8750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.8755161711409449	0.2500580043860785	0.1654181865111111	T	T	T
0.8754298788500959	0.2501029746251292	0.3317064460434744	T	T	T
0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8754714191868208	0.4999614201501211	0.1654530409039451	T	T	T
0.8753179809933778	0.4998395566726535	0.3317452499086836	T	T	T
0.8750000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.8751994405984431	0.6248627684650060	0.2479217377130620	T	T	T
0.8702396470983551	0.6247359888734593	0.4109240484930599	T	T	T
0.8750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.8753792754188899	0.7499386588324551	0.1653596206753158	T	T	T
0.8749595827032481	0.7498742333744680	0.3314074272130790	T	T	T
0.8750000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.8750745847763667	0.8749945789729566	0.2477706177853058	T	T	T
0.8699547019147187	0.8750518900027341	0.4106084791002873	T	T	T
0.4770062208858565	0.3008322624687382	0.5024096922489251	T	T	T
0.4732524612826256	0.1820585754639187	0.5029275994842578	T	T	T
0.4500584742261016	0.5679435535297657	0.5360529262371457	T	T	T
0.4438018318159164	0.4506756057021248	0.5462474560913738	T	T	T
0.4453811079889240	0.2427616961653432	0.5025607054577770	T	T	T
0.4244190739675077	0.5077672558696732	0.5287526420888516	T	T	T

MS3-pbc-2CO2 (1,3 S) (-2698.6339 eV)

1.0000000000000000

19.2439999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.2439999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.2439999999999998

Ca O C

208 212 2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0001986343530279	0.9999720858440417	0.1656319971131001	T	T	T
0.9989859895169858	0.9999718564062591	0.3326956177950965	T	T	T
0.0000000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.0000802069034560	0.1249653365279335	0.2490901669435804	T	T	T
0.9925719449415183	0.1250416841844515	0.4202800360296898	T	T	T
0.1250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.1248337451377571	0.9999533457374731	0.2492447068706541	T	T	T
0.1240533528889070	0.9999868085778859	0.4141354504244854	T	T	T
0.1250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.1250120049342978	0.1249600853867450	0.1657597783278160	T	T	T
0.1236008128610729	0.1248949369459808	0.3328651543172610	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F

0.0001955582405439	0.2500000182933149	0.1656021432529173	T	T	T
0.9990722346959158	0.2499999620624130	0.3326766113608742	T	T	T
0.0000000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.0000802538417837	0.3750345987970634	0.2490902407929661	T	T	T
0.9925720164879638	0.3749582908257210	0.4202800559049625	T	T	T
0.1250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.1247787860099495	0.2499999976779585	0.2491378839611794	T	T	T
0.1242654809104349	0.2499998498656218	0.4140854721019917	T	T	T
0.1250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.1250119569841133	0.3750398278909088	0.1657598448589475	T	T	T
0.1236008258011442	0.3751050409152925	0.3328653590926059	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2498127759276236	0.9999700453181203	0.1657220366207395	T	T	T
0.2507358974857217	0.9999578583762879	0.3324323537250518	T	T	T
0.2500000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.2497969046409486	0.1248779579776680	0.2491362834648627	T	T	T
0.2516226823718228	0.1246526473479258	0.4142511432267753	T	T	T
0.3750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.3749455339146324	0.9999591838589096	0.2487130110958416	T	T	T
0.3820611280006121	0.9999932048533355	0.4167283936141144	T	T	T
0.3750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.3747189477333506	0.1249606723678340	0.1654980205265958	T	T	T
0.3763932515797810	0.1243495918053141	0.3318778018143260	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2497814621613347	0.249999221172071	0.1656785898858873	T	T	T
0.2504273727811000	0.2499997963509709	0.3319184105597475	T	T	T
0.2500000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.2497968115128191	0.3751219881083452	0.2491363348059929	T	T	T
0.2516228596874958	0.3753471944803816	0.4142512873432038	T	T	T
0.3750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.3748192151501576	0.2499999122649323	0.2485582155600840	T	T	T
0.3807059717811643	0.2499998197520194	0.4131181344429825	T	T	T
0.3750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.3747188679977526	0.3750392090301226	0.1654980292920304	T	T	T
0.3763933881042273	0.3756503382222072	0.3318778584126784	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.4997423104579011	0.9999735912075668	0.1652070564117798	T	T	T
0.5006692174797582	0.9999985438677785	0.3314984304486153	T	T	T
0.5000000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.4998852462233002	0.1247721703657023	0.2480306183048230	T	T	T
0.5054681617320006	0.1269648701095794	0.4148081957167908	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4997384546223513	0.2499998887243377	0.1651788855692655	T	T	T
0.5010321811294987	0.2499998885461354	0.3300342543959993	T	T	T
0.5000000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.4998852522086627	0.3752276692627303	0.2480305591986092	T	T	T
0.5054680369312564	0.3730349536642604	0.4148080724890810	T	T	T
0.6250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.6247200784799888	0.9999750586982180	0.2477158337259955	T	T	T
0.6254444757580848	0.0000511996048636	0.4125060150003639	T	T	T
0.6250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.6248914775907662	0.1249594624985027	0.1650368127523410	T	T	T
0.6247970524379739	0.1250753562553708	0.3303330168657599	T	T	T
0.6250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.6249407095190769	0.2499998796372256	0.2474755102279102	T	T	T
0.6254452186152215	0.2499998600448289	0.4128880114405857	T	T	T
0.6250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.6248915799369189	0.3750404183878428	0.1650368709118679	T	T	T
0.6247970117805351	0.3749244709684739	0.3303331555413294	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F

0.0001986221993795	0.5000278530672720	0.1656320038472602	T	T	T
0.9989860579748837	0.5000278818373970	0.3326957615256245	T	T	T
0.1250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.1248338361574023	0.5000464096308311	0.2492448483144980	T	T	T
0.1240536776031015	0.5000131150447714	0.4141356145970155	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2498126465101012	0.5000298744351576	0.1657220664539371	T	T	T
0.2507360053753542	0.5000422952107588	0.3324324978366338	T	T	T
0.3750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.3749454402456075	0.5000407447477460	0.2487131652133003	T	T	T
0.3820613435633245	0.5000069343185897	0.4167286016857706	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4997422724462760	0.5000263139784151	0.1652071551565198	T	T	T
0.5006692488312916	0.5000011863776097	0.3314983284087109	T	T	T
0.6250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.6247200635318420	0.5000247955635200	0.2477158521898296	T	T	T
0.6254445466639086	0.4999485297698160	0.4125060746589936	T	T	T
0.0000000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.0000736219083886	0.6250108809549135	0.2491438730444572	T	T	T
0.9925450956960670	0.6250278464069388	0.4204326264475756	T	T	T
0.1250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.1250073086081077	0.6249993481943136	0.1657917392791859	T	T	T
0.1235991617124203	0.6249436947755841	0.3329681551368137	T	T	T
0.2500000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.2498035412866590	0.6249489521500233	0.2491928959182435	T	T	T
0.2516464733927988	0.6246748766232387	0.4143683492034167	T	T	T
0.3750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.3747282747884259	0.6250137363853298	0.1655213103479103	T	T	T
0.3764107161685520	0.6244132524189665	0.3319593237657693	T	T	T
0.5000000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.4998869321338091	0.6248185826783890	0.2480906258654847	T	T	T
0.5055153238394061	0.6268755725573315	0.4148469696054440	T	T	T
0.6250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.6248925732573665	0.6249908140113196	0.1650647261920568	T	T	T
0.6248173694690164	0.6250764384531039	0.3304075984261702	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0001947145605539	0.7500000303779724	0.1656371822247344	T	T	T
0.9990706717839964	0.7499999218780902	0.3328000275427161	T	T	T
0.1250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.1247831786343608	0.7499999199544879	0.2492185768798342	T	T	T
0.1242550344090081	0.7499997250279515	0.4142557936884519	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2497888758537680	0.7499999604315353	0.1657199511570557	T	T	T
0.2504528446113294	0.7499996808128426	0.3320607029773443	T	T	T
0.3750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.3748347960711114	0.7499998358667382	0.2486538978694796	T	T	T
0.3807864795923232	0.7499997885301436	0.4133686068980337	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.4997473299517807	0.7500000280313642	0.1652231565050147	T	T	T
0.5010501026883324	0.7499997603360501	0.3301831883321490	T	T	T
0.6250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.6249385609766922	0.7499998484898799	0.2475585645623556	T	T	T
0.6254760113313819	0.7499997701053380	0.4130150328646446	T	T	T
0.0000000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.0000735450167942	0.8749889605878283	0.2491438207880171	T	T	T
0.9925449713740028	0.8749718354534414	0.4204324353292851	T	T	T
0.1250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.1250072748074476	0.8750005143610875	0.1657917051445693	T	T	T
0.1235988701615577	0.8750561408522061	0.3329680181667266	T	T	T
0.2500000000000000	0.8750000000000000	0.0822561893037914	F	F	F

0.2498034629231155	0.8750508952400612	0.2491927539739225	T	T	T
0.2516463747142610	0.8753249384030685	0.4143682506530004	T	T	T
0.3750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.3747282856577140	0.8749862526445397	0.1655212078787248	T	T	T
0.3764108652360887	0.8755865708715025	0.3319592363535858	T	T	T
0.5000000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.4998869327295670	0.8751812658242240	0.2480906000625169	T	T	T
0.5055151913609990	0.8731238347779038	0.4148474158648112	T	T	T
0.6250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.6248925317827460	0.8750091362601686	0.1650646760825531	T	T	T
0.6248172418189306	0.8749232339541924	0.3304077019589042	T	T	T
0.0107818878235205	0.0000650807771702	0.4997601396396643	T	T	T
0.0114955845813508	0.2499998386570477	0.4996580664421051	T	T	T
0.0107820378567556	0.4999346398536471	0.4997602372903424	T	T	T
0.0115195645232758	0.7499998276418356	0.4998399909047788	T	T	T
0.1283411305792781	0.1248545558268160	0.4960563372626412	T	T	T
0.1283412958688802	0.3751452656068411	0.4960564376058726	T	T	T
0.1283407584085283	0.6247786801670037	0.4961879813818131	T	T	T
0.1283407829396418	0.8752210361218291	0.4961878215680423	T	T	T
0.2475180664124696	0.0000486274258509	0.4954767184835523	T	T	T
0.2475169525571639	0.2499998825329087	0.4954583960944765	T	T	T
0.2475181268736475	0.4999516171387931	0.4954770424820430	T	T	T
0.2474797152954380	0.7500000786930605	0.4956487271241037	T	T	T
0.3706589219988629	0.1162252525626641	0.4987747544934015	T	T	T
0.3706586726839391	0.3837747177819432	0.4987746972782676	T	T	T
0.3706363440345925	0.6161420261711174	0.4989230276175873	T	T	T
0.3706356879393162	0.8838583136158275	0.4989223833799498	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7500761508004696	0.9999805195653744	0.1651024176585355	T	T	T
0.7489346695771139	-0.0000001252104773	0.3300787121697637	T	T	T
0.7500000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.7499852399580480	0.1249743996803537	0.2477501516826824	T	T	T
0.7481807475900559	0.1250555876854875	0.4121662647167953	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7501378834074023	0.2499999702188914	0.1650466825082335	T	T	T
0.7488843959066123	0.2499999249857297	0.3300343133829874	T	T	T
0.7500000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.7499852797802691	0.3750255005936200	0.2477501392918579	T	T	T
0.7481806853144758	0.3749442523284180	0.4121662691062942	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7500761368297240	0.5000193830760915	0.1651024512640963	T	T	T
0.7489347032081137	0.4999999152028989	0.3300787613492961	T	T	T
0.7500000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.7499913217478198	0.6250044677038438	0.2478034741259733	T	T	T
0.7481640530147764	0.6249832860371566	0.4122587355131401	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7501329573171820	0.7499999905929091	0.1650826341879648	T	T	T
0.7488738648944568	0.7499997906504573	0.3301449467098302	T	T	T
0.7500000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.7499913197355839	0.8749953469311299	0.2478035000928291	T	T	T
0.7481640400859397	0.8750162599263887	0.4122587814143830	T	T	T
0.8750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.8751165752265249	-0.0000236252419564	0.2481574885960201	T	T	T
0.8689676053218841	0.0000401401254396	0.4117225664335413	T	T	T
0.8750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.8752526615598855	0.1249703620914689	0.1653137253270810	T	T	T
0.8747640721099172	0.1250212577430180	0.3310176355327463	T	T	T
0.8750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.8751328832415212	0.2500000474144309	0.2481391321064145	T	T	T
0.8689880123384230	0.2499999769782699	0.4117122986708476	T	T	T

0.8750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.8752527031667472	0.3750295826302555	0.1653137481606002	T	T	T
0.8747641009807346	0.3749786682690922	0.3310176305827401	T	T	T
0.8750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.8751165788949876	0.5000234863061145	0.2481575266294265	T	T	T
0.8689675617374341	0.4999596698344844	0.4117226102358619	T	T	T
0.8750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.8752475775804174	0.6250073920879144	0.1653412736595944	T	T	T
0.8747609026655702	0.6250319302137560	0.3311048569082332	T	T	T
0.8750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.8751314161349587	0.7499999627685275	0.2482125161675054	T	T	T
0.8689553363727562	0.7499998100291274	0.4118510793208282	T	T	T
0.8750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.8752475710690582	0.8749924851986013	0.1653412925392435	T	T	T
0.8747609363890769	0.8749678033127999	0.3311048429409464	T	T	T
0.1250000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.1249507569328064	0.1250040857982759	0.2491385331623744	T	T	T
0.1260011098060992	0.1252015903386217	0.4151282533316047	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1249001245858450	0.9999784205667666	0.1658686847283293	T	T	T
0.1237728704211285	0.9999619159840470	0.3325207711183477	T	T	T
0.0000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.0002499010918127	0.1249845211588159	0.1657382219514923	T	T	T
0.9997266554479202	0.1250074820810398	0.3325426499881330	T	T	T
0.0000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.9998409689189032	0.9999719018786929	0.2494067259330430	T	T	T
0.9945220457325881	0.0000218983156144	0.4205106166542032	T	T	T
0.1250000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.1249508498022378	0.3749958086647768	0.2491384773749696	T	T	T
0.1260010590796727	0.3747983879027446	0.4151280334321567	T	T	T
0.1250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.1249152881811280	0.2499999473139072	0.1658728868133900	T	T	T
0.1241606799337852	0.2499997893165139	0.3326689444779738	T	T	T
0.0000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.0002499631748615	0.3750153662828602	0.1657381656708743	T	T	T
0.9997265594887479	0.3749922133086463	0.3325426536779942	T	T	T
0.0000000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.9999231922858633	0.249999674274379	0.2494274318635252	T	T	T
0.9950735555195236	0.2499997874675376	0.4204309471761485	T	T	T
0.3750000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.3749387727807019	0.1249890454076334	0.2490112099807905	T	T	T
0.3791226369627980	0.1253259816255163	0.4183864693320353	T	T	T
0.3750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3746231556724281	0.9999733747045623	0.1656474652121708	T	T	T
0.3749652504020394	0.9999691716613794	0.3321202463037498	T	T	T
0.2500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.2498923366945107	0.1249877068834445	0.1658055853695878	T	T	T
0.2508308083171846	0.1251188826420930	0.3322928064908193	T	T	T
0.2500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.2497976787519612	0.9999605431060730	0.2490737346316473	T	T	T
0.2492449026593982	0.9999811119780827	0.4148029398337983	T	T	T
0.3750000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.3749387872340128	0.3750109081911014	0.2490111703985488	T	T	T
0.3791231966582282	0.3746734383349808	0.4183868800555562	T	T	T
0.3750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.3745548214418684	0.2499999336250980	0.1656337035375142	T	T	T
0.3745180895494611	0.2499997054801365	0.3321627442174598	T	T	T
0.2500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.2498922942429097	0.3750122454458492	0.1658055909851213	T	T	T
0.2508305321716060	0.3748810170694216	0.3322928220766971	T	T	T

0.2500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.2497748088129014	0.2500001233478229	0.2490922502189905	T	T	T
0.2519921213692610	0.249997959479435	0.4157737032358696	T	T	T
0.5000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.4996265424161825	0.1249287181170056	0.1652437313068771	T	T	T
0.4997700984483421	0.1248391049912901	0.3313205336445466	T	T	T
0.5000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.4998214248249818	0.9999742158781589	0.2477638686228389	T	T	T
0.5040015690078820	0.0000195199392454	0.4112244583082968	T	T	T
0.5000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.4996265648617907	0.3750710698852502	0.1652438178924501	T	T	T
0.4997698793153038	0.3751606705536019	0.3313204139966505	T	T	T
0.5000000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.4997570129634851	0.249998899933755	0.2473555204699520	T	T	T
0.5026653857779081	0.249999560168826	0.4080843694892959	T	T	T
0.6250000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.6247967601142026	0.1249821036921328	0.2474793979820116	T	T	T
0.6260340685329526	0.1252543026029380	0.4111726115814947	T	T	T
0.6250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6249430758884097	0.9999840020655700	0.1651005206879971	T	T	T
0.6253303547184508	-0.0000103943659089	0.3305072950936627	T	T	T
0.6250000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.6247967267571227	0.3750177414719448	0.2474793182997183	T	T	T
0.6260344346572156	0.3747452871669100	0.4111723132101937	T	T	T
0.6250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.6250014803797680	0.249999586778889	0.1650281582578094	T	T	T
0.6255504728167477	0.2499995418881183	0.3302024879091796	T	T	T
0.0000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.9998411149839765	0.5000280173858829	0.2494068128869575	T	T	T
0.9945220911537059	0.4999778387150750	0.4205108745123653	T	T	T
0.1250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1249002757893355	0.5000214894282187	0.1658687002858494	T	T	T
0.1237729737809062	0.5000380134295398	0.3325209812155350	T	T	T
0.2500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.2497976720723322	0.5000393288102631	0.2490738760142100	T	T	T
0.2492451701151654	0.5000188620802934	0.4148028312649398	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3746230762813877	0.5000265953742964	0.1656475981879622	T	T	T
0.3749651808137685	0.5000307292066619	0.3321202597758730	T	T	T
0.5000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.4998213917434409	0.5000256268934045	0.2477638916546883	T	T	T
0.5040016855798483	0.4999805665388303	0.4112244221104825	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.6249429777406621	0.5000159159441320	0.1651005906619627	T	T	T
0.6253303656763309	0.5000103443165826	0.3305070821310165	T	T	T
0.0000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.0002433672764860	0.6250149199870605	0.1657598976463035	T	T	T
0.9997160084499902	0.6250334543028695	0.3326218213697064	T	T	T
0.1250000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.1249398914695747	0.6250545161850173	0.2491921890420083	T	T	T
0.1260028058401371	0.6252127346497324	0.4152538121782585	T	T	T
0.2500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.2498868866562537	0.6250269616007409	0.1658346590984069	T	T	T
0.2508447831411821	0.6251548008572507	0.3323964431455965	T	T	T
0.3750000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.3749477248492104	0.6250363959763008	0.2490723054904959	T	T	T
0.3791882223819242	0.6253470283704997	0.4185351417331695	T	T	T
0.5000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.4996279589831989	0.6249599028779889	0.1652738015905312	T	T	T
0.4997952960976124	0.6248688979598033	0.3314193057950691	T	T	T

0.6250000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.6248000473062364	0.6250104252780392	0.2475430786004411	T	T	T
0.6260516087382759	0.6252049017702747	0.4112684829124251	T	T	T
0.0000000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.9999155035460037	0.7500000342106538	0.2495071957306786	T	T	T
0.9950517782847035	0.7499999723783802	0.4206243723493636	T	T	T
0.1250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.1249168791038067	0.7499999920544584	0.1659252004955294	T	T	T
0.1241496057425080	0.7499998508661095	0.3328117614881969	T	T	T
0.2500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.2497841514372388	0.7499998701552115	0.2491938245487491	T	T	T
0.2519813998560832	0.7499997096159864	0.4159392030627898	T	T	T
0.3750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.3745699074094125	0.7499999516148856	0.1656668044521624	T	T	T
0.3745507954198952	0.7499996039801389	0.3322880215628847	T	T	T
0.5000000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.4997716512732842	0.7499998247262998	0.2474554952371129	T	T	T
0.5027086822560992	0.7499998655672174	0.4082972682456482	T	T	T
0.6250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.6250080658858750	0.7499999904949468	0.1650676404706547	T	T	T
0.6255614301423278	0.7499997061216144	0.3303178928423093	T	T	T
0.0000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.0002433231775594	0.8749851348354065	0.1657600059957515	T	T	T
0.9997159003635830	0.8749662884300400	0.3326216893347272	T	T	T
0.1250000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.1249396303749008	0.8749451291234431	0.2491921049762822	T	T	T
0.1260026205129919	0.8747871902100900	0.4152535677471921	T	T	T
0.2500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.2498868815828560	0.8749728408403853	0.1658345755624632	T	T	T
0.2508446684838928	0.8748452681821847	0.3323961842271640	T	T	T
0.3750000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.3749475805406887	0.8749634831540946	0.2490722934471612	T	T	T
0.3791885253342897	0.8746528311371375	0.4185355501065605	T	T	T
0.5000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.4996280433736373	0.8750399909910206	0.1652737231096062	T	T	T
0.4997951248098771	0.8751310067726877	0.3314191828584132	T	T	T
0.6250000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.6247999494253904	0.8749894464979339	0.2475431259643772	T	T	T
0.6260518831808888	0.8747947867870648	0.4112684207308470	T	T	T
0.0114052370132416	0.1253497673325799	0.4987324149717470	T	T	T
0.0114049420688747	0.3746501257433901	0.4987324594993829	T	T	T
0.0114026531226741	0.6252842334997882	0.4988366384277116	T	T	T
0.0114021509502399	0.8747155219376275	0.4988367731370236	T	T	T
0.1265059848849509	0.0000448274476602	0.4958516690852425	T	T	T
0.1282229556011225	0.2499996551425582	0.4957890118552331	T	T	T
0.1265062571570649	0.4999551853944466	0.4958517275826093	T	T	T
0.1282036913533793	0.7499996632782128	0.4959675522738244	T	T	T
0.2519148533502999	0.1262277593394905	0.4962417963365986	T	T	T
0.2519144820181725	0.3737721391633465	0.4962419212116211	T	T	T
0.2518756793850420	0.6261498834398728	0.4963745488894274	T	T	T
0.2518747051185461	0.8738501576606408	0.4963743984952590	T	T	T
0.3650342059417895	0.0000342485664403	0.4961386902336475	T	T	T
0.3702714043555109	0.2499997764153447	0.4997767478406435	T	T	T
0.3650342781954262	0.4999670508308937	0.4961388389569787	T	T	T
0.3701852339551456	0.7500008846980956	0.4999687267857800	T	T	T
0.7500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.7501037134505831	0.1249789034009388	0.1651167359522103	T	T	T
0.7494950585994284	0.1249726525109096	0.3304310789849830	T	T	T
0.7500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.7501354393522226	0.9999806550158619	0.2476231522023221	T	T	T

0.7485034042088770	0.0000370006541858	0.4114372051307049	T	T	T
0.7500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.7501036351581537	0.3750209333706797	0.1651167752254216	T	T	T
0.7494951520576851	0.3750272196190798	0.3304310166198428	T	T	T
0.7500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.7501990036952854	0.2499999433846807	0.2475450129859607	T	T	T
0.7484355448372363	0.2499998534983623	0.4113102686130633	T	T	T
0.7500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.7501353300640635	0.5000192744303319	0.2476231484250410	T	T	T
0.7485035225570423	0.4999630478267177	0.4114371329546774	T	T	T
0.7500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.7501042211162299	0.6250077120383415	0.1651400176862012	T	T	T
0.7494946185769558	0.6249766501572070	0.3305058556130357	T	T	T
0.7500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.7502010685067830	0.7499999248350947	0.2476134900767890	T	T	T
0.7484201736949431	0.7499995875793076	0.4114477012805312	T	T	T
0.7500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.7501043174080820	0.8749922426736789	0.1651400045165424	T	T	T
0.7494948745940694	0.8750232135466293	0.3305058556698389	T	T	T
0.8750000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.8750880391730933	0.1249951593028742	0.2479563006344856	T	T	T
0.8701895681699869	0.1250850681056277	0.4110074779817017	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.8753613073249543	0.9999823305724281	0.1654333265274770	T	T	T
0.8749721313912358	-0.0000108343800258	0.3316586757619291	T	T	T
0.8750000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.8750880432388178	0.3750047182162877	0.2479563390988067	T	T	T
0.8701896214565016	0.3749147401178981	0.4110075227400405	T	T	T
0.8750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.8753986302807472	0.2500001266512482	0.1654105738173253	T	T	T
0.8750792175161634	0.2499999508986090	0.3316349498358233	T	T	T
0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8753611513874682	0.5000177166081213	0.1654332161132263	T	T	T
0.8749722831590590	0.5000106741671366	0.3316585955419455	T	T	T
0.8750000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.8750877397293562	0.6250199098884096	0.2480126455882373	T	T	T
0.8701801094072075	0.6250520935628194	0.4110998185186120	T	T	T
0.8750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.8753909656656584	0.7499999659892257	0.1654558898375515	T	T	T
0.8750569855365822	0.7499999779610899	0.3317628003548907	T	T	T
0.8750000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.8750878001041236	0.8749799734586966	0.2480126596233497	T	T	T
0.8701801519918586	0.8749476420762885	0.4110997764237485	T	T	T
0.4697051179039695	0.3094898792372064	0.5109308685738512	T	T	T
0.4697045996908209	0.1905115272993042	0.5109307791257427	T	T	T
0.4694991990615573	0.8094871020638688	0.5115289812819289	T	T	T
0.4694984773573826	0.6905159559061164	0.5115304607878010	T	T	T
0.4402279487562860	0.2499992250509188	0.5079557587655250	T	T	T
0.4400576070307726	0.7500002235620363	0.5084524341756601	T	T	T

MS3-pbc-3CO2 (-2723.2372 eV)

1.0000000000000000

19.2439999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.2439999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.2439999999999998

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Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0001689857665837	0.0000425760796939	0.1655706025268125	T	T	T
0.9990882711184386	0.0000842018659239	0.3326111843559924	T	T	T
0.0000000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.0001823215602337	0.1250710437789894	0.2491352522383023	T	T	T
0.9927995967720471	0.1250334580521184	0.4203443137803128	T	T	T
0.1250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.1247708971290611	0.0000744180014171	0.2490450065376655	T	T	T
0.1244060938633321	-0.0000250106381640	0.4139128153575292	T	T	T
0.1250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.1250472721529094	0.1250604150294022	0.1657576147044282	T	T	T
0.1239891289259529	0.1251241367307198	0.3330144318628869	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0002553688298957	0.2500095764693985	0.1656416851576958	T	T	T
0.9992332817633192	0.2500252927029821	0.3327808586753551	T	T	T
0.0000000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.0002070062892526	0.3749620089653344	0.2491600880569957	T	T	T
0.9928010242610465	0.3750001729420027	0.4204134276169349	T	T	T
0.1250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.1250452788105345	0.2500287676275894	0.2493123359139380	T	T	T
0.1245718142948323	0.2500426412396670	0.4142812715190436	T	T	T
0.1250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.1250660234218520	0.3749599429886105	0.1657677995331571	T	T	T
0.1240255985987358	0.3749427553198820	0.3330632871139117	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2497806875551788	0.0000422118157417	0.1656046765344226	T	T	T
0.2503817922637957	0.0000202473187149	0.3316483914301127	T	T	T
0.2500000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.2499505975245148	0.1251570940839856	0.2491579906383429	T	T	T
0.2529112072320752	0.1250418835102059	0.4147239274948950	T	T	T
0.3750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.3748812971714797	0.9999676887149007	0.2483522097925587	T	T	T
0.3806740824707299	0.9993110067454435	0.4118671937166639	T	T	T
0.3750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.3748071176523514	0.1250346137397770	0.1654549364717892	T	T	T
0.3769129842975515	0.1254658785781987	0.3317850485374763	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2499046012435504	0.2500147791471968	0.1657081198212728	T	T	T
0.2512034572864000	0.2500440070960612	0.3325740997376920	T	T	T
0.2500000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.2499841268854285	0.3748905833404957	0.2491813226482588	T	T	T
0.2530063775800487	0.3750162235234640	0.4148177149907986	T	T	T
0.3750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.3752526189012830	0.2500240791190876	0.2486739984396003	T	T	T
0.3832154594416330	0.2500235234232492	0.4158833143998469	T	T	T
0.3750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.3748319493302533	0.3749818603040860	0.1654637125787131	T	T	T
0.3769606658274670	0.3745869715297702	0.3318179586007279	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.4997939645650440	0.9999970555802264	0.1650843451217997	T	T	T
0.5013506549279418	-0.0002855607729218	0.3294954326397821	T	T	T
0.5000000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.5000592053644201	0.1252419518868757	0.2480017594199188	T	T	T
0.5054699288940492	0.1216244874054583	0.4157583324575654	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4998615901770823	0.2500066779490293	0.1651742449270560	T	T	T
0.5012440091956850	0.2500011776512918	0.3317553315946141	T	T	T
0.5000000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.5001052285733789	0.3747762705491283	0.2480258495370797	T	T	T
0.5055534956770337	0.3783115139716236	0.4157572512443207	T	T	T

0.6250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.6250486140015626	-0.0000237022267373	0.2473544233388198	T	T	T
0.6253692272133865	-0.0002330032107963	0.4127504468482906	T	T	T
0.6250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.6249412295720367	0.1250335576962031	0.1650067396671969	T	T	T
0.6246702330859232	0.1248447459018760	0.3304477624108261	T	T	T
0.6250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.6248181354584866	0.2500081475405705	0.2477374059289535	T	T	T
0.6252960832451364	0.2499714364136955	0.4127830412254299	T	T	T
0.6250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.6249658685076616	0.3749713362682239	0.1650161806977813	T	T	T
0.6247341810308661	0.3751573694197060	0.3304859187736682	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0001923686299278	0.4999623041545236	0.1655831822956129	T	T	T
0.9991264468630506	0.4999386736219934	0.3326629145318687	T	T	T
0.1250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.1248085534022392	0.4999409900654432	0.2490785756203562	T	T	T
0.1244728281735545	0.5000480532879480	0.4139982875060159	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2498079383739430	0.4999648939755457	0.1656177294609860	T	T	T
0.2504514934176030	0.4999921489932959	0.3317147258075764	T	T	T
0.3750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.3749377374665254	0.5000391453757522	0.2483877253513607	T	T	T
0.3807852398145774	0.5007060562426060	0.4119901641200158	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4998287792315398	0.5000007113696363	0.1651002688321712	T	T	T
0.5014208407214501	0.5002778266561443	0.3295782166908157	T	T	T
0.6250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.6250973374279566	0.5000162415510039	0.2473924115303280	T	T	T
0.6254451702792726	0.5002133535759494	0.4128377640556368	T	T	T
0.0000000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.0000087483422574	0.6249708134357485	0.2490097950417854	T	T	T
0.9925002846247607	0.6249352883660774	0.4201552739325383	T	T	T
0.1250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.1249767435967738	0.6249896283806765	0.1656965945123392	T	T	T
0.1235112487151208	0.6250735573789882	0.3326589140202416	T	T	T
0.2500000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.2498062913833260	0.6250615109123232	0.2489747072915247	T	T	T
0.2515136404558757	0.6256659668023066	0.4137409752225816	T	T	T
0.3750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.3747577938012833	0.6250123184521311	0.1653974051741262	T	T	T
0.3767037131034143	0.6258325647239015	0.3315979711634916	T	T	T
0.5000000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.4999704994325904	0.6253160283540113	0.2479053000949671	T	T	T
0.5055232402339757	0.6226717053182342	0.4159937687018982	T	T	T
0.6250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.6249202181749642	0.6250231790580646	0.1649815315234107	T	T	T
0.6245545259243495	0.6249604784883114	0.3303762142172937	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0001317641412703	0.7499959017211469	0.1655617659836410	T	T	T
0.9988368244184428	0.7500009321460641	0.3324909662689639	T	T	T
0.1250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.1247222855038094	0.7499878559647715	0.2490464379984074	T	T	T
0.1237214503355532	0.7499959964182379	0.4137551281300278	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2497822287377656	0.7499924998613173	0.1656098279952125	T	T	T
0.2505681570619683	0.7499775684925369	0.3319900660985340	T	T	T
0.3750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.3750048231054097	0.7499789119994438	0.2484697966413160	T	T	T
0.3819556711495325	0.7500010598449406	0.4157941170776402	T	T	T

0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.4997811266333382	0.7499897123417877	0.1650909221200313	T	T	T
0.5008147316773797	0.7499721206895773	0.3315112690363497	T	T	T
0.6250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.6246927879526697	0.7499798010476117	0.2476345858235777	T	T	T
0.6252732636460927	0.7500097159376480	0.4124279423115698	T	T	T
0.0000000000000000	0.8750000000000000	0.0822561893037914	F	F	F
-0.0000137092364349	0.8750247066550176	0.2489891397778431	T	T	T
0.9924965125737226	0.8750980021025889	0.4201042820114409	T	T	T
0.1250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.1249599545433031	0.8750044789134065	0.1656883858205312	T	T	T
0.1234809075676912	0.8749113474796628	0.3326204759858021	T	T	T
0.2500000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.2497744109028263	0.8749182481459996	0.2489494412765643	T	T	T
0.2514492896380225	0.8743279327281719	0.4136759851169426	T	T	T
0.3750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.3747370977745114	0.8749776523560588	0.1653867958952934	T	T	T
0.3766512310963750	0.8741327128032389	0.3315465863207757	T	T	T
0.5000000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.4999313347361842	0.8746491774841509	0.2478772790516495	T	T	T
0.5054630333964761	0.8773301717150493	0.4159131403663952	T	T	T
0.6250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.6248994624229856	0.8749607440083287	0.1649707593249980	T	T	T
0.6245106833503030	0.8750106124175016	0.3303250728189595	T	T	T
0.0117172711830232	-0.0001246882402097	0.4996264651864982	T	T	T
0.0119076795184711	0.2499995288826580	0.4999259792326725	T	T	T
0.0117788260681296	0.5001751002138610	0.4997020589431087	T	T	T
0.0104373161107044	0.7500382866215927	0.4995689512138948	T	T	T
0.1290570584824639	0.1242927142772467	0.4960880977022942	T	T	T
0.1291080687089700	0.3757263790214617	0.4961610668862437	T	T	T
0.1281200249073907	0.6255699111952265	0.4958418976043583	T	T	T
0.1280772750133618	0.8744883167752859	0.4957928562005149	T	T	T
0.2474812031407467	0.9983804100438438	0.4952572830105776	T	T	T
0.2459963030938548	0.2499964789505777	0.4964544127257042	T	T	T
0.2475931198163049	0.5016592183662383	0.4953674201908718	T	T	T
0.2470059712943146	0.7500344602079497	0.4949720858521768	T	T	T
0.3719366507700506	0.1230335232251598	0.5019681170449100	T	T	T
0.3721775249639961	0.3770137690942279	0.5020551929107234	T	T	T
0.3705022198278749	0.6350450285948543	0.4979964757147384	T	T	T
0.3704408159701434	0.8650603059666689	0.4979290731761559	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7501571823581336	0.0000090704967266	0.1650026955269107	T	T	T
0.7488413121777201	-0.0000160345542424	0.3299635202925041	T	T	T
0.7500000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.7499978272606010	0.1250432578354541	0.2477780571032082	T	T	T
0.7481155069102483	0.1249151070717669	0.4122019336428508	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7501207739639900	0.2500046554430393	0.1650930054670279	T	T	T
0.7489131036353729	0.2500003323763112	0.3301606476152990	T	T	T
0.7500000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.7500360526241696	0.3749676587429684	0.2478014476495196	T	T	T
0.7481570357306719	0.3750477146796665	0.4122549997171022	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7501828262988772	0.4999862054577439	0.1650178382228185	T	T	T
0.7488955546852128	0.5000177776680406	0.3300205425585701	T	T	T
0.7500000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.7499417058803001	0.6250150384768324	0.2477391891301378	T	T	T
0.7481357240286171	0.6250316361453406	0.4121298375890174	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7500494627488887	0.7499910444454169	0.1650456662835892	T	T	T

0.7488144530811985	0.7499985877759024	0.3299992298100345	T	T	T
0.7500000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.7499105085940639	0.8749671448068628	0.2477141965941198	T	T	T
0.7480947827531035	0.8750067854551238	0.4120799273945788	T	T	T
0.8750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.8751180565148989	0.0000480855216641	0.2481026707650056	T	T	T
0.8689416927330027	0.0000122451368318	0.4116834521086083	T	T	T
0.8750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.8752752532855658	0.1250353295333454	0.1653181280912357	T	T	T
0.8748130962511409	0.1250359080915840	0.3310738539919190	T	T	T
0.8750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.8751911274079868	0.2500110197055655	0.2482055379074392	T	T	T
0.8690201695453466	0.2499775107335725	0.4118572612647719	T	T	T
0.8750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.8752921728148926	0.3749729303237742	0.1653280359379077	T	T	T
0.8748450444450662	0.3749765412584581	0.3311175939317344	T	T	T
0.8750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.8751568182527588	0.4999589084302927	0.2481376181202591	T	T	T
0.8689756293784583	0.5000096102275163	0.4117435756231006	T	T	T
0.8750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.8752213388159777	0.6249882003763072	0.1652850826838772	T	T	T
0.8746960516593926	0.6249642488568256	0.3309735348481284	T	T	T
0.8750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.8750205941651644	0.7499956414966324	0.2480746778342013	T	T	T
0.8688696140072724	0.7500356400712799	0.4116004513548782	T	T	T
0.8750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.8752068659875089	0.8750022168646751	0.1652750780142306	T	T	T
0.8746684890872792	0.8750537742155674	0.3309401499585303	T	T	T
0.1250000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.1251101227741389	0.1251132451428248	0.2492731756935672	T	T	T
0.1267901840963593	0.1250190478134225	0.4152876614598576	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1249060012604210	0.0000868818604087	0.1658899521012640	T	T	T
0.1243112179517375	0.0001238463167618	0.3326778590846490	T	T	T
0.0000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.0003291338073158	0.1250571833710555	0.1658122523073221	T	T	T
0.0000222761390208	0.1250980204784014	0.3327119950657754	T	T	T
0.0000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.9999814367628655	0.0000971401672744	0.2494403580981291	T	T	T
0.9953147738522650	0.0001443253542104	0.4204963463981666	T	T	T
0.1250000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.1251438001409460	0.3749294683889169	0.2492990787334576	T	T	T
0.1268516372789016	0.3750413488693976	0.4153567119753634	T	T	T
0.1250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.1250566731367580	0.2500126206576917	0.1660187215908427	T	T	T
0.1246487153277951	0.2500358980902398	0.3330444196011622	T	T	T
0.0000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.0003506894327736	0.3749585271491405	0.1658224877551398	T	T	T
0.0000509419283256	0.3749414075147427	0.3327521879613012	T	T	T
0.0000000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.0001335108488856	0.2500179985427987	0.2496116814400385	T	T	T
0.9954389805079232	0.2500174106552796	0.4208007951159967	T	T	T
0.3750000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.3750150086185838	0.1252107677709616	0.2491153724558013	T	T	T
0.3795253752852533	0.1249266199153341	0.4191336664975921	T	T	T
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0.3744969144756565	0.0000999296991200	0.1655897522413889	T	T	T
0.3743390173801899	0.0001147620538961	0.3317713508334608	T	T	T
0.2500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.2499278533322559	0.1251133653887430	0.1658885751843062	T	T	T

0.2512257801903308	0.1251832486714670	0.3325344627325382	T	T	T
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0.2497463482427857	0.0001470456489205	0.2490645997351975	T	T	T
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0.3750561578083719	0.3748258172356230	0.2491403246325279	T	T	T
0.3796477348323713	0.3751083506598255	0.4192348772281210	T	T	T
0.3750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.3746502255643676	0.2500149380749258	0.1658152826094166	T	T	T
0.3753226468232248	0.2500305611213810	0.3333045995846016	T	T	T
0.2500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.2499524758537885	0.3749123597918467	0.1658990774894877	T	T	T
0.2512766440468389	0.3748684032238486	0.3325865636467137	T	T	T
0.2500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.2501432234392240	0.2500310608160686	0.2495066977679987	T	T	T
0.2523395597903619	0.2500345366122825	0.4171188949979737	T	T	T
0.5000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.4996339288714491	0.1251408492421303	0.1652380153684427	T	T	T
0.4998004580244237	0.1252516658737357	0.3312195277640696	T	T	T
0.5000000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.4997825620950658	0.0000494122277563	0.2470406357040630	T	T	T
0.5025829752494405	-0.0005467649665331	0.4067035732966571	T	T	T
0.5000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.4996596367725668	0.3748713800350383	0.1652473757251000	T	T	T
0.4998557312292193	0.3747510901253241	0.3312609587007599	T	T	T
0.5000000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.4998217987010437	0.2500138853787826	0.2479090648682059	T	T	T
0.5033703654034218	0.2499868827436456	0.4119971354401407	T	T	T
0.6250000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.6248743239268355	0.1250718916804062	0.2474717383028224	T	T	T
0.6260306222428074	0.1246555734241047	0.4111860837598568	T	T	T
0.6250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6250568597982910	0.0000360383830766	0.1649821620392287	T	T	T
0.6257603903861233	-0.0000125763562455	0.3299901753373493	T	T	T
0.6250000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.6249146334122859	0.3749344797661550	0.2474935979505817	T	T	T
0.6261001511874713	0.3753006780217181	0.4112273984031334	T	T	T
0.6250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.6249762634929940	0.2500055404847488	0.1651516344755746	T	T	T
0.6252921757814489	0.2499994112355712	0.3307239468515585	T	T	T
0.0000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.0000215091434482	0.4999183818195713	0.2494713601068102	T	T	T
0.9953361886134059	0.4998890953220416	0.4205757934848515	T	T	T
0.1250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1249362708535464	0.4999200722160822	0.1659025894194793	T	T	T
0.1243544807853347	0.4998965905913604	0.3327393566096011	T	T	T
0.2500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.2497989778545485	0.4998645540589599	0.2491004236113700	T	T	T
0.2525642141333832	0.5002450393509967	0.4159108941019847	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3745295949118137	0.4999049515300913	0.1656042232752468	T	T	T
0.3744184918891086	0.4998879881514457	0.3318443065145668	T	T	T
0.5000000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.4998319278662701	0.4999424284977462	0.2470793703453925	T	T	T
0.5026727224999281	0.5005130748412356	0.4068072671655450	T	T	T
0.6250000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.6250831955558620	0.4999585326146709	0.1649978585048142	T	T	T
0.6258234968415941	0.4999963267586081	0.3300495736400870	T	T	T
0.0000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.0002417623723762	0.6249475976586346	0.1657491179767658	T	T	T

0.9997088027561157	0.6249049698779654	0.3325123592854740	T	T	T
0.1250000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.1248751091008063	0.6248952798242723	0.2490669179799405	T	T	T
0.1258749189836287	0.6247504941116993	0.4149638122488851	T	T	T
0.2500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.2498386483782698	0.6249308090880589	0.1657549831002892	T	T	T
0.2506413024940165	0.6247912308507081	0.3320097320407135	T	T	T
0.3750000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.3748778475260932	0.6249450298031706	0.2487823587095578	T	T	T
0.3783000331062779	0.6250185545834629	0.4174587811924436	T	T	T
0.5000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.4996393197343135	0.6250332986146767	0.1651381155027926	T	T	T
0.4997755600376779	0.6253135758545915	0.3308735809008826	T	T	T
0.6250000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.6248779068504142	0.6249884622775904	0.2473862543431480	T	T	T
0.6261349038192704	0.6247763000887114	0.4111320119245779	T	T	T
0.0000000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.9997848921407611	0.7499984535269282	0.2493504358942107	T	T	T
0.9944338670537061	0.7500165388208686	0.4204181502913290	T	T	T
0.1250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.1248450895003680	0.7499936872153201	0.1658348497732091	T	T	T
0.1236084987709967	0.7499907422595032	0.3322965122420652	T	T	T
0.2500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.2496774018559775	0.7499854729472886	0.2488906746928936	T	T	T
0.2487518290510402	0.7500013482553163	0.4143740604458232	T	T	T
0.3750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.3745663521449688	0.7499887711915850	0.1655464427961611	T	T	T
0.3747828517965816	0.7499870178143440	0.3317340050477335	T	T	T
0.5000000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.4998198400697164	0.7499774550267081	0.2475470359917323	T	T	T
0.5038391769432484	0.7499982321175194	0.4112683527271504	T	T	T
0.6250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.6249668965503680	0.7499885002890928	0.1650491247752839	T	T	T
0.6253271576818829	0.7499862379177830	0.3304396122671751	T	T	T
0.0000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.0002246418616107	0.8750479589359378	0.1657407425646660	T	T	T
0.9996841109833907	0.8751016909013138	0.3324854466028995	T	T	T
0.1250000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.1248490950033404	0.8750924934029308	0.2490473487776597	T	T	T
0.1258378674984324	0.8752606130977523	0.4149143960295659	T	T	T
0.2500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.2498172000549287	0.8750565686625180	0.1657461794104724	T	T	T
0.2506004122388669	0.8751962335306137	0.3319720656374189	T	T	T
0.3750000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.3748391686102548	0.8750321333990906	0.2487576058462723	T	T	T
0.3782373841047597	0.8750068509452158	0.4173989272401094	T	T	T
0.5000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.4996187244234634	0.8749458316713492	0.1651276297541124	T	T	T
0.4997262083842229	0.8746471058409514	0.3308271505881997	T	T	T
0.6250000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.6248440097445880	0.8749848570613901	0.2473621507250652	T	T	T
0.6260787650381614	0.8752313454484443	0.4110802378528936	T	T	T
0.0123885758703921	0.1248913979178967	0.4987303270064423	T	T	T
0.0124398316923698	0.3751372811766076	0.4987895009106016	T	T	T
0.0113677206350566	0.6245902026008026	0.4986207873050612	T	T	T
0.0113380922349883	0.8754699755178429	0.4985760999594639	T	T	T
0.1287346250618593	-0.0003138984065681	0.4956227435045132	T	T	T
0.1284322210998005	0.2500106791459202	0.4960609790292392	T	T	T
0.1287866135155313	0.5003520941128428	0.4957193023262253	T	T	T
0.1261949128448700	0.7500300765044909	0.4955363612026066	T	T	T

0.2529433405617775	0.1232272328487664	0.4959635045774634	T	T	T
0.2530730327797154	0.3767574580234088	0.4960799475183355	T	T	T
0.2517190757454605	0.6241032336350294	0.4959191511324588	T	T	T
0.2516752124029743	0.8759694148347296	0.4958540033432864	T	T	T
0.3738097589943210	0.9958892545912807	0.4998432743693975	T	T	T
0.3711414392732191	0.2500020994831752	0.5004969049477255	T	T	T
0.3739048053624205	0.5042170482318953	0.4999298134559075	T	T	T
0.3644526450782994	0.7500736608258259	0.4953352688546948	T	T	T
0.7500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.7501782461152547	0.1250478331145689	0.1651394804444853	T	T	T
0.7495964271671876	0.1250743080735473	0.3304627071231188	T	T	T
0.7500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.7502834860669908	0.0000384136379483	0.2474829610626503	T	T	T
0.7484442979314888	0.0000061716059204	0.4112110427226583	T	T	T
0.7500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.7501999574122705	0.3749566365175720	0.1651500842840724	T	T	T
0.7496449029251246	0.3749267784122085	0.3304987719861701	T	T	T
0.7500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.7502095746683702	0.2500052767489029	0.2476840473388103	T	T	T
0.7485540453058716	0.2499769538271331	0.4114465422205013	T	T	T
0.7500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.7503260553879615	0.4999589668330916	0.2475180124157266	T	T	T
0.7485080473335716	0.4999956722650898	0.4112776975224803	T	T	T
0.7500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.7501554431081433	0.6249843650144210	0.1651031519408093	T	T	T
0.7495463151297596	0.6250302240427427	0.3303999360861054	T	T	T
0.7500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.7501223832217774	0.7499906739516382	0.2475633131527370	T	T	T
0.7484970342103321	0.7500220750495704	0.4113349725687186	T	T	T
0.7500000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.7501391366233950	0.8750016360607580	0.1650923974367054	T	T	T
0.7495027744278469	0.8749693728208622	0.3303628001068907	T	T	T
0.8750000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.8752250569285274	0.1250730789689853	0.2480292247629033	T	T	T
0.8704174149630671	0.1250025642613178	0.4111191122583711	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.8754366409009766	0.0000449564285463	0.1654229534306184	T	T	T
0.8751948987465388	0.0000868347213287	0.3316445418486106	T	T	T
0.8750000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.8752571729645942	0.3749420630378125	0.2480548536699312	T	T	T
0.8704435918066554	0.3749777858137841	0.4111678870458376	T	T	T
0.8750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.8754731998396291	0.2500027670154674	0.1655041374741562	T	T	T
0.8752733678768105	0.2500039189448626	0.3318090018641466	T	T	T
0.8750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.8754607048002155	0.4999540595703821	0.1654391008319438	T	T	T
0.8752402069340685	0.4999296715741773	0.3316962300326310	T	T	T
0.8750000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.8751177717142384	0.6249604963506596	0.2479491075058710	T	T	T
0.8702516469691470	0.6249019558869348	0.4109774762282069	T	T	T
0.8750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.8753562157682681	0.7499937161830044	0.1654161690057144	T	T	T
0.8749713374961660	0.7500137743128069	0.3315797588591752	T	T	T
0.8750000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.8750931155749543	0.8750378434352346	0.2479301465052045	T	T	T
0.8702296360702199	0.8751501997494223	0.4109411737569535	T	T	T
0.4738308333334180	0.5657530786386353	0.5033269921948316	T	T	T
0.4760642367675008	0.4468900197973049	0.5032130373974700	T	T	T
0.3931462964937106	0.3090878422095095	0.5659554507238448	T	T	T
0.3921001009784927	0.1908174194073282	0.5660616391418291	T	T	T

0.4759321502228759	0.0533118521010565	0.5028324244851790	T	T	T
0.4738064295376545	0.9344255520569148	0.5031196755522467	T	T	T
0.4452836884955515	0.5055304187449656	0.5027469272579324	T	T	T
0.3872344383844706	0.2499677988174887	0.5471721077823853	T	T	T
0.4452016160369857	0.9946182866849389	0.5024928473209260	T	T	T

MS3-pbc-4CO2 (-2747.7349 eV)

1.0000000000000000		
19.243999999999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	19.243999999999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.243999999999998

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Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0001628110384734	0.0000088166359624	0.1655741746177038	T	T	T
0.9989421880149649	0.0000194194716799	0.3325542813702971	T	T	T
0.0000000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.0000736435182823	0.1250067269442283	0.2490542241651318	T	T	T
0.9925219126677349	0.1250652298688637	0.4201375497959500	T	T	T
0.1250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.1248710418179335	0.0000158136789763	0.2491348539684657	T	T	T
0.1239314371618463	0.0000365332504260	0.4139695853071751	T	T	T
0.1250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.1250138702478928	0.1249905566306806	0.1657072346262507	T	T	T
0.1237855944711093	0.1249620724637174	0.3328314877427949	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0001745365289962	0.2500114945003735	0.1655520188498674	T	T	T
0.9990646822120423	0.2500191106910007	0.3325981661463985	T	T	T
0.0000000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.0001127040373757	0.3750190908490950	0.2490902425109554	T	T	T
0.9925732433251142	0.3749844366612907	0.4202174611316588	T	T	T
0.1250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.1247820732717470	0.2500235770072449	0.2490302670480690	T	T	T
0.1244002665937228	0.2500403301235737	0.4138790085923952	T	T	T
0.1250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.1250372433191342	0.3750293508285228	0.1657229991322287	T	T	T
0.1238672487891390	0.3750943934470513	0.3328927322477555	T	T	T
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2498570893467316	0.0000091167019008	0.1656252559889421	T	T	T
0.2508585056112080	0.0000282656065372	0.3322360326879144	T	T	T
0.2500000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.2499005831974002	0.1249192532211766	0.2490436655206019	T	T	T
0.2525464215557098	0.1246848347411733	0.4143458400932361	T	T	T
0.3750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.3751846236397202	0.0000018471149836	0.2485123630095757	T	T	T
0.3828328748379471	0.9999895000674663	0.4151610142562016	T	T	T
0.3750000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.3748074606178136	0.1249811676232758	0.1653824787274199	T	T	T
0.3769957287070466	0.1243977024747413	0.3315966765661240	T	T	T
0.2500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.2497990922008063	0.2500162053635486	0.1655855657345643	T	T	T
0.2503660122354435	0.2500290468570923	0.3315900782517512	T	T	T
0.2500000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.2499469670854151	0.3751134959040363	0.2490809355006561	T	T	T
0.2527111040181669	0.3753447693673038	0.4144629019667593	T	T	T
0.3750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.3749474718316880	0.2500114617629602	0.2482528899802926	T	T	T

0.3807236014835678	0.2499905652532982	0.4112314782453134	T	T	T
0.3750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.3748306571729226	0.3750256136994991	0.1653929921559867	T	T	T
0.3770637681740357	0.3756187457264693	0.3316347571437409	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.4998276345054096	0.0000018204150196	0.1650700629833345	T	T	T
0.5012015190842520	-0.0000031561332130	0.3316909072283504	T	T	T
0.5000000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.5000642781889321	0.1246650431224631	0.2478844294138270	T	T	T
0.5054376814339692	0.1283242201253547	0.4164470954779348	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.4998635066506468	0.2500039031550256	0.1650388329361800	T	T	T
0.5015809156425423	0.2499857648830895	0.3291677208019356	T	T	T
0.5000000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.5001161171271202	0.3753283864496390	0.2479002221575696	T	T	T
0.5055278143256645	0.3716524694445478	0.4164017186155063	T	T	T
0.6250000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.6247112660919175	-0.0000062326268136	0.2476628328070128	T	T	T
0.6250458078993787	-0.0000384853299681	0.4127623428310412	T	T	T
0.6250000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.6249493991677780	0.1249608303251841	0.1649548994854243	T	T	T
0.6244524240156976	0.1250959611342699	0.3304448523856412	T	T	T
0.6250000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.6251588244644148	0.2499973461418591	0.2472953258684406	T	T	T
0.6252866026434452	0.2499697290164845	0.4127736368512894	T	T	T
0.6250000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.6249768898180740	0.3750374615551859	0.1649655219991329	T	T	T
0.6245374192768769	0.3748884794367313	0.3304691908269820	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0001991050647924	0.4999862840557158	0.1655955952246759	T	T	T
0.9990233062645835	0.4999850104688253	0.3326387890193276	T	T	T
0.1250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.1249354492294552	0.4999831529573868	0.2491931770028642	T	T	T
0.1241138117663560	0.4999865706312395	0.4140888030543542	T	T	T
0.2500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2498869406472023	0.4999901974084422	0.1656466553323436	T	T	T
0.2509890372663633	0.4999821436799006	0.3323195373463750	T	T	T
0.3750000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.3752529850916297	0.4999904476127717	0.2485387190831101	T	T	T
0.3830163342038242	0.5000236529945566	0.4152976755979686	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.4998668931224127	0.4999922608189112	0.1650856377501129	T	T	T
0.5012923033664489	0.4999881606258504	0.3317135929624278	T	T	T
0.6250000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.6247853051625823	0.4999895836097832	0.2476891074361600	T	T	T
0.6251542072919528	0.5000221922831756	0.4128080509988505	T	T	T
0.0000000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.0000701959736451	0.6249498330907588	0.2490634173147471	T	T	T
0.9925094775121092	0.6249975926402190	0.4201769339388101	T	T	T
0.1250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.1250058920620756	0.6249500352930082	0.1657100952742408	T	T	T
0.1237819068885312	0.6248764274610779	0.3328502975234545	T	T	T
0.2500000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.2498889822235363	0.6248686055350884	0.2490549156947493	T	T	T
0.2525460738885820	0.6246883566244980	0.4143855997916202	T	T	T
0.3750000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.3748000907323477	0.6249656684139866	0.1653819410910054	T	T	T
0.3769735386468864	0.6243686405952842	0.3316017179630144	T	T	T
0.5000000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.5000619180052099	0.6246613211946264	0.2478882052849423	T	T	T

0.5054001254132544	0.6283722933645334	0.4163617993960251	T	T	T
0.6250000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.6249459796234460	0.6249501271148197	0.1649544779245977	T	T	T
0.6244679771282007	0.6250937036030154	0.3304377731838672	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0001326200021246	0.7499832275682353	0.1655372734956405	T	T	T
0.9989685893338253	0.7499815468904366	0.3325332881920698	T	T	T
0.1250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.1247074775047057	0.7499774526472784	0.2489898064967372	T	T	T
0.1242018570130738	0.7499848449653066	0.4137956867481457	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.2497524347416755	0.7499821097939521	0.1655631974741628	T	T	T
0.2502248336790174	0.7499805622667827	0.3315381256094046	T	T	T
0.3750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.3748613464242246	0.7499877070244867	0.2482385020347599	T	T	T
0.3805366837696800	0.7500190668244169	0.4111511255157821	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.4998200617037408	0.7499890954268914	0.1650210023063802	T	T	T
0.5014817894641862	0.7500100206257861	0.3291301916777838	T	T	T
0.6250000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.6250997504058581	0.7499865572217124	0.2472750729512302	T	T	T
0.6251826089999941	0.7500170642254026	0.4127177863991709	T	T	T
0.0000000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.0000277872236438	0.8750134745118026	0.2490290379108527	T	T	T
0.9924503537432507	0.8749893305651351	0.4201017553769216	T	T	T
0.1250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.1249846746573935	0.8750241240120565	0.1656940733698864	T	T	T
0.1236960628873000	0.8750890657259318	0.3327865319403224	T	T	T
0.2500000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.2498478764029578	0.8751008239730627	0.2490192846808292	T	T	T
0.2523730204227353	0.8753396704292705	0.4142656626901067	T	T	T
0.3750000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.3747789375981258	0.8750193970801744	0.1653683976587385	T	T	T
0.3769080193093889	0.8756217754532181	0.3315715961431129	T	T	T
0.5000000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.5000138777580899	0.8753236104491258	0.2478696499416093	T	T	T
0.5053078445465901	0.8716327982646431	0.4164303046686721	T	T	T
0.6250000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.6249218586050703	0.8750326135999927	0.1649416529280146	T	T	T
0.6243837125210572	0.8748897320065316	0.3304155240975425	T	T	T
0.0109630509255178	0.0000468823605840	0.4997218792778899	T	T	T
0.0115368377866993	0.2500292644598069	0.4996602050434862	T	T	T
0.0111846075370826	0.4999911766729730	0.4998330936861368	T	T	T
0.0113244492572879	0.7500010466957030	0.4995847029473102	T	T	T
0.1283515600787009	0.1253141314386211	0.4959236073012892	T	T	T
0.1285083134216412	0.3747073111159505	0.4960098395797451	T	T	T
0.1283383776390366	0.6253361545605483	0.4959573129560684	T	T	T
0.1281786199531278	0.8747262999727087	0.4958713068875934	T	T	T
0.2450585239243553	0.9999794826192961	0.4961491885546517	T	T	T
0.2470231011639652	0.2499703301480738	0.4953276365631563	T	T	T
0.2453486854384702	0.5000701221075040	0.4962862059901432	T	T	T
0.2467301496945582	0.7500739566356157	0.4952122409277031	T	T	T
0.3716187309198725	0.1251201543158819	0.5012933681859215	T	T	T
0.3719047511499616	0.3747358936495843	0.5014557029403687	T	T	T
0.3715486441181410	0.6253744445381988	0.5014306577250238	T	T	T
0.3712598266604221	0.8748474779869639	0.5012563521397767	T	T	T
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7500545080929754	-0.0000017273353598	0.1650451338929949	T	T	T
0.7486813680617976	-0.0000080305180118	0.3300785886647143	T	T	T
0.7500000000000000	0.1250000000000000	0.0822561893037914	F	F	F

0.7499192865231390	0.1249730289272830	0.2477506690550539	T	T	T
0.7479646206967765	0.1249944219764659	0.4121840237626143	T	T	T
0.7500000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.7502002851448631	0.2500037010806168	0.1649809014877341	T	T	T
0.7488027988264082	0.2499892993298192	0.3299816916079953	T	T	T
0.7500000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.7499748757872650	0.3750245542036185	0.2477751801118928	T	T	T
0.7480209267533073	0.3749540208846115	0.4122350836125824	T	T	T
0.7500000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7500931990200719	0.4999944437977115	0.1650606366224405	T	T	T
0.7487730688923294	0.4999917463916264	0.3301362930247156	T	T	T
0.7500000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.7499228384532843	0.6249520492057001	0.2477615714906046	T	T	T
0.7479539817359636	0.6250613170122880	0.4122040532932288	T	T	T
0.7500000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.7501642378757684	0.7499866692739274	0.1649624707107279	T	T	T
0.7487293646980696	0.7499943911395438	0.3299383117219082	T	T	T
0.7500000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.7498683703671424	0.8750206376279124	0.2477372934550558	T	T	T
0.7478997381928583	0.8749673609586731	0.4121540927374683	T	T	T
0.8750000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.8750191370729085	0.0000013057059133	0.2481065344434657	T	T	T
0.8687528247655131	-0.0000166817462865	0.4116820299633003	T	T	T
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0.8752277458121095	0.1249893462604134	0.1652840328196124	T	T	T
0.8746418778453326	0.1249969879424971	0.3309951922516884	T	T	T
0.8750000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.8751192142584125	0.2500074761950445	0.2481106178453107	T	T	T
0.8688199637451999	0.2499743030171268	0.4117011681560852	T	T	T
0.8750000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.8752531690381575	0.3750166066585683	0.1652982878660839	T	T	T
0.8746942764445826	0.3749983179659747	0.3310564931596960	T	T	T
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0.8750862934199607	0.4999877151946346	0.2481555930757151	T	T	T
0.8688150482848382	0.5000169873228887	0.4117790912327846	T	T	T
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0.8752258688872003	0.6249663957768038	0.1652895811901208	T	T	T
0.8746414713324268	0.6249878509734533	0.3310168733798015	T	T	T
0.8750000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.8750492572223285	0.7499841243258899	0.2480754490141191	T	T	T
0.8687387664496111	0.7500192686214721	0.4116464387152696	T	T	T
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0.8752009748058014	0.8750146548252832	0.1652748260944454	T	T	T
0.8745894091513440	0.8749974812181730	0.3309615173012002	T	T	T
0.1250000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.1250156936086518	0.1250010777259881	0.2492233034232849	T	T	T
0.1264143735674485	0.1250623729022850	0.4151575919254285	T	T	T
0.1250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1249679853227492	0.0000096551645059	0.1659858513873822	T	T	T
0.1243334439147788	0.0000263830540592	0.3328385965851702	T	T	T
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0.0003099967684620	0.1249929323065015	0.1658168343310949	T	T	T
-0.0001010633396128	0.1249988289176072	0.3326549388957759	T	T	T
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0.9999933743131640	0.0000127022086088	0.2495133229544159	T	T	T
0.9950655042705685	0.0000398425163366	0.4206188291039523	T	T	T
0.1250000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.1250612375093346	0.3750325334557771	0.2492653061017750	T	T	T
0.1265706827899614	0.3749919470689747	0.4152431640160346	T	T	T
0.1250000000000000	0.2500000000000000	0.0000000000000000	F	F	F

0.1249445037568459	0.2500140167905888	0.1659534409865296	T	T	T
0.1244000340074304	0.2500309514121021	0.3327720424500824	T	T	T
0.0000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.0003352022877411	0.3750224722927043	0.1658369387669419	T	T	T
-0.0000423357899043	0.3750346946785875	0.3327197781775889	T	T	T
0.0000000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.0000471736491517	0.2500168812156031	0.2495276097884083	T	T	T
0.9953833980770809	0.2500379621300060	0.4205803369747818	T	T	T
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0.3748876216309699	0.1248664218922112	0.2489446253110653	T	T	T
0.3787224695704415	0.1245963449744294	0.4182511869349164	T	T	T
0.3750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3745595889179578	0.0000034563814857	0.1657436141869775	T	T	T
0.3749979306780027	0.0000137894182234	0.3329251528181861	T	T	T
0.2500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.2498767823884465	0.1249763727961958	0.1658763759523069	T	T	T
0.2509233952849845	0.1249254829663430	0.3323603665724426	T	T	T
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0.2499447933747880	0.0000129546228298	0.2493744307795457	T	T	T
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0.3750000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.3749425398494975	0.3751500865653329	0.2489741441266474	T	T	T
0.3788944742816905	0.3753715360307698	0.4183950694713224	T	T	T
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0.3744709656235938	0.2500100134950513	0.1656075855025513	T	T	T
0.3742086064472923	0.2500182968827976	0.3315834794157060	T	T	T
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0.2499001262585078	0.3750495218904576	0.1658955268291499	T	T	T
0.2510184716399142	0.3751156608708508	0.3324177850930988	T	T	T
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0.2497426663227437	0.2500222257382902	0.2491382708574739	T	T	T
0.2527297023542206	0.2500147564634234	0.4160557889136367	T	T	T
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0.4996207478904705	0.1248770428688036	0.1651590731751154	T	T	T
0.4997212812554618	0.1245701843482566	0.3307969232757220	T	T	T
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0.4997215112987513	0.0000036661840054	0.2477300520931775	T	T	T
0.5030183018931751	-0.0000126689258602	0.4119799253925727	T	T	T
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0.4996470068960180	0.3751275115782677	0.1651709005929152	T	T	T
0.4997843180910076	0.3754168852925180	0.3308291670233255	T	T	T
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0.4998087990879993	0.2500054638251125	0.2468576102369032	T	T	T
0.5025027902132408	0.2500011694277215	0.4058564046222309	T	T	T
0.6250000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.6248860920047649	0.1249412013551225	0.2473843325184632	T	T	T
0.6260109726643625	0.1252248674039149	0.4110911992914573	T	T	T
0.6250000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6249498027141788	-0.0000009081737689	0.1651156889877786	T	T	T
0.6251510995511849	-0.0000130432894480	0.3306506372463388	T	T	T
0.6250000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.6249386308015973	0.3750515176547140	0.2474048905071529	T	T	T
0.6260875629942820	0.3747406799128805	0.4111149985231894	T	T	T
0.6250000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.6251221156994844	0.2500020927408234	0.1649802571914764	T	T	T
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0.0000613701900452	0.4999804810796310	0.2495757143796614	T	T	T
0.9951781305178058	0.4999798161062367	0.4207320922777709	T	T	T
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0.1250078409270381	0.4999882239444224	0.1660106649079991	T	T	T
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0.2500169940708556	0.4999895704487717	0.2494369138300248	T	T	T
0.2518003301625211	0.5000072647645458	0.4169653353901289	T	T	T
0.3750000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3745911628694905	0.4999928385608031	0.1657627516136933	T	T	T
0.3751238971150350	0.4999879693770068	0.3330084767228667	T	T	T
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0.4997949688838943	0.4999845340223029	0.2477546745844019	T	T	T
0.5031507643441931	0.5000015699629314	0.4119977144334534	T	T	T
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0.6249871394352102	0.4999924243067071	0.1651299593283458	T	T	T
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0.1250105605399048	0.6249364756292690	0.2492309518855492	T	T	T
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0.3748768133767468	0.6248201938724267	0.2489580277155502	T	T	T
0.3787444250691634	0.6246652427199554	0.4183259552454885	T	T	T
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0.6248883974845729	0.6249159508165630	0.2473947859154297	T	T	T
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0.9999725589572325	0.7499793525867229	0.2494857582123877	T	T	T
0.9952567173886765	0.7499807699915330	0.4205318156636315	T	T	T
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0.1248903551073954	0.7499803029185860	0.1659339877388113	T	T	T
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0.2496450254131534	0.7499807843672400	0.2490896291434174	T	T	T
0.2525186062242707	0.7500085678667994	0.4159543723448793	T	T	T
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0.3744196101683620	0.7499863120074366	0.1655928914509018	T	T	T
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0.4997484480826574	0.7499843798887487	0.2468293001939433	T	T	T
0.5023367305773887	0.7499863376002113	0.4058116587495312	T	T	T
0.6250000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.6250899527418917	0.7499872487975366	0.1649669656462846	T	T	T
0.6257926223794792	0.7499919466520391	0.3298620894663438	T	T	T
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0.0002814378125828	0.8750140728934844	0.1658018669930164	T	T	T
0.9998366479914044	0.8750301724591032	0.3326140128866460	T	T	T
0.1250000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.1249650311551365	0.8750277946369033	0.2491891876873473	T	T	T
0.1262533777311342	0.8749933106626453	0.4150973981960135	T	T	T
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0.2498442437688128	0.8750366614682231	0.1658623676348827	T	T	T
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0.3750000000000000	0.8750000000000000	0.0822561893037914	F	F	F

0.3748313964422306	0.8751518117835435	0.2489288958464558	T	T	T
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0.4995918010582006	0.8751263932310079	0.1651518167637213	T	T	T
0.4996470091432366	0.8754065756787998	0.3307669869464708	T	T	T
0.6250000000000000	0.8750000000000000	0.0822561893037914	F	F	F
0.6248419610152293	0.8750541220355735	0.2473735130837642	T	T	T
0.6259240052355755	0.8747320872882886	0.4110722548184996	T	T	T
0.0118465350071457	0.1252673977729949	0.4985685188503509	T	T	T
0.0120208704783921	0.3747981881243218	0.4986535969277265	T	T	T
0.0118539752035144	0.6251971615546694	0.4986064241312753	T	T	T
0.0116831998831417	0.8748118394035683	0.4985308498003081	T	T	T
0.1274876666874996	0.0000243590185541	0.4958213618652281	T	T	T
0.1287764508857899	0.2500098970874130	0.4956029520167567	T	T	T
0.1277566020307743	0.5000150673759023	0.4959474705135380	T	T	T
0.1285189995502254	0.7500306343572082	0.4954995120988988	T	T	T
0.2523075448999772	0.1262906702947613	0.4958353435938686	T	T	T
0.2525732710179179	0.3736826265640435	0.4959661333246325	T	T	T
0.2522886461073903	0.6264326112930678	0.4958594555646679	T	T	T
0.2520375569841538	0.8736845793138917	0.4957224610619058	T	T	T
0.3700094558957764	0.9999775204207997	0.5003562689622442	T	T	T
0.3766321323710263	0.2498886816501802	0.4991011463925647	T	T	T
0.3703107163111518	0.5000799964450444	0.5004605189120233	T	T	T
0.3762824001137316	0.7501340121097545	0.4989980940486992	T	T	T
0.7500000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.7501901034373019	0.1249741286589566	0.1651372301542859	T	T	T
0.7495507261382327	0.1249208353929965	0.3304206149071235	T	T	T
0.7500000000000000	0.0000000000000000	0.0822561893037914	F	F	F
0.7501234210720512	-0.0000039109443743	0.2476179327155989	T	T	T
0.7483893664774808	-0.0000240429982148	0.4113514849913099	T	T	T
0.7500000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.7502200460664703	0.3750292487133527	0.1651503187827965	T	T	T
0.7496236541574448	0.3750622469948979	0.3304613442096828	T	T	T
0.7500000000000000	0.2500000000000000	0.0822561893037914	F	F	F
0.7503705095159791	0.2500014721124263	0.2474854858989513	T	T	T
0.7484156260242480	0.2499751120857741	0.4111994474612316	T	T	T
0.7500000000000000	0.5000000000000000	0.0822561893037914	F	F	F
0.7501986310516531	0.4999897168760032	0.2476584425455080	T	T	T
0.7484708029362060	0.5000086057100946	0.4114102315361777	T	T	T
0.7500000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.7501866922114623	0.6249586337495955	0.1651397397845325	T	T	T
0.7495452965679069	0.6249228047094432	0.3304362435946446	T	T	T
0.7500000000000000	0.7500000000000000	0.0822561893037914	F	F	F
0.7503102445264305	0.7499834610510292	0.2474571490307935	T	T	T
0.7483211968280385	0.7500126067941483	0.4111575913269572	T	T	T
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0.7501611198533452	0.8750215287546808	0.1651256200201288	T	T	T
0.7494751665411118	0.8750586396299471	0.3303957412193330	T	T	T
0.8750000000000000	0.1250000000000000	0.0822561893037914	F	F	F
0.8751960748825620	0.1249901738743955	0.2480012288475753	T	T	T
0.8703073281651768	0.1250205322573505	0.4110310834154934	T	T	T
0.8750000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.8754258979834063	-0.0000002606760489	0.1654846415925655	T	T	T
0.8751043016834912	-0.0000011600514525	0.3316790017068643	T	T	T
0.8750000000000000	0.3750000000000000	0.0822561893037914	F	F	F
0.8752438973990463	0.3750170336473513	0.2480407077404786	T	T	T
0.8703571166705630	0.3749584404295908	0.4111053564528486	T	T	T
0.8750000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.8755085198688837	0.2500060920356759	0.1654645650693749	T	T	T
0.8752671624451906	0.2499980760156701	0.3316956267376479	T	T	T

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0.8754635462008273	0.4999937899124209	0.1655065523055594	T	T	T
0.8751951490248199	0.4999944891335847	0.3317655005582831	T	T	T
0.8750000000000000	0.6250000000000000	0.0822561893037914	F	F	F
0.8751930887342794	0.6249629858998788	0.2480130022040804	T	T	T
0.8703034917631344	0.6250520780442436	0.4110479598997858	T	T	T
0.8750000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.8754701555186840	0.7499872383382750	0.1654447969932707	T	T	T
0.8751662189128930	0.7499906285517272	0.3316400046719808	T	T	T
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0.8751468714260751	0.8750138431750885	0.2479740120838750	T	T	T
0.8702490120974919	0.8749625791591098	0.4109787423448304	T	T	T
0.4775617445661618	0.8097199234673502	0.4988037940880844	T	T	T
0.4777345781132579	0.6908798568200545	0.4990845003627047	T	T	T
0.3953626843397664	0.5592477770151980	0.5654996674564038	T	T	T
0.3967422641169111	0.4409921138181228	0.5653138444384359	T	T	T
0.4780880432106532	0.3091300878999776	0.4991172948546110	T	T	T
0.4779005076235320	0.1903433537717197	0.4989017032036786	T	T	T
0.3958932016413573	0.0590455430466973	0.5653181070343521	T	T	T
0.3946242843698816	0.9407920332025037	0.5654756191415359	T	T	T
0.4482605079486185	0.7502451724712045	0.4994638104843138	T	T	T
0.3893978819116076	0.5001115697070307	0.5468651745454726	T	T	T
0.4486071362167502	0.2497865864167143	0.4995384983701097	T	T	T
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