

**Electronic Supporting Information (ESI)**

For

**Theoretical study on the surface stabilities, electronic structures and water  
adsorption behavior of the Ta<sub>3</sub>N<sub>5</sub> (110) surface**

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by

Jiajia Wang,<sup>ab</sup> Aibin Ma,<sup>\*ac</sup> Zhaosheng Li,<sup>\*b</sup> Jinghua Jiang,<sup>ac</sup> Jianyong Feng<sup>b</sup> and Zhigang  
Zou<sup>b</sup>

<sup>a</sup> *College of Mechanics and Materials, Hohai University, Nanjing 210098, P. R. of  
China.*

<sup>b</sup> *National Laboratory of Solid State Microstructures, Department of Physics,  
Ecomaterials and Renewable Energy Research Center (ERERC), and College of  
Engineering and Applied Sciences, Nanjing University, Nanjing 210093, P. R. of China.*

<sup>c</sup> *Jiangsu collaborative innovation center of advanced micro/nano materials &  
equipment, Nanjing 210094, P. R. of China.*

\* Corresponding Authors: Tel: +86-25-83787239, Fax: +86-25-83786046. E-mail:[aibin-  
ma@hhu.edu.cn](mailto:aibin-ma@hhu.edu.cn)(A.B. MA) or [zsli@nju.edu.cn](mailto:zsli@nju.edu.cn)(Z. S. Li)

### SI-1 Details of the Ta<sub>3</sub>N<sub>5</sub> (110) and (100) surface models

As can be seen in the **Fig. S1**, it is very difficult to clarify all terminations of the Ta<sub>3</sub>N<sub>5</sub> (110) surface. Then, based on the repeated atomic layer (the atoms inside the two black lines), we select ten possible terminations to calculate their surface energies. The detailed atomic structures of these ten terminations are shown in **Fig. S2a to j**. It is seen that, the termination in Fig. S2a is equal to the first black line in Fig. S1. From Fig. S2a to j, the surface atoms with the same vertical coordinates (in the same plane) are gradually removed.

Before calculating the surface energies of these ten terminations, we must test how many atomic layers are sufficient to simulate the Ta<sub>3</sub>N<sub>5</sub> (110) surface. Using the termination in Fig. S2a as a probe, the slab models with 5, 7, 9 and 11 atomic layers are constructed. Surface energies calculations reveal that 7 atomic layers with a vacuum space of 15 Å at each side of the slab model are sufficient to simulate the Ta<sub>3</sub>N<sub>5</sub> (110) surface. Then, all the other nine terminations are constructed based on the slab model that contains 7 atomic layers with a vacuum space of 15 Å at each side of the slab model.

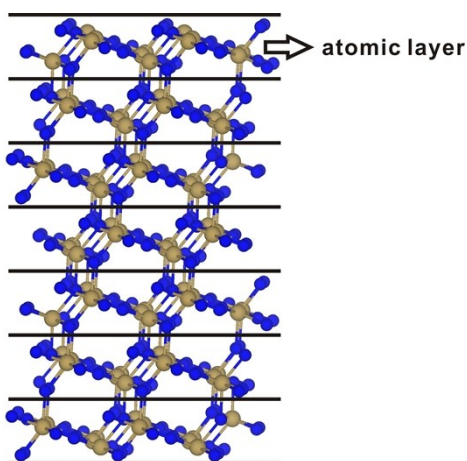
The surface energies of these ten terminations are listed in **Table S1**. It is seen that, the surface energy of the termination in Fig. S2a is the smallest, suggesting that this termination is theoretically most stable. Then, the termination in Fig. S2a is adopted to construct all Ta<sub>3</sub>N<sub>5</sub> (110) surfaces in this study. **Fig. S3a** shows the slab model of the Ta<sub>3</sub>N<sub>5</sub> (110) surface used in this study.

When we investigate the water adsorption on the Ta<sub>3</sub>N<sub>5</sub> (110) surface, we do not use the slab model in Fig. S3a but that in **Fig. S3b**. It is seen that, the slab model in Fig. S3b also contains 7 atomic layers but with a vacuum space of 20 Å *only* at one side of the slab model. Furthermore, to keep the nearly same neighboring image interactions along different directions<sup>1</sup>, the 1×2 slab model of the Ta<sub>3</sub>N<sub>5</sub> (110) surface is adopted for the water adsorption calculations. The surface size of the 1×1 Ta<sub>3</sub>N<sub>5</sub> (110) surface is 10.35(*u*)×5.52(*v*) Å<sup>2</sup>. Thus, the neighboring water interaction along the *u* direction is largely different from that along the *v* direction. Using the 1×2 slab model, whose surface size becomes 10.35(*u*)×11.04(*v*) Å<sup>2</sup>, the neighboring water interaction along the *u* direction is nearly the same as that along the *v* direction. When we perform the water adsorption calculation, the water molecule is put onto one side of the slab and the two bottom atomic layers are fixed.

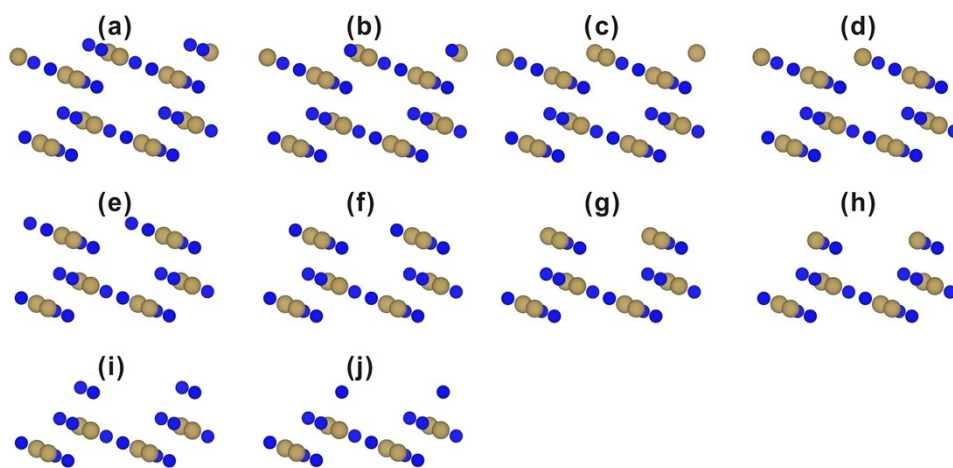
Using the slab model in Fig. S3b is able to reduce the computational costs of water adsorption calculations.

In this study, the surface energies and water adsorption energies associated with the  $\text{Ta}_3\text{N}_5$  (100) surface are all cited from our previous work.<sup>2,3</sup> Except the surface energies and water adsorption energies, some important properties of the (100) surface, for example the water splitting energy barriers, are calculated in this study. The slab models of the  $\text{Ta}_3\text{N}_5$  (100) surface for surface calculation and water adsorption calculation are shown in **Fig. S3c and d**, which are cited from Ref. 2 and 3, respectively. It is seen that, similar with the  $\text{Ta}_3\text{N}_5$  (110) surface model, the (100) surface model also contains 7 atomic layers.

The CONTCARs of clean and oxygen contained (110) and (100) surfaces, and the molecular and dissociative water adsorption on the (110) and (100) surfaces are listed at the end of this supporting information.



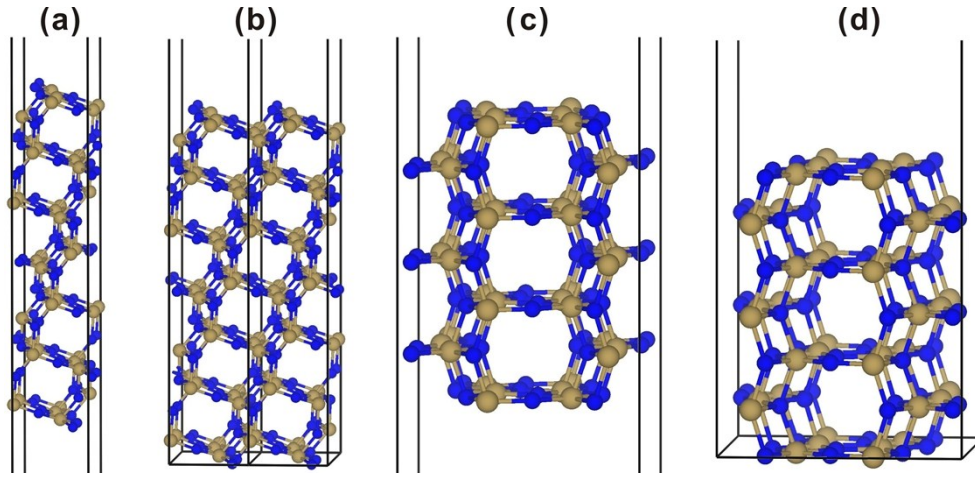
**Fig. S1** Atomic structure of the  $\text{Ta}_3\text{N}_5$  (110) surface.



**Fig. S2** The selected ten terminations of the  $\text{Ta}_3\text{N}_5$  (110) surface.

**Table S1** Surface energies of ten terminations of the Ta<sub>3</sub>N<sub>5</sub> (110) surface shown in Fig. S2.

Surface terminations	$E_{\text{surf}}$ (J/m <sup>2</sup> )	Surface terminations	$E_{\text{surf}}$ (J/m <sup>2</sup> )
<b>(a)</b>	<b><u>1.04</u></b>	(f)	2.01
(b)	2.49	(g)	3.21
(c)	3.53	(h)	2.71
(d)	2.93	(i)	2.68
(e)	3.21	(j)	1.73



**Fig. S3** The slab models of the Ta<sub>3</sub>N<sub>5</sub> (110) surface for (a) surface calculation and (b) water adsorption calculation. The slab models of the Ta<sub>3</sub>N<sub>5</sub> (100) surface for (c) surface calculation and (d) water adsorption calculation.

### SI-2 Chemical potential calculation details

Under the thermal equilibrium growth conditions, the bulk Ta<sub>3</sub>N<sub>5</sub> should satisfy:

$$3\Delta\mu_{\text{Ta}} + 5\Delta\mu_{\text{N}} = E_{\text{Ta}_3\text{N}_5}^f = -8.47\text{eV} \quad (\text{S1})$$

where  $E_{\text{Ta}_3\text{N}_5}^f$  is the formation energy of bulk Ta<sub>3</sub>N<sub>5</sub>. Then, we can get  $\Delta\mu_{\text{N}}$  and  $\Delta\mu_{\text{Ta}}$  under different growth conditions: under the N-poor (Ta-rich) growth condition,  $\Delta\mu_{\text{N}} = -1.69$  and  $\Delta\mu_{\text{Ta}} = 0$  eV; under the N-rich (Ta-poor) growth condition,  $\Delta\mu_{\text{N}} = 0$  and  $\Delta\mu_{\text{Ta}} = -2.82$  eV. To calculate the  $\Delta\mu_{\text{O}}$ , precipitation of secondary phases such as TaON and Ta<sub>2</sub>O<sub>5</sub> should be avoided:

$$\Delta\mu_N + \Delta\mu_O + \Delta\mu_{Ta} < E_{TaON}^f = -5.79eV \quad (S2)$$

$$5\Delta\mu_O + 2\Delta\mu_{Ta} < E_{Ta_2O_5}^f = -20.20eV \quad (S3)$$

where  $E_{Ta_2O_5}^f$  and  $E_{TaON}^f$  are formation energies of  $Ta_2O_5$  and TaON, respectively. Then,  $\Delta\mu_O$  can be calculated from the lower bound for each growth condition: -4.10 and -2.97 eV under N-poor and N-rich growth conditions, respectively. More discussion of the chemical potential calculations of  $Ta_3N_5$  can be found in Ref. 2.

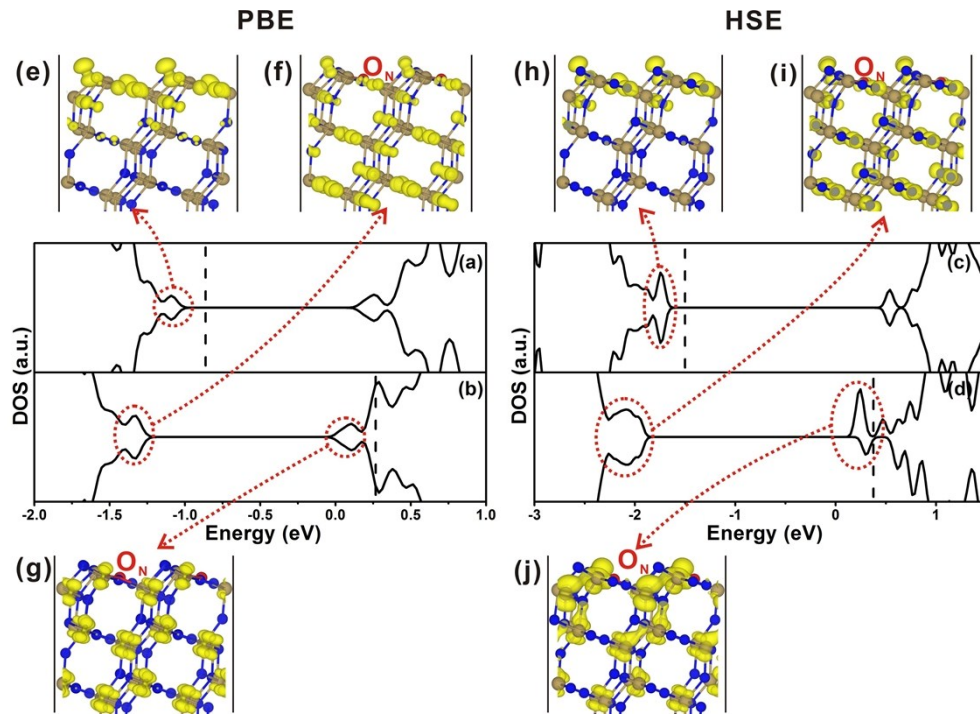
### SI-3 The HSE calculation

In this study, the HSE calculations are performed to verify the GGA results. Due to the large cell size of surface slab model, the HSE calculations of the  $Ta_3N_5$  (110) surface need large amount of computational resources, especially when many  $k$ -points are used for HSE calculations. Then, to reduce the computational costs, the  $\Gamma$ -centered  $k$ -point meshes of  $1 \times 2 \times 1$ , which contains the (0, 0, 0) and (0, 0.5, 0)  $k$ -points, are adopted for the HSE calculations. The accuracy of the HSE method is mainly determined by two important parameters  $\alpha$  and  $\omega$ , where  $\alpha$  represents the fraction of the semilocal PBE exchange interaction replaced by a screened nonlocal functional, and  $\omega$  is the inverse screening length. The parameters  $\alpha$  and  $\omega$  are set as 25% and  $0.2 \text{ \AA}^{-1}$ , respectively, which refers to the HSE06<sup>4</sup> functional. The band gap of the pure bulk  $Ta_3N_5$  calculated by the HSE06 functional is 2.2 eV, which is very close to the experimental results (about 2.1 eV), suggesting that the HSE method is very accurate. In the HSE06 calculations, the NKRED<sup>5</sup> flag was not used in this study. The future research will include a broader spectrum of HSE06 calculations on a limited K-point grid using the NKRED flag.

**Fig. S4a and b** show the DOS of (110) and (100)+ $O_{N3}$ , respectively, calculated by the PBE functional. The DOS results of (110) and (100)+ $O_{N3}$  calculated by the HSE functional are shown in **Fig. S4c and d**, respectively. Due to the insufficient  $k$ -points, the DOS curves calculated by the HSE method are discontinuous. For example, the energy regions near the CBM in **Fig. S4c and d** should have DOS curves. However, the discontinuous DOS curves of the HSE results do not affect any qualitative analysis. The comparisons between HSE

and PBE results reveal that: (i) the charge densities of the VBM in the (110) surface calculated by PBE (**Fig. S4e**) and HSE (**Fig. S4h**) are both localized on the top atomic layers; (ii) the charge densities of the VBM in the (100)+O<sub>N3</sub> surface calculated by PBE (**Fig. S4f**) and HSE (**Fig. S4i**) are both uniformly distributed on N atoms; (iii) the charge densities of the CBM in the (100)+O<sub>N3</sub> surface calculated by PBE (**Fig. S4g**) and HSE (**Fig. S4j**) are both uniformly distributed on Ta atoms.

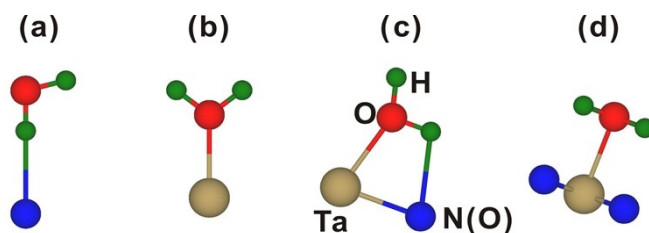
Therefore, the comparisons between the PBE and HSE results reveal that, although the PBE functional has its limitations, our calculated electronic structures by the PBE functional are theoretically reliable. The HSE calculation results of the Ta<sub>3</sub>N<sub>5</sub> (100) surface have been given in our previous theoretical work.<sup>2</sup>



**Fig. S4** Calculated DOS of the Ta<sub>3</sub>N<sub>5</sub> (a) (110) and (b) (110)+O<sub>N3</sub> surfaces at the PBE level. Calculated DOS of the Ta<sub>3</sub>N<sub>5</sub> (c) (110) and (d) (110)+O<sub>N3</sub> at the HSE level. The vertical dashed line in each case is the Fermi level. For the PBE and HSE results, the horizontal axes of (110)+O<sub>N3</sub> are aligned with that of the clean (110) by the electrostatic potential calculations. The partial charge densities of some labeled states (e to j) are also shown. (For PBE: isosurface level = 0.0005 electron/Å<sup>3</sup>; For HSE: isosurface level = 0.001 electron/Å<sup>3</sup>)

#### SI-4 Initial adsorption sites and configurations of water molecule

**Fig. S5** shows the four possible initial adsorption configurations of water adsorption on the  $\text{Ta}_3\text{N}_5$  (110) surface. In **Fig. S5a**, one H is put on the top of one N (or O) atom. In **Fig. S5b**, the O atom of water is put on the top of the Ta atom. Considering that water is usually decomposed to one OH and one H, the water molecule interacting with the surface *via* both the O and H atoms is considered as shown in **Fig. S5c**. Since water molecule is reported to molecularly adsorbed onto  $\text{TiO}_2$  surface with its O atom bonding to the Ti atom and two H atoms bonding to the two surface O atoms,<sup>6,7</sup> the fourth initial adsorption model shown in **Fig. S5d** is constructed with the O atom bonding with the Ta atom and two H atoms bonding with two surface anion atoms. These four initial adsorption configurations of water adsorption on the  $\text{Ta}_3\text{N}_5$  (110) surface are the same as that on the (100) surface in our previous theoretical work.<sup>3</sup> Furthermore, on the (110)+ $\text{O}_{\text{N}_3}$  surface, the Ta site that is far away from the  $\text{O}_{\text{N}_3}$  atom are also considered and the calculation results are discussed in the following SI-5.



**Fig. S5** Initial adsorption configurations of water adsorption on the  $\text{Ta}_3\text{N}_5$  (110) surface

#### SI-5 Atomic structures of water adsorption and dissociation on the $\text{Ta}_3\text{N}_5$ (100) and (110) surfaces

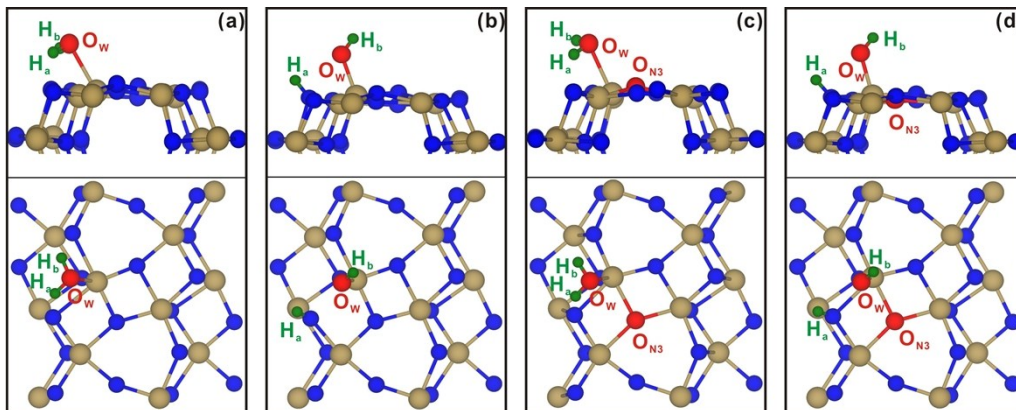
**Fig. S6a to d** show the four models of water adsorption and dissociation on the  $\text{Ta}_3\text{N}_5$  (100) surfaces, which are all cited from our previous theoretical work.<sup>3</sup> What should be mentioned is that, the  $[100]_{\text{mol}}$ ,  $[100]_{\text{dis}}$  and  $[100+\text{O}_{\text{N}_3}]_{\text{dis}}$  models are cited from the main text of our previous theoretical work, while the  $[100+\text{O}_{\text{N}_3}]_{\text{mol}}$  model is cited from the supporting information of our previous work. It is seen that, in the  $[100]_{\text{mol}}$  model, the water is molecularly adsorbed with the  $\text{O}_w$  atom bonding with surface Ta atom. In the  $[100]_{\text{dis}}$  model, the water is decomposed into one OH and one H, which bonds with surface Ta and N atoms, respectively. In the  $[100+\text{O}_{\text{N}_3}]_{\text{mol}}$  and  $[100+\text{O}_{\text{N}_3}]_{\text{dis}}$  models, the adsorption sites and



configurations of the adsorbed water on the (100)+O<sub>N3</sub> surfaces are nearly the same as that on the clean (100) surfaces. The adsorption sites and configurations of water adsorption on the (100) and (100)+O<sub>N3</sub> surfaces are close to that on the (110) and (110)+O<sub>N3</sub> surfaces.

**Table S2** lists the structural parameters of water on the different Ta<sub>3</sub>N<sub>5</sub> (110) and (100) surfaces. It is seen that, regardless of the clean or deficient surfaces, the structural parameters of water on the Ta<sub>3</sub>N<sub>5</sub> (110) surfaces are close to that on the (100) surfaces. Beside the structural parameters of water, the number of electrons that the water molecule accepts from the (110) and (100) surfaces are also listed in Table S2. The number of electrons that the water molecule accepts from the (110) and (100) surfaces are calculated by the Bader<sup>8</sup> population analysis. Note that, for clarity purpose, our calculated Bader charge is the sum of Bader charge of three atoms of one water molecule. Therefore, the Bader charge in Table S2 reflects the electron gain and loss for one whole water molecule. The positive and negative values of Bader charge mean acceptance and donation of electrons of the water, respectively. It is seen that, the water molecule on the (110) surface accepts almost the same number of electrons as that on the (100) surface.

What should be mentioned is that, on the (110)+O<sub>N3</sub> surface, the Ta site that is far away from the O<sub>N3</sub> atom are also considered and carefully tested. The results showed that, on the Ta site that was far away from the O<sub>N3</sub> atom, the most stable molecular and dissociative water adsorption energies were 0.60 and 1.46 eV, respectively, which were smaller than that near the O<sub>N3</sub> atom (0.69 and 1.49, respectively).



**Fig. S6** The optimized structures of water adsorption models: (a) [100]<sub>mol</sub>, (b) [100]<sub>dis</sub>, (c) [100+O<sub>N3</sub>]<sub>mol</sub> and (d) [100+O<sub>N3</sub>]<sub>dis</sub> (upper: side-view; lower: top-view). Here, the ‘mol’ and ‘dis’ refer to the molecular and dissociative adsorptions, respectively.



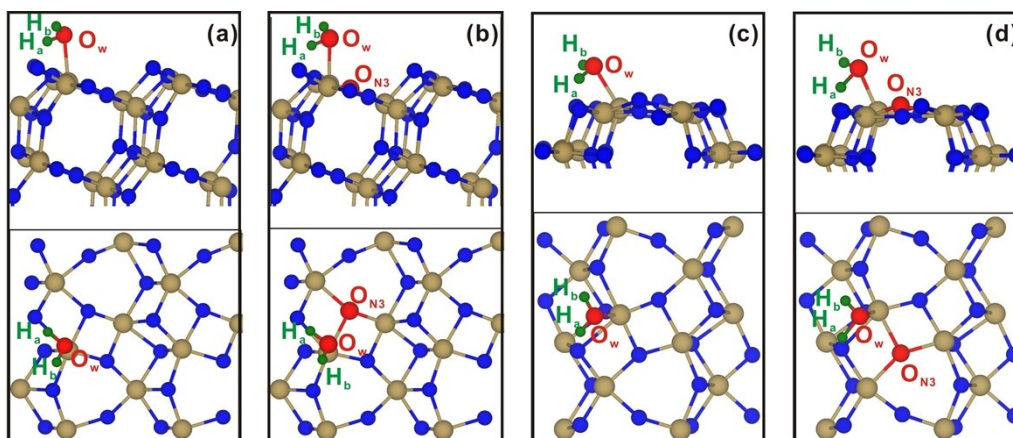
**Table S2** Structural parameters of water [ $d(\text{H}_a\text{-O}_w)$  and  $d(\text{H}_b\text{-O}_w)$  in Å;  $\angle\text{H}_a\text{-O}_w\text{-H}_b$  in degree( $^\circ$ )] and Bader charge of water (in eV) for water adsorption on the different  $\text{Ta}_3\text{N}_5$  (110) and (100) surfaces.

Surfaces	Structural parameters of water <sup>a</sup>			Bader charge	
	$d(\text{H}_a\text{-O}_w)$	$d(\text{H}_b\text{-O}_w)$	$\angle\text{H}_a\text{-O}_w\text{-H}_b$		
(110)	$[\text{110}]_{\text{mol}}$	0.99	0.99	105.98	-0.04
	$[\text{110}]_{\text{dis}}$	2.59	0.97	138.87	0.13
	$[\text{110}+\text{O}_{\text{N}_3}]_{\text{mol}}$	1.00	0.98	106.89	-0.02
	$[\text{110}+\text{O}_{\text{N}_3}]_{\text{dis}}$	2.71	0.97	125.82	0.14
(100)	$[\text{100}]_{\text{mol}}$	0.99	1.02	106.44	-0.03
	$[\text{100}]_{\text{dis}}$	2.60	0.97	158.25	0.13
	$[\text{100}+\text{O}_{\text{N}_3}]_{\text{mol}}$	1.00	0.98	107.37	-0.03
	$[\text{100}+\text{O}_{\text{N}_3}]_{\text{dis}}$	2.58	0.97	162.44	0.13

<sup>a</sup>For free water:  $d(\text{H}_a\text{-O}_w) = d(\text{H}_b\text{-O}_w) = 0.97$  Å,  $\angle\text{H}_a\text{-O}_w\text{-H}_b = 104.5^\circ$ .

### SI-6 Atomic structures and frequencies of transition states

The atomic structures of the four transition states  $[\text{110}]_{\text{TS}}$ ,  $[\text{110}+\text{O}_{\text{N}_3}]_{\text{TS}}$ ,  $[\text{100}]_{\text{TS}}$  and  $[\text{100}+\text{O}_{\text{N}_3}]_{\text{TS}}$  are shown in the following **Fig. S7**. The detailed structural parameters of these four transition states are listed in **Table S3**.



**Fig. S7** The atomic structures of four transition states: (a)  $[\text{110}]_{\text{TS}}$ , (b)  $[\text{110}+\text{O}_{\text{N}_3}]_{\text{TS}}$ , (c)  $[\text{100}]_{\text{TS}}$  and (d)  $[\text{100}+\text{O}_{\text{N}_3}]_{\text{TS}}$  (upper: side-view; lower: top-view). Here, the ‘TS’ refers to the transition state.

**Table S3** Structural parameters of water [ $d(\text{H}_a\text{-O}_w)$  and  $d(\text{H}_b\text{-O}_w)$  in Å;  $\angle\text{H}_a\text{-O}_w\text{-H}_b$  in degree( $^\circ$ )] for transition states shown in Fig. S7.

Transition states	Structural parameters of water <sup>a</sup>		
	$d(\text{H}_a\text{-O}_w)$	$d(\text{H}_b\text{-O}_w)$	$\angle\text{H}_a\text{-O}_w\text{-H}_b$
$[110]_{\text{TS}}$	1.09	0.98	109.22
$[110+\text{O}_{\text{N}_3}]_{\text{TS}}$	1.12	0.97	112.65
$[100]_{\text{TS}}$	1.09	0.98	108.51
$[100+\text{O}_{\text{N}_3}]_{\text{TS}}$	1.50	0.97	105.05

<sup>a</sup>For free water:  $d(\text{H}_a\text{-O}_w) = d(\text{H}_b\text{-O}_w) = 0.97$  Å,  $\angle\text{H}_a\text{-O}_w\text{-H}_b = 104.5^\circ$ .

The frequency calculations should be performed to confirm whether a good transition state is found. Frequencies of four transition states  $[100]_{\text{TS}}$ ,  $[100+\text{O}_{\text{N}_3}]_{\text{TS}}$ ,  $[110]_{\text{TS}}$  and  $[110+\text{O}_{\text{N}_3}]_{\text{TS}}$  are calculated. For the frequency calculations, most of the surface is frozen, but the atoms that undergo major changes during the transition state are relaxed. Using the  $[110]_{\text{TS}}$  as example, the bottom six atomic layers are fixed, while the one top atomic layer (32 atoms) and the adsorbed water (3 atoms) are relaxed. Then, for the transition state  $[110]_{\text{TS}}$ , the total number of calculated frequencies is 105 ( $105=35\times 3$ ). The 105 frequencies of the transition state  $[110]_{\text{TS}}$  are listed below (partly):

1 f =	111.365466 THz	699.729857 2PiTHz	3714.751965 cm-1	460.570710 meV
2 f =	57.864160 THz	363.571238 2PiTHz	1930.140547 cm-1	239.307014 meV
3 f =	43.376931 THz	272.545293 2PiTHz	1446.898616 cm-1	179.392629 meV
...				
103 f =	1.835970 THz	11.535743 2PiTHz	61.241381 cm-1	7.592966 meV
104 f =	1.645280 THz	10.337596 2PiTHz	54.880616 cm-1	6.804332 meV
105 f/i =	8.166483 THz	51.311526 2PiTHz	272.404545 cm-1	33.773871 meV

The transition state is defined as having one and only one negative (imaginary) vibration frequency. The above results yield one and only one negative frequency (No. 105: the 'f/i' means imaginary frequency), confirming that the transition state  $[110]_{\text{TS}}$  is a good transition state. Other three transition states also have one and only one negative frequency, proving that they are all good transition states:

The frequencies of the transition state  $[110+\text{O}_{\text{N}_3}]_{\text{TS}}$  (partly):

1 f =	112.251643 THz	705.297871 2PiTHz	3744.311645 cm-1	464.235644 meV
2 f =	53.115897 THz	333.737021 2PiTHz	1771.755542 cm-1	219.669770 meV
3 f =	39.693480 THz	249.401490 2PiTHz	1324.031930 cm-1	164.159096 meV

...	...	...	...	...
103 f =	1.797953 THz	11.296870 2PiTHz	59.973247 cm-1	7.435738 meV
104 f =	1.662779 THz	10.447550 2PiTHz	55.464344 cm-1	6.876705 meV
105 f/i =	19.984737 THz	125.567803 2PiTHz	666.619037 cm-1	82.650257 meVs

The frequencies of the transition state [100]<sub>TS</sub> (partly):

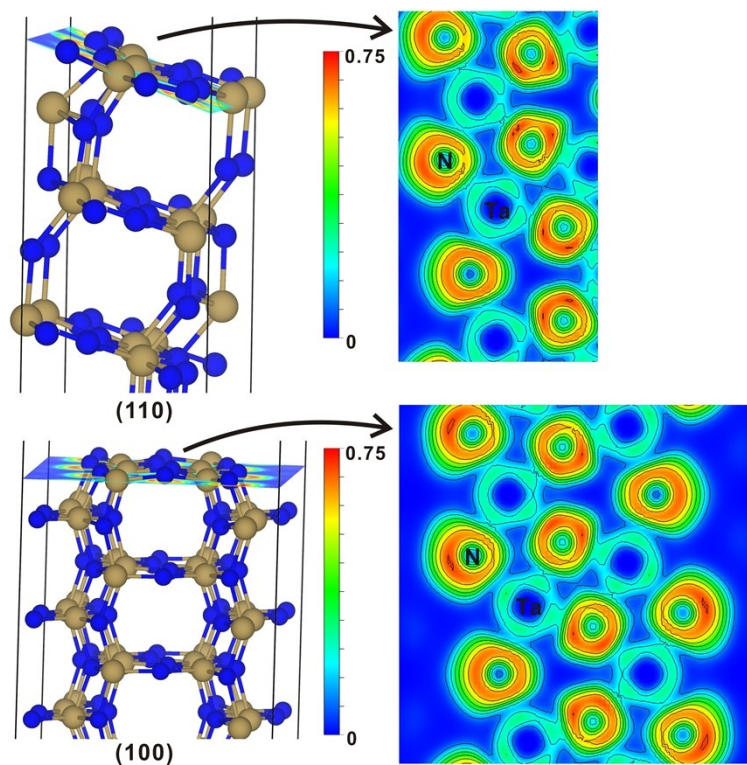
1 f =	108.634541 THz	682.570955 2PiTHz	3623.658142 cm-1	449.276511 meV
2 f =	57.656072 THz	362.263785 2PiTHz	1923.199494 cm-1	238.446433 meV
3 f =	44.039597 THz	276.708948 2PiTHz	1469.002786 cm-1	182.133198 meV
...	...	...	...	...
55 f =	2.578326 THz	16.200098 2PiTHz	86.003685 cm-1	10.663102 meV
56 f =	1.356385 THz	8.522417 2PiTHz	45.244126 cm-1	5.609559 meV
57 f/i =	7.960605 THz	50.017956 2PiTHz	265.537191 cm-1	32.922428 meV

The frequencies of the transition state [100+O<sub>N3</sub>]<sub>TS</sub> (partly):

1 f =	112.355378 THz	705.949658 2PiTHz	3747.771874 cm-1	464.664658 meV
2 f =	56.814041 THz	356.973150 2PiTHz	1895.112375 cm-1	234.964073 meV
3 f =	34.739174 THz	218.272669 2PiTHz	1158.774088 cm-1	143.669728 meV
...	...	...	...	...
55 f =	2.789564 THz	17.527345 2PiTHz	93.049822 cm-1	11.536712 meV
56 f =	2.660221 THz	16.714662 2PiTHz	88.735420 cm-1	11.001794 meV
57 f/i =	3.026927 THz	19.018745 2PiTHz	100.967425 cm-1	12.518370 meV

### SI-7 Electron localization function (ELF)

The ELF is a measure of the spatial distribution of an electron. The value of ELF varies in the range of 0 to 1, corresponding to the delocalized and localized limit of electron gas.<sup>9</sup> In the water splitting reaction, the water molecule usually accepts electrons from surface to break the H-O bond. Therefore, the surface with smaller ELF, *i.e.*, more delocalized electron distribution, is expected to have strong water splitting ability, because the electrons are relatively easier transferred from surface to the adsorbed water molecule. **Fig. S8a and b** are the ELF of selected planes on the (110) and (100) surfaces, respectively. For the comparison purpose, the energy scales in Fig. S8a and b are both set from 0 to 0.75. It is seen that, the ELF on the (110) surface is nearly the same as that on the (100) surface. Therefore, the surface electron localization does not account for the different water splitting ability between the (110) and (100) surfaces.



**Fig. S8** The Electron localization function (ELF) of selected planes on the (a) (110) and (b) (100) surfaces. The isosurface level are both set from 0 to 0.75.

## References

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**The CONTCARs of 12 discussed slab models are listed below:**

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Direct
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  0.7500000000000000   0.8093973981883923   0.3135333224072218
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  0.3806845186218517   0.6649839609126291   0.4351522426554381
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  0.3804509535230721   0.1639347912415557   0.5711758201809860
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  0.4254439125501136   0.2401558086833923   0.7249581137584107
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N O Ta

68 2 42

Direct

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**(3) (100)**

100

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N    Ta  
70    42

Direct

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0.5461959468704976	0.3804914457284596	0.5548541938285041
0.5423817518412832	0.3813944451314057	0.6727962160389183
0.7967783097919252	0.4207040570777139	0.3293403924464613
0.8100278676124617	0.4251935142295409	0.4427374078613084
0.8100278676124617	0.4251935142295409	0.5572625921386916
0.7967783097919252	0.4207040570777139	0.6706596075535387
0.9502686641142901	0.8818868103450015	0.3837114537108803
0.9529993992229606	0.8803943707624526	0.5000000000000000
0.9502686641142901	0.8818868103450015	0.6162885462891197
0.6849524416913511	0.9305792501948460	0.3873858796585026
0.6939278816355170	0.9266547310455877	0.5000000000000000
0.6849524416913511	0.9305792501948460	0.6126141203414974

0.4576182481587168	0.8813944451314057	0.3272037839610817
0.4538040531295024	0.8804914457284596	0.4451458061714959
0.4538040531295024	0.8804914457284596	0.5548541938285041
0.4576182481587168	0.8813944451314057	0.6727962160389183
0.2032216902080748	0.9207040570777139	0.3293403924464613
0.1899721323875383	0.9251935142295409	0.4427374078613084
0.1899721323875383	0.9251935142295409	0.5572625921386916
0.2032216902080748	0.9207040570777139	0.6706596075535387
0.0497313358857170	0.1181131896549985	0.3837114537108803
0.0470006007770394	0.1196056292375474	0.5000000000000000
0.0497313358857170	0.1181131896549985	0.6162885462891197
0.3150475583086489	0.0694207498051540	0.3873858796585026
0.3060721183644830	0.0733452689544123	0.5000000000000000
0.3150475583086489	0.0694207498051540	0.6126141203414974
0.5423817518412832	0.1186055548685943	0.3272037839610817
0.5461959468704976	0.1195085542715404	0.4451458061714959
0.5461959468704976	0.1195085542715404	0.5548541938285041
0.5423817518412832	0.1186055548685943	0.6727962160389183
0.7967783097919252	0.0792959429222861	0.3293403924464613
0.8100278676124617	0.0748064857704591	0.4427374078613084
0.8100278676124617	0.0748064857704591	0.5572625921386916
0.7967783097919252	0.0792959429222861	0.6706596075535387
0.9502686641142901	0.6181131896549985	0.3837114537108803
0.9529993992229606	0.6196056292375474	0.5000000000000000
0.9502686641142901	0.6181131896549985	0.6162885462891197
0.6849524416913511	0.5694207498051540	0.3873858796585026
0.6939278816355170	0.5733452689544123	0.5000000000000000
0.6849524416913511	0.5694207498051540	0.6126141203414974
0.4576182481587168	0.6186055548685943	0.3272037839610817
0.4538040531295024	0.6195085542715404	0.4451458061714959
0.4538040531295024	0.6195085542715404	0.5548541938285041
0.4576182481587168	0.6186055548685943	0.6727962160389183
0.2032216902080748	0.5792959429222861	0.3293403924464613
0.1899721323875383	0.5748064857704591	0.4427374078613084
0.1899721323875383	0.5748064857704591	0.5572625921386916
0.2032216902080748	0.5792959429222861	0.6706596075535387
0.1983732929609872	0.2500000000000000	0.3844614097993428
0.1965157769180763	0.2500000000000000	0.5000000000000000
0.1983732929609872	0.2500000000000000	0.6155385902006572
0.6939148871477272	0.2500000000000000	0.3346689145283932
0.6974682665211773	0.2500000000000000	0.4447350560625907
0.6974682665211773	0.2500000000000000	0.5552649439374093
0.6939148871477272	0.2500000000000000	0.6653310854716068
0.8016267070390128	0.7500000000000000	0.3844614097993428
0.8034842230819237	0.7500000000000000	0.5000000000000000
0.8016267070390128	0.7500000000000000	0.6155385902006572
0.3060851128522728	0.7500000000000000	0.3346689145283932
0.3025317334788227	0.7500000000000000	0.4447350560625907
0.3025317334788227	0.7500000000000000	0.5552649439374093
0.3060851128522728	0.7500000000000000	0.6653310854716068
0.1339068177944256	0.9394205631286781	0.3836993237531132
0.1325600883915428	0.9402983366497679	0.5000000000000000
0.1339068177944256	0.9394205631286781	0.6163006762468868
0.6387702311087224	0.9402098455793535	0.3336764532395406
0.6337790296402659	0.9414881102613180	0.4445284724383143
0.6337790296402588	0.9414881102613180	0.5554715275616857
0.6387702311087153	0.9402098455793535	0.6663235467604594
0.8660931822055815	0.4394205631286781	0.3836993237531132

0.8674399116084643	0.4402983366497679	0.5000000000000000
0.8660931822055815	0.4394205631286781	0.6163006762468868
0.3612297688912847	0.4402098455793535	0.3336764532395406
0.3662209703597412	0.4414881102613180	0.4445284724383143
0.3662209703597412	0.4414881102613180	0.5554715275616857
0.3612297688912847	0.4402098455793535	0.6663235467604594
0.1339068177944256	0.5605794368713219	0.3836993237531132
0.1325600883915428	0.5597016633502321	0.5000000000000000
0.1339068177944256	0.5605794368713219	0.6163006762468868
0.6387702311087224	0.5597901544206465	0.3336764532395406
0.6337790296402659	0.5585118897386820	0.4445284724383143
0.6337790296402588	0.5585118897386820	0.5554715275616857
0.6387702311087153	0.5597901544206465	0.6663235467604594
0.8660931822055815	0.0605794368713219	0.3836993237531132
0.8674399116084643	0.0597016633502321	0.5000000000000000
0.8660931822055815	0.0605794368713219	0.6163006762468868
0.3612297688912847	0.0597901544206465	0.3336764532395406
0.3662209703597412	0.0585118897386820	0.4445284724383143
0.3662209703597412	0.0585118897386820	0.5554715275616857
0.3612297688912847	0.0597901544206465	0.6663235467604594

**(4) (100)+O<sub>N3</sub>**

100-on

1.0000000000000000		
10.3189349201333993	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.3476600646972994	0.0000000000000000
0.0000000000000000	0.0000000000000000	34.5370260389971975

N O Ta

68 2 42

Direct

0.7513311296279837	0.2484547775598507	0.3873863531093513
0.7657956978083684	0.2493441929350877	0.5000000000000000
0.7513311296279837	0.2484547775598507	0.6126136468906486
0.2802375066088215	0.2501274070837847	0.3303609453911612
0.2639751736591089	0.2501844003250935	0.4428187813529499
0.2639751736591089	0.2501844003250935	0.5571812186470502
0.2802375066088215	0.2501274070837847	0.6696390546088383
0.2500239188251851	0.7490840816836122	0.3873343386549628
0.2344320253763904	0.7482523816351412	0.5000000000000000
0.2500239188251851	0.7490840816836122	0.6126656613450374
0.7199474735521447	0.7504592333577488	0.3298896482339109
0.7367738944004671	0.7499383126507236	0.4428229107855567
0.7367738944004671	0.7499383126507236	0.5571770892144434
0.7199474735521447	0.7504592333577488	0.6701103517660891
0.0492931933907886	0.3821774110705915	0.3831144962704990
0.0471801538892062	0.3799515264215856	0.5000000000000000
0.0492931933907886	0.3821774110705915	0.6168855037295011
0.3157080074876779	0.4314750485149201	0.3870343592236301
0.3059228617818372	0.4296719125291005	0.5000000000000000
0.3157080074876779	0.4314750485149201	0.6129656407763701
0.5465071407625692	0.3799567735713343	0.4446958498977664
0.5465071407625692	0.3799567735713343	0.5553041501022338
0.7889673089602195	0.4210997369288133	0.3291156429493525
0.8109661473276876	0.4234821596508224	0.4422146982515984
0.8109661473276876	0.4234821596508224	0.5577853017484018
0.7889673089602195	0.4210997369288133	0.6708843570506479
0.9498514910858126	0.8822017534284620	0.3837057635123680
0.9527031178053195	0.8798642127235646	0.5000000000000000

0.9498514910858126	0.8822017534284620	0.6162942364876318
0.6854367836608645	0.9317558703011516	0.3870148924874430
0.6944536485005093	0.9299005970545668	0.5000000000000000
0.6854367836608645	0.9317558703011516	0.6129851075125567
0.4585519602578569	0.8831829636897225	0.3255676312798773
0.4538075742122171	0.8801865812904526	0.4448119216195520
0.4538075742122171	0.8801865812904526	0.5551880783804486
0.4585519602578569	0.8831829636897225	0.6744323687201231
0.2040323051256962	0.9199814650269346	0.3291999875358959
0.1887737675989025	0.9227791924086179	0.4425121086815180
0.1887737675989025	0.9227791924086179	0.5574878913184815
0.2040323051256962	0.9199814650269346	0.6708000124641043
0.0501788141616823	0.1179861902093950	0.3836311008351626
0.0479030869557570	0.1187939450388650	0.5000000000000000
0.0501788141616823	0.1179861902093950	0.6163688991648378
0.3132621203435643	0.0681420115941256	0.3872860592790403
0.3059315100239264	0.0705450884192852	0.5000000000000000
0.3132621203435643	0.0681420115941256	0.6127139407209601
0.5410469919815931	0.1220698429855049	0.3296534306560268
0.5466005947199453	0.1189791850978507	0.4447550944013993
0.5466005947199453	0.1189791850978507	0.5552449055986012
0.5410469919815931	0.1220698429855049	0.6703465693439732
0.7967267146866112	0.0808597946205768	0.3282242186666241
0.8128890496348758	0.0757618373228733	0.4423281254751135
0.8128890496348758	0.0757618373228733	0.5576718745248870
0.7967267146866112	0.0808597946205768	0.6717757813333760
0.9498107693520328	0.6182813908026173	0.3833478694890782
0.9520305184065984	0.6189373121415570	0.5000000000000000
0.9498107693520328	0.6182813908026173	0.6166521305109215
0.6860539235421749	0.5699365668497829	0.3871195612743192
0.6942509447537704	0.5702293478035250	0.5000000000000000
0.6860539235421749	0.5699365668497829	0.6128804387256812
0.4596100104607937	0.6151841856921400	0.3283390550038561
0.4538242678184635	0.6187963818876738	0.4448748388176699
0.4538242678184635	0.6187963818876738	0.5551251611823296
0.4596100104607937	0.6151841856921400	0.6716609449961438
0.2075556368433928	0.5761984254640760	0.3284520579278868
0.1871793771282030	0.5753169071682499	0.4421845678897633
0.1871793771282030	0.5753169071682499	0.5578154321102368
0.2075556368433928	0.5761984254640760	0.6715479420721127
0.5415978597231752	0.3857204296869869	0.3222923467056323
0.5415978597231752	0.3857204296869869	0.6777076532943680
0.1997894934954096	0.2497098958826579	0.3845293537394068
0.1972972605733715	0.2499247549305401	0.5000000000000000
0.1997894934954096	0.2497098958826579	0.6154706462605927
0.6931096479645671	0.2434375440214345	0.3343921183651811
0.6976552185344367	0.2492517779682349	0.4446092803337420
0.6976552185344367	0.2492517779682349	0.5553907196662575
0.6931096479645671	0.2434375440214345	0.6656078816348192
0.8004713789537604	0.7511205695523002	0.3851101555709762
0.8026247662050776	0.7501435365102916	0.5000000000000000
0.8004713789537604	0.7511205695523002	0.6148898444290238
0.3096368692887065	0.7506501752094580	0.3344122168020927
0.3029276009018841	0.7495542723378879	0.4445819424426962
0.3029276009018841	0.7495542723378879	0.5554180575573036
0.3096368692887065	0.7506501752094580	0.6655877831979075
0.1344597152680122	0.9382600945196931	0.3838585669341052
0.1331675117045379	0.9398386074724341	0.5000000000000000

0.1344597152680122	0.9382600945196931	0.6161414330658951
0.6400061728158719	0.9414357153508289	0.3334396947659800
0.6336891382196657	0.9395459621482062	0.4444476035774684
0.6336891382196586	0.9395459621482062	0.5555523964225311
0.6400061728158648	0.9414357153508289	0.6665603052340199
0.8637477503699845	0.4389827667781896	0.3833819413772110
0.8664274865769475	0.4397647718860447	0.5000000000000000
0.8637477503699845	0.4389827667781896	0.6166180586227890
0.3540429541599189	0.4432685780132097	0.3332383703614917
0.3668921498666879	0.4397070797952312	0.4445122617581424
0.3668921498666879	0.4397070797952312	0.5554877382418576
0.3540429541599189	0.4432685780132097	0.6667616296385083
0.1323947611017125	0.5597061702451019	0.3843002946281602
0.1320956777503345	0.5591076947373302	0.5000000000000000
0.1323947611017125	0.5597061702451019	0.6156997053718395
0.6449863983539161	0.5684987981788705	0.3331940358114016
0.6341316078659643	0.5593364893242598	0.4444968802045010
0.6341316078659572	0.5593364893242598	0.5555031197954984
0.6449863983539090	0.5684987981788705	0.6668059641885985
0.8673230240236096	0.0613113893009957	0.3842623525010389
0.8676122713412245	0.0589190321294247	0.5000000000000000
0.8673230240236096	0.0613113893009957	0.6157376474989612
0.3578338072931454	0.0603237123710389	0.3336211409641818
0.3664671348556762	0.0595442338937415	0.4445348530780952
0.3664671348556762	0.0595442338937415	0.5554651469219052
0.3578338072931454	0.0603237123710389	0.6663788590358181

**(5) [110]<sub>mol</sub>**

110-water-mol

1.0000000000000000		
10.3476600646972994	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.0339593887328995	0.0000000000000010
0.0000000000000000	0.0000000000000000	44.1809380160793026

H	N	O	Ta
2	140	1	84

Selective dynamics

Direct

0.5232339543039612	0.1826456656239864	0.5879160229570530	T	T	T
0.6707875710832404	0.2135951665319027	0.5837182607822383	T	T	T
0.2500000000000000	0.3293039861898137	0.0059393964048695	F	F	F
0.2500000000000000	0.4547089975823013	0.0886492757288480	F	F	F
0.2485756132093741	0.0932759249978512	0.5002025953947150	T	T	T
0.2499438158634626	0.0802160786716339	0.1713195782158242	T	T	T
0.2498933955846248	0.2058156869228910	0.2540061251476893	T	T	T
0.2499509255668232	0.3310145741985084	0.3367016718523012	T	T	T
0.2497126951618213	0.4540811007739936	0.4194096566371752	T	T	T
0.7500000000000000	0.0404308394626796	0.1278272917373684	F	F	F
0.7499193783578177	0.1637747890850856	0.2105956894167309	T	T	T
0.7498008281615351	0.2883852668063700	0.2933591538827077	T	T	T
0.7497180953913226	0.4133456160711568	0.3761514578200040	T	T	T
0.7500000000000000	0.4150258280701919	0.0451174124133900	F	F	F
0.7494949876321613	0.0386348301866077	0.4596776019896588	T	T	T
0.7552117516050098	0.1828429148452652	0.5397028254381065	T	T	T
0.3805899955332279	0.0811638913835608	0.0294058438053355	F	F	F
0.3805899955332279	0.2065689027760556	0.1121157231293139	F	F	F
0.3815798133836322	0.3308143693484951	0.1947622133430762	T	T	T
0.3814918301479959	0.4557731942192876	0.2774665865562971	T	T	T
0.4252809836911807	0.1025248990101832	0.2165479620004255	T	T	T

0.4253414520077075	0.2275903676091326	0.2992990526559427	T	T	T
0.4255585521112922	0.3530902826920956	0.3820463203048484	T	T	T
0.4251545278866863	0.4779256046138037	0.4654334420623875	T	T	T
0.3810922134450341	0.0809137656943484	0.3601933555090058	T	T	T
0.3814079674107234	0.2048986820381654	0.4421781522898495	T	T	T
0.3794154471561279	0.3381600029889892	0.5267902503759085	T	T	T
0.4261699933558702	0.3522211622490019	0.0510568088182595	F	F	F
0.4261699933558702	0.4776261736414895	0.1337666881422379	F	F	F
0.4188030739350211	0.1173328777999458	0.5479037256419832	T	T	T
0.8805899955332279	0.1631659228764377	0.0216509650129240	F	F	F
0.8805899955332279	0.2885709342689324	0.1043608443369095	F	F	F
0.8814531687658637	0.4136250335246522	0.1870938419217721	T	T	T
0.9261699933558702	0.3921086520110038	0.0000000000000000	F	F	F
0.9245133971466502	0.0153244207660494	0.4133087664099836	T	T	T
0.9290982539111063	0.1525865167031456	0.4943777391422380	T	T	T
0.8815179166637140	0.0384364934713409	0.2698086800315306	T	T	T
0.8816465775617333	0.1635426438264896	0.3525449717217932	T	T	T
0.8815242892433164	0.2880179348806631	0.4347197879498619	T	T	T
0.8817444556742760	0.4215515694516982	0.5195158023043838	T	T	T
0.9261699933558702	0.0175136634034914	0.0827098793239784	F	F	F
0.9257581482604543	0.1418536193457071	0.1654672607297409	T	T	T
0.9253376420976003	0.2666803758051363	0.2481184548087854	T	T	T
0.9248495126000129	0.3920817812800206	0.3307255127086584	T	T	T
0.1194100044667721	0.0811638913835608	0.0294058438053355	F	F	F
0.1194100044667721	0.2065689027760556	0.1121157231293139	F	F	F
0.1182797195401265	0.3308394484530712	0.1947867486702083	T	T	T
0.1182458536164539	0.4558360524723373	0.2774905942878357	T	T	T
0.0745725549800427	0.1025119484314297	0.2165466824186401	T	T	T
0.0744370810661472	0.2277106291859486	0.2992715340436944	T	T	T
0.0740377478347662	0.3535899369486923	0.3818733724440220	T	T	T
0.0742772135130206	0.4774748643861995	0.4654278407265119	T	T	T
0.1183993925286065	0.0809991147205749	0.3601770650557949	T	T	T
0.1184061908231624	0.2046968220504803	0.4415810368092221	T	T	T
0.1226905270115491	0.3406211999035598	0.5274338135395572	T	T	T
0.0738300066441298	0.3522211622490019	0.0510568088182595	F	F	F
0.0738300066441298	0.4776261736414895	0.1337666881422379	F	F	F
0.0739675541457452	0.1202165327267807	0.5472671441789099	T	T	T
0.6194100044667721	0.1631659228764377	0.0216509650129240	F	F	F
0.6194100044667721	0.2885709342689324	0.1043608443369095	F	F	F
0.6184274363944772	0.4136591550857294	0.1871160509627013	T	T	T
0.5738300066441298	0.3921086520110038	0.0000000000000000	F	F	F
0.5743647855074900	0.0169119782422619	0.4137105607776995	T	T	T
0.5718304352647029	0.1526050054117506	0.4960237061686223	T	T	T
0.6182054634989306	0.0384818741093259	0.2698715659927710	T	T	T
0.6179355677532887	0.1636772280328352	0.3527406305359245	T	T	T
0.6180332550605263	0.2885739996391686	0.4356493882550164	T	T	T
0.6173064097999326	0.4216341586116705	0.5201926949797528	T	T	T
0.5738300066441298	0.0175136634034914	0.0827098793239784	F	F	F
0.5741603688450855	0.1418717849777124	0.1654650790238329	T	T	T
0.5743910792472222	0.2666761882770842	0.2481204789749218	T	T	T
0.5746047596018823	0.3920862885770878	0.3307539616467646	T	T	T
0.2500000000000000	0.8293039861898137	0.0059393964048695	F	F	F
0.2500000000000000	0.9547089975823013	0.0886492757288480	F	F	F
0.2497635799818550	0.5929605669562158	0.5005037758596801	T	T	T
0.2499432847015195	0.5802095589866146	0.1713189934845172	T	T	T
0.2499139580828494	0.7058200266972844	0.2540009006298055	T	T	T
0.2500466869851750	0.8308076127043791	0.3367038293488775	T	T	T
0.2499606812486087	0.9535789223324741	0.4193835618539700	T	T	T



0.7500000000000000	0.5404308394626796	0.1278272917373684	F	F	F
0.7499035110270879	0.6637848649081429	0.2105929955863484	T	T	T
0.7496869468441201	0.7883987787764438	0.2933686140596979	T	T	T
0.7492257602632447	0.9140357383441663	0.3761183985366862	T	T	T
0.7500000000000000	0.9150258280701919	0.0451174124133900	F	F	F
0.7497028793460019	0.5381353330232163	0.4596200836449510	T	T	T
0.7498229600316020	0.6844003267016976	0.5395347228826958	T	T	T
0.3805899955332279	0.5811638913835608	0.0294058438053355	F	F	F
0.3805899955332279	0.7065689027760556	0.1121157231293139	F	F	F
0.3815686875289824	0.8308156119982245	0.1947588880922774	T	T	T
0.3814441604645270	0.9557617526256250	0.2774676317838076	T	T	T
0.4252732284785230	0.6025249556334006	0.2165416349444627	T	T	T
0.4253620878807418	0.7276025531658191	0.2992841921026013	T	T	T
0.4259088781196871	0.8536509094432722	0.3819766279823825	T	T	T
0.4255415130675611	0.9780761921898298	0.4656045034072794	T	T	T
0.3812677047381395	0.5809209430700737	0.3601962301448801	T	T	T
0.3810347575953827	0.7053644972360571	0.4419138933913349	T	T	T
0.3776615424038761	0.8385247256170335	0.5268812006391927	T	T	T
0.4261699933558702	0.8522211622490019	0.0510568088182595	F	F	F
0.4261699933558702	0.9776261736414895	0.1337666881422379	F	F	F
0.4251100559375184	0.6203866951326695	0.5473140561148847	T	T	T
0.8805899955332279	0.6631659228764377	0.0216509650129240	F	F	F
0.8805899955332279	0.7885709342689324	0.1043608443369095	F	F	F
0.8814490787386038	0.9136369080689923	0.1870973184288481	T	T	T
0.9261699933558702	0.8921086520110038	0.0000000000000000	F	F	F
0.9245701726737648	0.5157155310928692	0.4133853272383490	T	T	T
0.9281192954327511	0.6532282569140466	0.4946726155382589	T	T	T
0.8815100201608830	0.5384389843136409	0.2698014264826740	T	T	T
0.8814927996307167	0.6636036394665590	0.3525865566827325	T	T	T
0.8810785190366764	0.7882337641126999	0.4348687871689169	T	T	T
0.8816085909334298	0.9216177462990204	0.5199811038818251	T	T	T
0.9261699933558702	0.5175136634034985	0.0827098793239784	F	F	F
0.9257524003856392	0.6418570741497656	0.1654679435837049	T	T	T
0.9252599420848888	0.7667142267037356	0.2481212648955464	T	T	T
0.9246928166575771	0.8919852846914950	0.3307259349946061	T	T	T
0.1194100044667721	0.5811638913835608	0.0294058438053355	F	F	F
0.1194100044667721	0.7065689027760556	0.1121157231293139	F	F	F
0.1182673925372504	0.8308378404475920	0.1947853690471956	T	T	T
0.1182114841129697	0.9558293581146270	0.2775031318099642	T	T	T
0.0745489098609161	0.6025409571462915	0.2165436365413804	T	T	T
0.0744017962032087	0.7276848576591577	0.2992687975274927	T	T	T
0.0740362501103014	0.8535425600494085	0.3818366742874765	T	T	T
0.0739269471071983	0.9771673930001693	0.4652752571722997	T	T	T
0.1183323081323693	0.5809801553352006	0.3602064886434213	T	T	T
0.1180872810918633	0.7047377320275202	0.4417795153640464	T	T	T
0.1219349416455206	0.8390433902839824	0.5270386244247895	T	T	T
0.0738300066441298	0.8522211622490019	0.0510568088182595	F	F	F
0.0738300066441298	0.9776261736414895	0.1337666881422379	F	F	F
0.0741787302324882	0.6209917869066772	0.5474218682841629	T	T	T
0.6194100044667721	0.6631659228764377	0.0216509650129240	F	F	F
0.6194100044667721	0.7885709342689324	0.1043608443369095	F	F	F
0.6184206186728762	0.9136728161839098	0.1871220846423092	T	T	T
0.5738300066441298	0.8921086520110038	0.0000000000000000	F	F	F
0.5748336403586857	0.5158456712372956	0.4134067236063216	T	T	T
0.5708974552098006	0.6527733229184970	0.4947387670221380	T	T	T
0.6182245648956454	0.5384466926833393	0.2698429774045815	T	T	T
0.6180148791975546	0.6636214822289103	0.3526490832339563	T	T	T
0.6180189959016609	0.7884706955062776	0.4349535986441611	T	T	T

0.6175778668086384	0.9219177299804502	0.5207474095386599	T	T	T
0.5738300066441298	0.5175136634034985	0.0827098793239784	F	F	F
0.5741543705865160	0.6418658751682544	0.1654652068863750	T	T	T
0.5743705346946523	0.7666873427199729	0.2481214059504754	T	T	T
0.5743695814402839	0.8921149287165522	0.3307876512486317	T	T	T
0.5837647047035456	0.2501362358991451	0.5843092229864116	T	T	T
0.2500000000000000	0.0746099933052733	0.1245949913851589	F	F	F
0.2499470486089535	0.2003011941361209	0.2072847130079058	T	T	T
0.2499668498982262	0.3252902001707830	0.2899753436560584	T	T	T
0.2498667509267353	0.4496074624362172	0.3725340751424324	T	T	T
0.2500000000000000	0.4492049819127857	0.0418851120611805	F	F	F
0.2498981492224495	0.0746865740400080	0.4544362069103058	T	T	T
0.2477216438648361	0.1948640769305386	0.5348724129886606	T	T	T
0.7500000000000000	0.2951248323472200	0.0091716967570790	F	F	F
0.7500000000000000	0.4205298437397076	0.0918815760810574	F	F	F
0.7494388576580472	0.0453149224146931	0.5073671461025230	T	T	T
0.7499394357149365	0.0443995834400016	0.1745504644120598	T	T	T
0.7498484403219950	0.1688580363225761	0.2573729381895938	T	T	T
0.7497052628809876	0.2935885407998888	0.3401804620594778	T	T	T
0.7495173731773591	0.4178656774272942	0.4231546621445664	T	T	T
0.9406099943444133	0.0054327150181379	0.0365676919062707	F	F	F
0.9406099943444133	0.1308377264106326	0.1192775712302492	F	F	F
0.9392488804774323	0.2555315576609467	0.2018981024760052	T	T	T
0.9392430990936323	0.3801765340342960	0.2845473147834331	T	T	T
0.9394226223298092	0.0044244966198135	0.3670319304342166	T	T	T
0.9403534300336366	0.1292773536202964	0.4488302306615032	T	T	T
0.9389158149602784	0.2436425697458471	0.5302168127055737	T	T	T
0.4406099943444133	0.2388970992418606	0.0144891169119887	F	F	F
0.4406099943444133	0.3643021106343554	0.0971989962359672	F	F	F
0.4393443773211954	0.4891618750252467	0.1800451638361076	T	T	T
0.4392697472591816	0.1140023823844658	0.2627805924064004	T	T	T
0.4392589041447479	0.2387142728917317	0.3456235678233265	T	T	T
0.4396041927426286	0.3637206500292836	0.4286588138970191	T	T	T
0.4410742691867534	0.4910898034935413	0.5128720145202892	T	T	T
0.5593900056555867	0.0054327150181379	0.0365676919062707	F	F	F
0.5593900056555867	0.1308377264106326	0.1192775712302492	F	F	F
0.5606046175150649	0.2555328257238547	0.2019025741131872	T	T	T
0.5604784369268034	0.3801335021088554	0.2845712842638978	T	T	T
0.5605378884100831	0.0045379510320561	0.3673571640045154	T	T	T
0.5602399830897227	0.1290880390469855	0.4501763450265686	T	T	T
0.5570972957122697	0.2481861486040356	0.5321306281518640	T	T	T
0.0593900056555867	0.2388970992418606	0.0144891169119887	F	F	F
0.0593900056555867	0.3643021106343554	0.0971989962359672	F	F	F
0.0605348391281305	0.4891508024219778	0.1800434200814210	T	T	T
0.0604707318785457	0.1140470268751755	0.2627637228906587	T	T	T
0.0603054147943937	0.2389427589438252	0.3455550223565779	T	T	T
0.0604384443036950	0.3646454546372797	0.4285042193424072	T	T	T
0.0585135012417064	0.4903069135669594	0.5131368593593836	T	T	T
0.2500000000000000	0.5746099933052733	0.1245949913851589	F	F	F
0.2499319632732174	0.7003090892421228	0.2072778233683802	T	T	T
0.2499240573656586	0.8252491398407440	0.2899559298440303	T	T	T
0.2499507060401095	0.9495446679779516	0.3725062841259292	T	T	T
0.2500000000000000	0.9492049819127857	0.0418851120611805	F	F	F
0.2493284166490808	0.5745559248784082	0.4544391163864956	T	T	T
0.2496106868940614	0.6956097667708400	0.5351062481756825	T	T	T
0.7500000000000000	0.7951248323472200	0.0091716967570790	F	F	F
0.7500000000000000	0.9205298437397076	0.0918815760810574	F	F	F
0.7500054516192449	0.5442334000389608	0.5068294726782568	T	T	T

0.7499271724624320	0.5443939604874584	0.1745502137772121	T	T	T
0.7497807622007496	0.6688938563827324	0.2573690820496787	T	T	T
0.7494332207822453	0.7939006629729302	0.3401738661381478	T	T	T
0.7489739020999095	0.9190893873130461	0.4231972952403001	T	T	T
0.9406099943444133	0.5054327150181379	0.0365676919062707	F	F	F
0.9406099943444133	0.6308377264106326	0.1192775712302492	F	F	F
0.9392309980273477	0.7555316753562684	0.2018982423654414	T	T	T
0.9392609371469391	0.8801579337209231	0.2845430570053047	T	T	T
0.9391600518220056	0.5044947555306514	0.3670658618873361	T	T	T
0.9398000266597920	0.6295079624430535	0.4489123277413590	T	T	T
0.9381514389790754	0.7436979928738741	0.5305958604816263	T	T	T
0.4406099943444133	0.7388970992418606	0.0144891169119887	F	F	F
0.4406099943444133	0.8643021106343554	0.0971989962359672	F	F	F
0.4393456605435558	0.9891659816979849	0.1800476907683438	T	T	T
0.4393060709424231	0.6140358613429373	0.2627658608281656	T	T	T
0.4391984176725952	0.7391627784124993	0.3455879705027383	T	T	T
0.4389833545076331	0.8654454957039384	0.4286602309710225	T	T	T
0.4412458488944091	0.9901487271865056	0.5134336266278046	T	T	T
0.5593900056555867	0.5054327150181379	0.0365676919062707	F	F	F
0.5593900056555867	0.6308377264106326	0.1192775712302492	F	F	F
0.5606015088618260	0.7555426893134283	0.2019055727273826	T	T	T
0.5605084689282166	0.8801671374969540	0.2846065582700932	T	T	T
0.5602299602124641	0.5045673826042499	0.3670942189155302	T	T	T
0.5587788276149928	0.6297214290033561	0.4488954952218340	T	T	T
0.5610474296354702	0.7438137022530735	0.5306731987107420	T	T	T
0.0593900056555867	0.7388970992418606	0.0144891169119887	F	F	F
0.0593900056555867	0.8643021106343554	0.0971989962359672	F	F	F
0.0605376147868868	0.9891576270457844	0.1800447166733412	T	T	T
0.0604345514836475	0.6139966132206561	0.2627621188815766	T	T	T
0.0601389280024584	0.7388144162693628	0.3455589249281433	T	T	T
0.0598780636724802	0.8644855508401780	0.4284867627766173	T	T	T
0.0578943120967560	0.9892861572179481	0.5129164730207931	T	T	T

(6) [110]<sub>dis</sub>

110-water-dis

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10.3476600646972994	0.0000000000000000	0.0000000000000000
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H	N	O	Ta
2	140	1	84

Selective dynamics

Direct

0.5562780278892000	0.3623958983509207	0.5890380502926515	T	T	T
0.4354575426667362	0.0866352025057846	0.5716400337269124	T	T	T
0.2500000000000000	0.3293039861898137	0.0059393964048695	F	F	F
0.2500000000000000	0.4547089975823013	0.0886492757288480	F	F	F
0.2534864841112432	0.0971614745075656	0.5000494295357808	T	T	T
0.2499979202232230	0.0804240415792366	0.1713210952254717	T	T	T
0.2500557084718013	0.2062975118349616	0.2539987133270704	T	T	T
0.2503083635649606	0.3317307774077401	0.3366557030980096	T	T	T
0.2498509955186024	0.4553270958675257	0.4192798525553705	T	T	T
0.7500000000000000	0.0404308394626796	0.1278272917373684	F	F	F
0.7499990189911013	0.1640871425183790	0.2105918625333337	T	T	T
0.7500027033358790	0.2888281098527341	0.2933540678502585	T	T	T
0.7500849658095803	0.4134848420971531	0.3762048968160678	T	T	T
0.7500000000000000	0.4150258280701919	0.0451174124133900	F	F	F
0.7491073649204687	0.0407588710936982	0.4597269099864779	T	T	T

0.7578096360424278	0.1838020957100195	0.5392331744842155	T	T	T
0.3805899955332279	0.0811638913835608	0.0294058438053355	F	F	F
0.3805899955332279	0.2065689027760556	0.1121157231293139	F	F	F
0.3816404567026762	0.3311138462358860	0.1947698439711128	T	T	T
0.3817036248746695	0.4563292614941738	0.2774511499011809	T	T	T
0.4253906434248108	0.1028389424064829	0.2165552967231985	T	T	T
0.4256086280160193	0.2281362503885053	0.2992987485096784	T	T	T
0.4259240056192895	0.3535076174269617	0.3820583459613877	T	T	T
0.4254371523489725	0.4785418536125232	0.4651837503130948	T	T	T
0.3813647968082152	0.0814988300093341	0.3601551800156624	T	T	T
0.3823803726636645	0.2049051157612965	0.4418751728749122	T	T	T
0.3833327949726709	0.3351520819142910	0.5259137300770410	T	T	T
0.4261699933558702	0.3522211622490019	0.0510568088182595	F	F	F
0.4261699933558702	0.4776261736414895	0.1337666881422379	F	F	F
0.4109480737715758	0.1084966625859921	0.5498875887831873	T	T	T
0.8805899955332279	0.1631659228764377	0.0216509650129240	F	F	F
0.8805899955332279	0.2885709342689324	0.1043608443369095	F	F	F
0.8814923472506538	0.4139197060859422	0.1871073903734067	T	T	T
0.9261699933558702	0.3921086520110038	0.0000000000000000	F	F	F
0.9249451383627717	0.0161946457581332	0.4134371015685036	T	T	T
0.9282993245591963	0.1526019704216914	0.4942550334178258	T	T	T
0.8816685073813310	0.0389135209505128	0.2698003757543160	T	T	T
0.8819750729884200	0.1640199980948075	0.3524733662522418	T	T	T
0.8818487100139321	0.2885032634325486	0.4343495793913069	T	T	T
0.8811657298510260	0.4214003517292854	0.5182436414853656	T	T	T
0.9261699933558702	0.0175136634034914	0.0827098793239784	F	F	F
0.9258149475868988	0.1420620477456311	0.1654646008092959	T	T	T
0.9254516204270009	0.2671669685335258	0.2481047988886376	T	T	T
0.9249508807494057	0.3927609596002050	0.3306974474296758	T	T	T
0.1194100044667721	0.0811638913835608	0.0294058438053355	F	F	F
0.1194100044667721	0.2065689027760556	0.1121157231293139	F	F	F
0.1183461729859393	0.3311239577897169	0.1947859426162176	T	T	T
0.1183637198892468	0.4564056358102280	0.2774915170082305	T	T	T
0.0746655075582471	0.1028398929694887	0.2165522583104177	T	T	T
0.0746287522781597	0.2282977906622266	0.2992603724488753	T	T	T
0.0745010122619886	0.3542941646433579	0.3818155058200497	T	T	T
0.0748368789463141	0.4787287092495630	0.4652884575714316	T	T	T
0.1186747448114958	0.0818172951689647	0.3602250335799039	T	T	T
0.1187338848102854	0.2062983296950523	0.4418345574722641	T	T	T
0.1224743013011105	0.3435717322862855	0.5282300262402464	T	T	T
0.0738300066441298	0.3522211622490019	0.0510568088182595	F	F	F
0.0738300066441298	0.4776261736414895	0.1337666881422379	F	F	F
0.0737763775154028	0.1211274549486540	0.5467542902596492	T	T	T
0.6194100044667721	0.1631659228764377	0.0216509650129240	F	F	F
0.6194100044667721	0.2885709342689324	0.1043608443369095	F	F	F
0.6184893128804939	0.4139477846762410	0.1871218894837659	T	T	T
0.5738300066441298	0.3921086520110038	0.0000000000000000	F	F	F
0.5740312641035562	0.0181736886021904	0.4141094067155287	T	T	T
0.5702469575316653	0.1484154627104308	0.4976943941705553	T	T	T
0.6183469786959673	0.0390914045387001	0.2699546930631243	T	T	T
0.6182211592668815	0.1646383267343111	0.3530173872487801	T	T	T
0.6185936070923871	0.2910348193333295	0.4370227292992531	T	T	T
0.6179049927875006	0.4236675001147355	0.5203968659376490	T	T	T
0.5738300066441298	0.0175136634034914	0.0827098793239784	F	F	F
0.5741952075063781	0.1420830912281175	0.1654631045409765	T	T	T
0.5745784751893042	0.2672081165036326	0.2481084068732384	T	T	T
0.5750729042428853	0.3927997369943252	0.3307299868909755	T	T	T
0.2500000000000000	0.8293039861898137	0.0059393964048695	F	F	F

0.2500000000000000	0.9547089975823013	0.0886492757288480	F	F	F
0.2510909894376927	0.5913143590550898	0.5004575283646506	T	T	T
0.2499864080079615	0.5804467300504856	0.1713227897526916	T	T	T
0.2500280912683743	0.7063255466995372	0.2540060944625828	T	T	T
0.2503493115455252	0.8313121128699400	0.3366971020464127	T	T	T
0.2505888774268579	0.9546831300336887	0.4192668178910857	T	T	T
0.7500000000000000	0.5404308394626796	0.1278272917373684	F	F	F
0.7499567364493650	0.6641125040800724	0.2106075199471499	T	T	T
0.7498476640133575	0.7891874398684214	0.2933941124269654	T	T	T
0.7494732568322852	0.9153387381207051	0.3761846929628304	T	T	T
0.7500000000000000	0.9150258280701919	0.0451174124133900	F	F	F
0.7502298233458187	0.5403077281490456	0.4593255382848347	T	T	T
0.7504292657394033	0.6846435347168600	0.5394372163871857	T	T	T
0.3805899955332279	0.5811638913835608	0.0294058438053355	F	F	F
0.3805899955332279	0.7065689027760556	0.1121157231293139	F	F	F
0.3816158674678471	0.8311067835384066	0.1947770326951520	T	T	T
0.3815773490857053	0.9562995623656655	0.2774819150326445	T	T	T
0.4253701381739577	0.6028664244131222	0.2165481282167164	T	T	T
0.4256206435627544	0.7282592118086770	0.2992707467361534	T	T	T
0.4262900804720245	0.8544318266922781	0.3819623777266085	T	T	T
0.4255282891607881	0.9787332884618120	0.4655593525547920	T	T	T
0.3817545825248422	0.5816179395767063	0.3601047425449694	T	T	T
0.3816220163356626	0.7064492959259732	0.4417513939324594	T	T	T
0.3779527923109514	0.8344545931511420	0.5241845522604498	T	T	T
0.4261699933558702	0.8522211622490019	0.0510568088182595	F	F	F
0.4261699933558702	0.9776261736414895	0.1337666881422379	F	F	F
0.4243124552452107	0.6201222753464619	0.5475777373373092	T	T	T
0.8805899955332279	0.6631659228764377	0.0216509650129240	F	F	F
0.8805899955332279	0.7885709342689324	0.1043608443369095	F	F	F
0.8814965557216337	0.9139109229811289	0.1871106818528909	T	T	T
0.9261699933558702	0.8921086520110038	0.0000000000000000	F	F	F
0.9249807282106353	0.5165610802034070	0.4132889022359568	T	T	T
0.9277140686627978	0.6540555481557725	0.4945192310506523	T	T	T
0.8815949870193528	0.5390192207325226	0.2698028321971436	T	T	T
0.8816282276963994	0.6644602187918341	0.3525788237948372	T	T	T
0.8812757710854764	0.7896144819492400	0.4347617877142491	T	T	T
0.8813437425947267	0.9207355815671066	0.5188994000954094	T	T	T
0.9261699933558702	0.5175136634034985	0.0827098793239784	F	F	F
0.9257721906798821	0.6421055215274604	0.1654685469340620	T	T	T
0.9253467211056065	0.7672774309269456	0.2481257331607563	T	T	T
0.9249292037352760	0.8927373775018231	0.3307765179679450	T	T	T
0.1194100044667721	0.5811638913835608	0.0294058438053355	F	F	F
0.1194100044667721	0.7065689027760556	0.1121157231293139	F	F	F
0.1183277475436037	0.8311188144462541	0.1947886965532139	T	T	T
0.1183722591708693	0.9563984813106059	0.2775237465026566	T	T	T
0.0746119197152489	0.6028636413032215	0.2165574189473320	T	T	T
0.0744740225411191	0.7283381930900159	0.2992786622842211	T	T	T
0.0743615081069307	0.8543887551435755	0.3818833809989132	T	T	T
0.0758173272886135	0.9781901052493062	0.4654618044856226	T	T	T
0.1185344625766164	0.5817859372983097	0.3601727645929235	T	T	T
0.1183992738803655	0.7062260639045357	0.4418766114054827	T	T	T
0.1224154828880400	0.8412170350735220	0.5284529229652014	T	T	T
0.0738300066441298	0.8522211622490019	0.0510568088182595	F	F	F
0.0738300066441298	0.9776261736414895	0.1337666881422379	F	F	F
0.0737862111888447	0.6212854190098887	0.5469365957293600	T	T	T
0.6194100044667721	0.6631659228764377	0.0216509650129240	F	F	F
0.6194100044667721	0.7885709342689324	0.1043608443369095	F	F	F
0.6184732412880201	0.9139529174603293	0.1871384790847213	T	T	T

0.5738300066441298	0.8921086520110038	0.0000000000000000	F	F	F
0.5754637821396742	0.5169793375365622	0.4132909397956364	T	T	T
0.5712467517230793	0.6514673440301926	0.4948249394491481	T	T	T
0.6184149485095020	0.5390601998616518	0.2698562727568025	T	T	T
0.6185032346668020	0.6644212976938744	0.3526298369329628	T	T	T
0.6189005699018998	0.7896317767822569	0.4351270836509814	T	T	T
0.6171272239752288	0.9226380383782543	0.5230398887747741	T	T	T
0.5738300066441298	0.5175136634034985	0.0827098793239784	F	F	F
0.5741943740402932	0.6421092187767110	0.1654683502614961	T	T	T
0.5744865626916735	0.7673039324277948	0.2481446098363207	T	T	T
0.5744659512097356	0.8929021841897400	0.3309136312661731	T	T	T
0.5669765416223891	0.2831484931983363	0.5797701139298084	T	T	T
0.2500000000000000	0.0746099933052733	0.1245949913851589	F	F	F
0.2500454977596919	0.2005790662423302	0.2072798973876702	T	T	T
0.2501827919542333	0.3258575641376216	0.2899315572647394	T	T	T
0.2501879163168231	0.4504217687504204	0.3723738224191701	T	T	T
0.2500000000000000	0.4492049819127857	0.0418851120611805	F	F	F
0.2509413273129570	0.0761962796265891	0.4541344275788833	T	T	T
0.2436152193699615	0.1975532574462785	0.5343709211761276	T	T	T
0.7500000000000000	0.2951248323472200	0.0091716967570790	F	F	F
0.7500000000000000	0.4205298437397076	0.0918815760810574	F	F	F
0.7459172184953757	0.0493862174533772	0.5077725742040086	T	T	T
0.7499734654549802	0.0446464608557880	0.1745486091574334	T	T	T
0.7499564386913903	0.1693415753505907	0.2573700086805597	T	T	T
0.7499144556118300	0.2940501570174979	0.3401814756263485	T	T	T
0.7496805209730989	0.4184593647726186	0.4230704135136243	T	T	T
0.9406099943444133	0.0054327150181379	0.0365676919062707	F	F	F
0.9406099943444133	0.1308377264106326	0.1192775712302492	F	F	F
0.9393034863548116	0.2558174275738204	0.2018871254880774	T	T	T
0.9393189962261379	0.3807439806256024	0.2845072183608560	T	T	T
0.9397764420266725	0.0050847568143008	0.3671051453737265	T	T	T
0.9410698308911249	0.130677782382106	0.4488167257694296	T	T	T
0.9378994090816483	0.2451944855886843	0.5298419441775249	T	T	T
0.4406099943444133	0.2388970992418606	0.0144891169119887	F	F	F
0.4406099943444133	0.3643021106343554	0.0971989962359672	F	F	F
0.4394174649630839	0.4894351607417630	0.1800421154873149	T	T	T
0.4394534699775255	0.1144352740035988	0.2627877197244645	T	T	T
0.4397008195152767	0.2390106914787182	0.3456120236586928	T	T	T
0.4409333648941809	0.3628843080917679	0.4285240930887185	T	T	T
0.4381083192567817	0.4905134514786562	0.5119984855203528	T	T	T
0.5593900056555867	0.0054327150181379	0.0365676919062707	F	F	F
0.5593900056555867	0.1308377264106326	0.1192775712302492	F	F	F
0.5606781776715783	0.2558162974000227	0.2018994184242048	T	T	T
0.5606682746520015	0.3807100901546867	0.2845546284337855	T	T	T
0.5611292296867516	0.0055968963578884	0.3678832501461808	T	T	T
0.5624269006792459	0.1306989822252809	0.4523372715034335	T	T	T
0.5672434860990987	0.2620429853638396	0.5358864519333570	T	T	T
0.0593900056555867	0.2388970992418606	0.0144891169119887	F	F	F
0.0593900056555867	0.3643021106343554	0.0971989962359672	F	F	F
0.0605789557415251	0.4894105171831011	0.1800485470931885	T	T	T
0.0605732610345211	0.1145477450366195	0.2627634595701513	T	T	T
0.0604878854551192	0.2395957420074966	0.3455290677015430	T	T	T
0.0608353428365818	0.3660591379378260	0.4284064180075526	T	T	T
0.0578579461897930	0.4921378867816216	0.5130148368796897	T	T	T
0.2500000000000000	0.5746099933052733	0.1245949913851589	F	F	F
0.2499790263217463	0.7005893423965776	0.2072713851293445	T	T	T
0.2500527103861698	0.8258006735759805	0.2899334524364290	T	T	T
0.2502760484571197	0.9503771829731217	0.3724439871722096	T	T	T

0.2500000000000000	0.9492049819127857	0.0418851120611805	F	F	F
0.2494422422338411	0.5755289797042732	0.4540257960832657	T	T	T
0.2501543102085240	0.6953032250294924	0.5348822474695163	T	T	T
0.7500000000000000	0.7951248323472200	0.0091716967570790	F	F	F
0.7500000000000000	0.9205298437397076	0.0918815760810574	F	F	F
0.7519464656770857	0.5477204964334724	0.5061604200859160	T	T	T
0.7499520041811462	0.5446870490072226	0.1745466745134799	T	T	T
0.7498031481552317	0.6695821735462358	0.2573697572926500	T	T	T
0.7492844477518590	0.7952014495756575	0.3402011568538845	T	T	T
0.7478185126453336	0.9216874877253299	0.4233056763540979	T	T	T
0.9406099943444133	0.5054327150181379	0.0365676919062707	F	F	F
0.9406099943444133	0.6308377264106326	0.1192775712302492	F	F	F
0.9392915214125305	0.7558216283832639	0.2018994964722005	T	T	T
0.9393897798061988	0.8806678777022622	0.2845601578213061	T	T	T
0.9393702233547950	0.5054168138919943	0.3669275134794175	T	T	T
0.9397685110010110	0.6311089713663142	0.4485443182667420	T	T	T
0.9367487007838158	0.7454481640348312	0.5304517064182632	T	T	T
0.4406099943444133	0.7388970992418606	0.0144891169119887	F	F	F
0.4406099943444133	0.8643021106343554	0.0971989962359672	F	F	F
0.4393860680960769	0.9894112976428291	0.1800491260259823	T	T	T
0.4394949578806296	0.6146545695062721	0.2627526463237706	T	T	T
0.4396172031442997	0.7403385839483182	0.3455313095456264	T	T	T
0.4399008176193263	0.8674389835380166	0.4285277109163524	T	T	T
0.4439928860764048	0.9882313182191436	0.5128747648772296	T	T	T
0.5593900056555867	0.5054327150181379	0.0365676919062707	F	F	F
0.5593900056555867	0.6308377264106326	0.1192775712302492	F	F	F
0.5606823976616397	0.7558491558242728	0.2019287506510584	T	T	T
0.5607442279163831	0.8807775706191592	0.2847309008958760	T	T	T
0.5603725727622701	0.5055437895538526	0.3669942482728865	T	T	T
0.5585757607094179	0.6308352372713633	0.4486472209827660	T	T	T
0.5597579379926492	0.7426176181518591	0.5308252609603915	T	T	T
0.0593900056555867	0.7388970992418606	0.0144891169119887	F	F	F
0.0593900056555867	0.8643021106343554	0.0971989962359672	F	F	F
0.0605931162619348	0.9894291942695829	0.1800458162237137	T	T	T
0.0605112052619447	0.6145640679858635	0.2627726146324649	T	T	T
0.0602443425197109	0.7398017426371468	0.3455719645438153	T	T	T
0.0598449739999349	0.8661366619992459	0.4285504002497362	T	T	T
0.0565103240415764	0.9885489672258351	0.5129814670442617	T	T	T

**(7) [110+O<sub>N3</sub>]<sub>mol</sub>**

110-on-water-mol

1.0000000000000000		
10.3476600646972994	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.0339593887328995	0.0000000000000010
0.0000000000000000	0.0000000000000000	44.1809380160793026

H N O Ta  
2 139 2 84

Selective dynamics

Direct

0.5010909851631896	0.1868361356930883	0.5842666852152524	T	T	T
0.6453768178188097	0.2221781757659558	0.5926261439835012	T	T	T
0.2500000000000000	0.3293039861898137	0.0059393964048695	F	F	F
0.2500000000000000	0.4547089975823013	0.0886492757288480	F	F	F
0.2486921471551420	0.0951550042120329	0.5004642255087000	T	T	T
0.2499556317603680	0.0800123622206920	0.1713579069174860	T	T	T
0.2499340683408022	0.2053951763197110	0.2541099154859289	T	T	T
0.2500260792166610	0.3307244240621890	0.3369052854711653	T	T	T
0.2499518688081026	0.4550933598073821	0.4196975020104182	T	T	T



0.7500000000000000	0.0404308394626796	0.1278272917373684	F	F	F
0.7498873107607666	0.1631568071161802	0.2106903686920134	T	T	T
0.7497438264965255	0.2877211736958292	0.2935707722751554	T	T	T
0.7495576114949007	0.4132649272351336	0.3765128951335197	T	T	T
0.7500000000000000	0.4150258280701919	0.0451174124133900	F	F	F
0.7508121494639921	0.0391021064212475	0.4600173982833349	T	T	T
0.7556620989039825	0.1858119491145832	0.5404062479071128	T	T	T
0.3805899955332279	0.0811638913835608	0.0294058438053355	F	F	F
0.3805899955332279	0.2065689027760556	0.1121157231293139	F	F	F
0.3816299369335281	0.3303952977903704	0.1948021846896461	T	T	T
0.3815693228677969	0.4552436006790695	0.2775878003388134	T	T	T
0.4252339127545909	0.1020325952479651	0.2166261831900450	T	T	T
0.4252488952227401	0.2269785835652018	0.2994840422690689	T	T	T
0.4254042861961103	0.3528111524595116	0.3823559513442314	T	T	T
0.4237392626313493	0.4773290396442352	0.4662052803031526	T	T	T
0.3814872986760239	0.0805703160798003	0.3604053246793142	T	T	T
0.3818807336181292	0.2059764822136457	0.4425160887945008	T	T	T
0.4261699933558702	0.3522211622490019	0.0510568088182595	F	F	F
0.4261699933558702	0.4776261736414895	0.1337666881422379	F	F	F
0.4218430158704121	0.1253194456066355	0.5472220210839263	T	T	T
0.8805899955332279	0.1631659228764377	0.0216509650129240	F	F	F
0.8805899955332279	0.2885709342689324	0.1043608443369095	F	F	F
0.8814377378306648	0.4132361456889269	0.1871089258126057	T	T	T
0.9261699933558702	0.3921086520110038	0.0000000000000000	F	F	F
0.9250493556509473	0.0161919369999066	0.4135404127093809	T	T	T
0.9303840811705707	0.1553737501134709	0.4947911709222672	T	T	T
0.8814831352987151	0.0379496220736917	0.2699008295240581	T	T	T
0.8816494537831946	0.1633398066141441	0.3526417794781916	T	T	T
0.8815856529596307	0.2894813988325516	0.4351115997229966	T	T	T
0.8843499838518295	0.4235776578954163	0.5206031706672428	T	T	T
0.9261699933558702	0.0175136634034914	0.0827098793239784	F	F	F
0.9256933961233691	0.1415507976565399	0.1655182294886214	T	T	T
0.9252685505054431	0.2661644147043359	0.2482471298523600	T	T	T
0.9249234040077189	0.3916455911545213	0.3309639707723065	T	T	T
0.1194100044667721	0.0811638913835608	0.0294058438053355	F	F	F
0.1194100044667721	0.2065689027760556	0.1121157231293139	F	F	F
0.1182143108877634	0.3304335277419616	0.1948295178421731	T	T	T
0.1181290002613390	0.4552468628217726	0.2775818723869386	T	T	T
0.0746148727067565	0.1020682774457666	0.2166167629611662	T	T	T
0.0745680644709734	0.2271401058737823	0.2994330126507115	T	T	T
0.0744158269432541	0.3533280741147491	0.3821720433556128	T	T	T
0.0746404391270404	0.4792913223310610	0.4657487937376452	T	T	T
0.1184393815134963	0.0807136464382224	0.3603217006344878	T	T	T
0.1186076462095818	0.2056769174508876	0.4417242014729644	T	T	T
0.1273054093236843	0.3411884162798705	0.5255330938917634	T	T	T
0.0738300066441298	0.3522211622490019	0.0510568088182595	F	F	F
0.0738300066441298	0.4776261736414895	0.1337666881422379	F	F	F
0.0773768552581235	0.1237135575255928	0.5477121732505852	T	T	T
0.6194100044667721	0.1631659228764377	0.0216509650129240	F	F	F
0.6194100044667721	0.2885709342689324	0.1043608443369095	F	F	F
0.6184489824197957	0.4132503181209016	0.1871430263933278	T	T	T
0.5738300066441298	0.3921086520110038	0.0000000000000000	F	F	F
0.5744347269847978	0.0165053466818082	0.4141152677024164	T	T	T
0.5741159509171488	0.1554525161473921	0.4960171240102085	T	T	T
0.6182586727820358	0.0379251071202476	0.2699491269164230	T	T	T
0.6181729790062758	0.1634132087958001	0.3529532454940949	T	T	T
0.6183457511938220	0.2892706685820473	0.4355387944491045	T	T	T
0.6169134166762603	0.4215226309073506	0.5195402442072965	T	T	T

0.5738300066441298	0.0175136634034914	0.0827098793239784	F	F	F
0.5741907852960204	0.1415278740466015	0.1655190231070192	T	T	T
0.5743704152241281	0.2661330976017706	0.2482528014194486	T	T	T
0.5744695789833412	0.3916540350855875	0.3309977864844901	T	T	T
0.2500000000000000	0.8293039861898137	0.0059393964048695	F	F	F
0.2500000000000000	0.9547089975823013	0.0886492757288480	F	F	F
0.2508831665271540	0.5949902055881452	0.5008996159686903	T	T	T
0.2499654093494680	0.5800144986939654	0.1713537385772561	T	T	T
0.2499796387725044	0.7054064733099411	0.2541001448888406	T	T	T
0.2501974018824334	0.8306188376109047	0.3369175367481774	T	T	T
0.2504463881403551	0.9540686805041184	0.4197283537154421	T	T	T
0.7500000000000000	0.5404308394626796	0.1278272917373684	F	F	F
0.7498653054509544	0.6631541665654065	0.2106875733530283	T	T	T
0.7496678650451666	0.7878289762231427	0.2935388919217137	T	T	T
0.7494849916257703	0.9135255000445218	0.3764087901741067	T	T	T
0.7500000000000000	0.9150258280701919	0.0451174124133900	F	F	F
0.7505338916053284	0.5400521959551002	0.4601794825476578	T	T	T
0.7505471989087129	0.6877812311414112	0.5395193376506678	T	T	T
0.3805899955332279	0.5811638913835608	0.0294058438053355	F	F	F
0.3805899955332279	0.7065689027760556	0.1121157231293139	F	F	F
0.3816257955045770	0.8304017602628376	0.1947959577211546	T	T	T
0.3815424647076435	0.9552330033535876	0.2775793225926577	T	T	T
0.4252352694584018	0.6020217508195962	0.2166217176446505	T	T	T
0.4252844377569346	0.7270066629381756	0.2994748366486643	T	T	T
0.4258581035923243	0.8531257255391176	0.3824026128568208	T	T	T
0.4252729322373557	0.9795822965734448	0.4661140873161358	T	T	T
0.3815451769799559	0.5807277350672603	0.3604122096897073	T	T	T
0.3821276874111441	0.7061821809033456	0.4426860046150048	T	T	T
0.3799642099797311	0.8434142542046905	0.5286371269287925	T	T	T
0.4261699933558702	0.8522211622490019	0.0510568088182595	F	F	F
0.4261699933558702	0.9776261736414895	0.1337666881422379	F	F	F
0.4263386004458429	0.6227487733372076	0.5473233088104054	T	T	T
0.8805899955332279	0.6631659228764377	0.0216509650129240	F	F	F
0.8805899955332279	0.7885709342689324	0.1043608443369095	F	F	F
0.8814310211586770	0.9132371948171030	0.1871142316693439	T	T	T
0.9261699933558702	0.8921086520110038	0.0000000000000000	F	F	F
0.9249864353681752	0.5164442459863607	0.4136463664748559	T	T	T
0.9301229049713173	0.6533308516581262	0.4951177019431563	T	T	T
0.8814736593599275	0.5379535729259339	0.2699108000810773	T	T	T
0.8814925908183947	0.6634523592051111	0.3527189118935266	T	T	T
0.8813726312725810	0.7892690438991151	0.4352075336150556	T	T	T
0.8835013952593338	0.9244195689339063	0.5204680350966447	T	T	T
0.9261699933558702	0.5175136634034985	0.0827098793239784	F	F	F
0.9256753206547094	0.6415423530582389	0.1655199004426220	T	T	T
0.9252615890523754	0.7661529344122223	0.2482389088686164	T	T	T
0.9249917824388774	0.8914980294914387	0.3309269919562038	T	T	T
0.1194100044667721	0.5811638913835608	0.0294058438053355	F	F	F
0.1194100044667721	0.7065689027760556	0.1121157231293139	F	F	F
0.1182096398073207	0.8304312865203670	0.1948245546040689	T	T	T
0.1181712351766561	0.9552707431710883	0.2775731446556234	T	T	T
0.0746602817532910	0.6020393179927818	0.2166192672731252	T	T	T
0.0746734933099848	0.7271016535505592	0.2994231062081985	T	T	T
0.0745292605887380	0.8532778076331823	0.3821261318152788	T	T	T
0.0741043057136412	0.9787479431653248	0.4655073115361110	T	T	T
0.1182192579187205	0.5806542656514970	0.3602751915127298	T	T	T
0.1183168870702959	0.7056025947812103	0.4418692921564894	T	T	T
0.1237455426718406	0.8401604259768257	0.5257214975749654	T	T	T
0.0738300066441298	0.8522211622490019	0.0510568088182595	F	F	F

0.0738300066441298	0.9776261736414895	0.1337666881422379	F	F	F
0.0756622394463208	0.6244819135070621	0.5478105723343774	T	T	T
0.6194100044667721	0.6631659228764377	0.0216509650129240	F	F	F
0.6194100044667721	0.7885709342689324	0.1043608443369095	F	F	F
0.6184516459738298	0.9132732772894868	0.1871484554088121	T	T	T
0.5738300066441298	0.8921086520110038	0.0000000000000000	F	F	F
0.5743485312849991	0.5167321548318814	0.4138404335694484	T	T	T
0.5686993224120781	0.6487182254176027	0.4956155460121856	T	T	T
0.6182655271823482	0.5378807993153327	0.2699168474664630	T	T	T
0.6182512038408572	0.6632930068145495	0.3527570442788855	T	T	T
0.6189582852425600	0.7887707857006427	0.4354079812153809	T	T	T
0.6189997357064608	0.9227285007761731	0.5197008706540782	T	T	T
0.5738300066441298	0.5175136634034985	0.0827098793239784	F	F	F
0.5741871304732317	0.6415362260944263	0.1655167634601924	T	T	T
0.5743496494939164	0.7661663342315459	0.2482481074510867	T	T	T
0.5743108133629752	0.8917600314643710	0.3310327130753272	T	T	T
0.3838681603647277	0.3458917892793442	0.5294065867550231	T	T	T
0.5634629714140753	0.2556583945640108	0.5854743791205971	T	T	T
0.2500000000000000	0.0746099933052733	0.1245949913851589	F	F	F
0.2499632176519745	0.1998142129263032	0.2072103728793148	T	T	T
0.2499866464626563	0.3246435766575390	0.2898508149473779	T	T	T
0.2500466495142661	0.4494022392889575	0.3723539749881702	T	T	T
0.2500000000000000	0.4492049819127857	0.0418851120611805	F	F	F
0.2504016007592478	0.0752642636199729	0.4542707927434585	T	T	T
0.2452115312693588	0.1975294567622332	0.5347626279304559	T	T	T
0.7500000000000000	0.2951248323472200	0.0091716967570790	F	F	F
0.7500000000000000	0.4205298437397076	0.0918815760810574	F	F	F
0.7512330700825975	0.0452194117223657	0.5065192074616680	T	T	T
0.7499404832719377	0.0441346547579005	0.1744848200832675	T	T	T
0.7498286814807458	0.1684270999790446	0.2572787923354082	T	T	T
0.7497590962470182	0.2934799312612858	0.3400336990356928	T	T	T
0.7496062024751262	0.4188917451752683	0.4229325695478844	T	T	T
0.9406099943444133	0.0054327150181379	0.0365676919062707	F	F	F
0.9406099943444133	0.1308377264106326	0.1192775712302492	F	F	F
0.9392585197042047	0.2552116001596360	0.2019187369436305	T	T	T
0.9392269167015629	0.3797892450291215	0.2845744339138647	T	T	T
0.9396777616760751	0.0046685154112306	0.3669904681970076	T	T	T
0.9406361354615305	0.1307477495253316	0.4487947328719304	T	T	T
0.9405541274488686	0.2459663353510708	0.5305445431867976	T	T	T
0.4406099943444133	0.2388970992418606	0.0144891169119887	F	F	F
0.4406099943444133	0.3643021106343554	0.0971989962359672	F	F	F
0.4394143462669036	0.4889432944062871	0.1800400233083828	T	T	T
0.4392209177551763	0.1137894796795998	0.2627836573138434	T	T	T
0.4392843439765725	0.2389213266464588	0.3456166718427990	T	T	T
0.4394420870869119	0.3650423335572383	0.4285803687936486	T	T	T
0.4426192441871309	0.4982396008476591	0.5126210026468641	T	T	T
0.5593900056555867	0.0054327150181379	0.0365676919062707	F	F	F
0.5593900056555867	0.1308377264106326	0.1192775712302492	F	F	F
0.5605788940131338	0.2551843598378805	0.2019272367798248	T	T	T
0.5604454176609333	0.3797339665028066	0.2845988992950086	T	T	T
0.5606386026958941	0.0044435012343590	0.3673529229408418	T	T	T
0.5603305465587924	0.1302224627468665	0.4500036069653830	T	T	T
0.5739616602830359	0.2480806307046981	0.5323720034355299	T	T	T
0.0593900056555867	0.2388970992418606	0.0144891169119887	F	F	F
0.0593900056555867	0.3643021106343554	0.0971989962359672	F	F	F
0.0605005721376317	0.4889328101657205	0.1800365925197081	T	T	T
0.0605758610800008	0.1138177711437040	0.2627527822864089	T	T	T
0.0606522324594082	0.2390648611141953	0.3454994661766583	T	T	T

0.0609330446051110	0.3657625871760583	0.4282948789173635	T	T	T
0.0602002395199759	0.4935765017947735	0.5126561365869642	T	T	T
0.2500000000000000	0.5746099933052733	0.1245949913851589	F	F	F
0.2499766321524764	0.6998009156208718	0.2071950387918178	T	T	T
0.2500593568089194	0.8245758590222969	0.2898278652848075	T	T	T
0.2504402453415029	0.9491425411909308	0.3723814292288050	T	T	T
0.2500000000000000	0.9492049819127857	0.0418851120611805	F	F	F
0.2490462960435237	0.5755743715591547	0.4542961481918848	T	T	T
0.2495400491330242	0.6989463849259887	0.5352881848816267	T	T	T
0.7500000000000000	0.7951248323472200	0.0091716967570790	F	F	F
0.7500000000000000	0.9205298437397076	0.0918815760810574	F	F	F
0.7522602943606120	0.5462362663934469	0.5068497220963282	T	T	T
0.7499208576068278	0.5441238931706995	0.1744811145090156	T	T	T
0.7497806535743449	0.6684109628687217	0.2572594992716177	T	T	T
0.7496184870367665	0.7936370741854758	0.3399671403859245	T	T	T
0.7496821810901471	0.9193781244763710	0.4228142164746284	T	T	T
0.9406099943444133	0.5054327150181379	0.0365676919062707	F	F	F
0.9406099943444133	0.6308377264106326	0.1192775712302492	F	F	F
0.9392904427038328	0.7552244898221631	0.2019114860304682	T	T	T
0.9393502837796243	0.8798339961192760	0.2845386793255731	T	T	T
0.9393135846525863	0.5047027367697794	0.3670511548914024	T	T	T
0.9397393678438091	0.6303311451829109	0.4489313622715119	T	T	T
0.9396040933875358	0.7459612790912197	0.5307618085888304	T	T	T
0.4406099943444133	0.7388970992418606	0.0144891169119887	F	F	F
0.4406099943444133	0.8643021106343554	0.0971989962359672	F	F	F
0.4393871924120556	0.9889759641434039	0.1800398227905755	T	T	T
0.4392267193645773	0.6138055481972426	0.2627727957809313	T	T	T
0.4392032619199397	0.7393552724584452	0.3456056785193613	T	T	T
0.4390227107714962	0.8665873361017675	0.4287863311663001	T	T	T
0.4418345925097652	0.9941090237129214	0.5136554561819424	T	T	T
0.5593900056555867	0.5054327150181379	0.0365676919062707	F	F	F
0.5593900056555867	0.6308377264106326	0.1192775712302492	F	F	F
0.5605757154222966	0.7552224221031664	0.2019215176414215	T	T	T
0.5604788222829521	0.8797609044934432	0.2846145944437474	T	T	T
0.5604272348065519	0.5046232935068369	0.3671258879832977	T	T	T
0.5597361120936257	0.6307065757914871	0.4490077466290087	T	T	T
0.5623274380782387	0.7465821993569965	0.5308564827147590	T	T	T
0.0593900056555867	0.7388970992418606	0.0144891169119887	F	F	F
0.0593900056555867	0.8643021106343554	0.0971989962359672	F	F	F
0.0605090061195972	0.9889624298231317	0.1800337190986760	T	T	T
0.0605204081359954	0.6137353015243119	0.2627516839406227	T	T	T
0.0604046628188284	0.7390625802229999	0.3454775875997975	T	T	T
0.0602013699549228	0.8654101657631269	0.4282522098738284	T	T	T
0.0600203314784579	0.9913478825837584	0.5122277945955713	T	T	T

**(8) [110+O<sub>N3</sub>]<sub>dis</sub>**

110-on-water-dis

1.0000000000000000		
10.3476600646972994	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.0339593887328995	0.0000000000000010
0.0000000000000000	0.0000000000000000	44.1809380160793026

H N O Ta  
2 139 2 84

Selective dynamics

Direct

0.5354998661852012	0.3747150093350051	0.5883748608714030	T	T	T
0.4343913730758849	0.0927324672058604	0.5708357376529228	T	T	T
0.2500000000000000	0.3293039861898137	0.0059393964048695	F	F	F

0.2500000000000000	0.4547089975823013	0.0886492757288480	F	F	F
0.2526860565000713	0.0979436166524543	0.5003733486345531	T	T	T
0.2499413533565511	0.0801992548063660	0.1713579416872016	T	T	T
0.2499318490012019	0.2058738048031121	0.2540893435491161	T	T	T
0.2500849715186227	0.3313576247108996	0.3368707685052844	T	T	T
0.2496821553281960	0.4554761716245648	0.4196038556526513	T	T	T
0.7500000000000000	0.0404308394626796	0.1278272917373684	F	F	F
0.7498510197798217	0.1636325948162420	0.2106716173225064	T	T	T
0.7496406797191133	0.2883630101355937	0.2935437224462401	T	T	T
0.7494199409794632	0.4137418814545287	0.3765093092210384	T	T	T
0.7500000000000000	0.4150258280701919	0.0451174124133900	F	F	F
0.7507422327561105	0.0406342907150706	0.4601292549110565	T	T	T
0.7591948653540086	0.1840149465711732	0.5403149950981465	T	T	T
0.3805899955332279	0.0811638913835608	0.0294058438053355	F	F	F
0.3805899955332279	0.2065689027760556	0.1121157231293139	F	F	F
0.3815928786890961	0.3307091162849800	0.1947829329697691	T	T	T
0.3815419908140215	0.4557614625842795	0.2775439288510742	T	T	T
0.4252267701243393	0.1024182354607450	0.2166160825624172	T	T	T
0.4252461735698090	0.2275408477429029	0.2994737140637415	T	T	T
0.4253897964925126	0.3531981573299283	0.3823772729415257	T	T	T
0.4235682634302271	0.4786637430622203	0.4657250561699150	T	T	T
0.3813894602015415	0.0813412823298068	0.3604496235484382	T	T	T
0.3825268035077132	0.2059128077387400	0.4427139606468348	T	T	T
0.4261699933558702	0.3522211622490019	0.0510568088182595	F	F	F
0.4261699933558702	0.4776261736414895	0.1337666881422379	F	F	F
0.4209572952114249	0.1207169164066188	0.5489400569052337	T	T	T
0.8805899955332279	0.1631659228764377	0.0216509650129240	F	F	F
0.8805899955332279	0.2885709342689324	0.1043608443369095	F	F	F
0.8814151125817129	0.4135533308842803	0.1871166045313603	T	T	T
0.9261699933558702	0.3921086520110038	0.0000000000000000	F	F	F
0.9245234192153540	0.0169803404109351	0.4135719248070087	T	T	T
0.9297336568827469	0.1551768100517263	0.4946396894992777	T	T	T
0.8813985202748230	0.0384957311397434	0.2698773756402771	T	T	T
0.8814858743988692	0.1639268020923176	0.3525553336202702	T	T	T
0.8813323578282861	0.2898463388874857	0.4347432829621047	T	T	T
0.8838368455058025	0.4232897582843179	0.5197693626027133	T	T	T
0.9261699933558702	0.0175136634034914	0.0827098793239784	F	F	F
0.9257288689799245	0.1417271973697998	0.1655162795955596	T	T	T
0.9252888787960588	0.2666199807541981	0.2482307957920833	T	T	T
0.9248440127847598	0.3921941160660496	0.3309347424533117	T	T	T
0.1194100044667721	0.0811638913835608	0.0294058438053355	F	F	F
0.1194100044667721	0.2065689027760556	0.1121157231293139	F	F	F
0.1182001566311102	0.3307643223811392	0.1948263170566165	T	T	T
0.1180725533777354	0.4558621767858835	0.2775975963987983	T	T	T
0.0746086244394865	0.1024457908147028	0.2166102447591556	T	T	T
0.0745685159407765	0.2278086646302377	0.2993884909552676	T	T	T
0.0743646667262083	0.3539864439530510	0.3820752424586033	T	T	T
0.0744907000647581	0.4799778132670801	0.4656318792016544	T	T	T
0.1181880187520739	0.0815184400146576	0.3603196478465576	T	T	T
0.1184761594517749	0.2068385971106186	0.4417681866652114	T	T	T
0.1259521615109605	0.3427937105238330	0.5260186837509836	T	T	T
0.0738300066441298	0.3522211622490019	0.0510568088182595	F	F	F
0.0738300066441298	0.4776261736414895	0.1337666881422379	F	F	F
0.0771897495573266	0.1231919641214413	0.5473695394840741	T	T	T
0.6194100044667721	0.1631659228764377	0.0216509650129240	F	F	F
0.6194100044667721	0.2885709342689324	0.1043608443369095	F	F	F
0.6184211476247884	0.4135783310351168	0.1871504117336416	T	T	T
0.5738300066441298	0.3921086520110038	0.0000000000000000	F	F	F

0.5738121288030184	0.0182790531405316	0.4147301748343821	T	T	T
0.5723100947232608	0.1504503426131990	0.4978725151688167	T	T	T
0.6182191606399629	0.0385928943825638	0.2699985637079370	T	T	T
0.6180966499165967	0.1643736469982461	0.3532102446464127	T	T	T
0.6184664372312270	0.2911753973630663	0.4368670637659616	T	T	T
0.6172558093209273	0.4208440950865933	0.5189822856052548	T	T	T
0.5738300066441298	0.0175136634034914	0.0827098793239784	F	F	F
0.5741311307053183	0.1417185354181311	0.1655122964612313	T	T	T
0.5742453544879976	0.2666150578143522	0.2482339392024470	T	T	T
0.5742547788520780	0.3921825376045399	0.3309800308295971	T	T	T
0.2500000000000000	0.8293039861898137	0.0059393964048695	F	F	F
0.2500000000000000	0.9547089975823013	0.0886492757288480	F	F	F
0.2508558465931133	0.5945974780518456	0.5006482815707735	T	T	T
0.2499365917596984	0.5803288797334889	0.1713675789790380	T	T	T
0.2499450657886579	0.7060507927069941	0.2541292007058659	T	T	T
0.2502042245450879	0.8312482808747947	0.3369371793456987	T	T	T
0.2505621705609348	0.9552877863866720	0.4195967914498789	T	T	T
0.7500000000000000	0.5404308394626796	0.1278272917373684	F	F	F
0.7498205885586463	0.6634672665278891	0.2107206055169107	T	T	T
0.7494369061782065	0.7884197737409547	0.2936121159665521	T	T	T
0.7488666183272132	0.9145810098674280	0.3765493533812503	T	T	T
0.7500000000000000	0.9150258280701919	0.0451174124133900	F	F	F
0.7503286595918399	0.5415361628784724	0.4598623284862534	T	T	T
0.7505895568736209	0.6866941635713593	0.5397434305375846	T	T	T
0.3805899955332279	0.5811638913835608	0.0294058438053355	F	F	F
0.3805899955332279	0.7065689027760556	0.1121157231293139	F	F	F
0.3816029708744708	0.8307229613367808	0.1948115478403822	T	T	T
0.3814817683583129	0.9558328930566218	0.2775991734790035	T	T	T
0.4252035537142293	0.6023784103577348	0.2166487181322150	T	T	T
0.4253510128188810	0.7276909322475762	0.2995005859300528	T	T	T
0.4259523922195751	0.8539972399245596	0.3823831933831773	T	T	T
0.4235647951531776	0.9775466881028221	0.4663748674570793	T	T	T
0.3815701053210175	0.5812889368883213	0.3603129943179617	T	T	T
0.3819483352701249	0.7068556170339627	0.4423583651653767	T	T	T
0.3814030145024571	0.8427071203781702	0.5300196927024385	T	T	T
0.4261699933558702	0.8522211622490019	0.0510568088182595	F	F	F
0.4261699933558702	0.9776261736414895	0.1337666881422379	F	F	F
0.4255850528863726	0.6183036868477680	0.5471197936904064	T	T	T
0.8805899955332279	0.6631659228764377	0.0216509650129240	F	F	F
0.8805899955332279	0.7885709342689324	0.1043608443369095	F	F	F
0.8813824973686540	0.9135333767985785	0.1871150993329309	T	T	T
0.9261699933558702	0.8921086520110038	0.0000000000000000	F	F	F
0.9250446802023899	0.5170708516153977	0.4135982917759947	T	T	T
0.9293270904622433	0.6535212386372922	0.4951020827620218	T	T	T
0.8813997895041086	0.5385461311648866	0.2699086188033699	T	T	T
0.8812706338535187	0.6642164881759497	0.3527224660759757	T	T	T
0.8809885575903263	0.7905331650290043	0.4352813820950415	T	T	T
0.8834337814082548	0.9239923401534457	0.5205668972874257	T	T	T
0.9261699933558702	0.5175136634034985	0.0827098793239784	F	F	F
0.9256298659981206	0.6418604393176309	0.1655305315718706	T	T	T
0.9250435458119588	0.7668547383220972	0.2482686102077665	T	T	T
0.9245129869723659	0.8923352681462926	0.3309884066518594	T	T	T
0.1194100044667721	0.5811638913835608	0.0294058438053355	F	F	F
0.1194100044667721	0.7065689027760556	0.1121157231293139	F	F	F
0.1181620906752497	0.8307722215207576	0.1948540827011641	T	T	T
0.1180401304830351	0.9559126898884971	0.2776348398775914	T	T	T
0.0746071176480099	0.6024107277263346	0.2166539789668089	T	T	T
0.0745297501089658	0.7277579594555404	0.2994661880999219	T	T	T

0.0744338226543007	0.8540210526430633	0.3821679413893388	T	T	T
0.0747886974260303	0.9799584383427294	0.4655555147187603	T	T	T
0.1180480171062058	0.5813871751804038	0.3603012087709370	T	T	T
0.1178891006617842	0.7066418535045625	0.4418327160802721	T	T	T
0.1248377397801723	0.8392972908447155	0.5252207817202467	T	T	T
0.0738300066441298	0.8522211622490019	0.0510568088182595	F	F	F
0.0738300066441298	0.9776261736414895	0.1337666881422379	F	F	F
0.0756795646780618	0.6244701563590003	0.5476847767149644	T	T	T
0.6194100044667721	0.6631659228764377	0.0216509650129240	F	F	F
0.6194100044667721	0.7885709342689324	0.1043608443369095	F	F	F
0.6184490541332763	0.9135785543292073	0.1871547447658826	T	T	T
0.5738300066441298	0.8921086520110038	0.0000000000000000	F	F	F
0.5738990650893766	0.5167841229659684	0.4137616540586419	T	T	T
0.5685657580088216	0.6479562878026957	0.4955558782990700	T	T	T
0.6182096944341539	0.5385498104230524	0.2699680126770991	T	T	T
0.6182280883772023	0.6640995780739212	0.3528163523816784	T	T	T
0.6190435897090052	0.7893668340684160	0.4353670198688421	T	T	T
0.6198930283803453	0.9190725067439064	0.5197102804751719	T	T	T
0.5738300066441298	0.5175136634034985	0.0827098793239784	F	F	F
0.5742059125764496	0.6418439122490057	0.1655261145192004	T	T	T
0.5743452811741390	0.7669022719856018	0.2482772629996653	T	T	T
0.5742138360113088	0.8929981443680640	0.3311714964389423	T	T	T
0.3823771709783265	0.3412423561748407	0.5269817667221802	T	T	T
0.5686974402793454	0.3011400323131309	0.5792360553849565	T	T	T
0.2500000000000000	0.0746099933052733	0.1245949913851589	F	F	F
0.2499583221991839	0.2001251454270628	0.2071906738478476	T	T	T
0.2500029155896164	0.3252019765147243	0.2898095174880271	T	T	T
0.2499851285291585	0.4501576125592524	0.3722533821744030	T	T	T
0.2500000000000000	0.4492049819127857	0.0418851120611805	F	F	F
0.2500777326685906	0.0763701929003305	0.4540219106682310	T	T	T
0.2412513750344818	0.1988641521372581	0.5343191156847132	T	T	T
0.7500000000000000	0.2951248323472200	0.0091716967570790	F	F	F
0.7500000000000000	0.4205298437397076	0.0918815760810574	F	F	F
0.7476357817471768	0.0476738243758040	0.5064331765452892	T	T	T
0.7499140912163063	0.04444484398497152	0.1744775118248232	T	T	T
0.7497618797921710	0.1690317765937927	0.2572714341699580	T	T	T
0.7496428707797405	0.2941490111713463	0.3400487665176444	T	T	T
0.7494634910549555	0.4195668702544625	0.4229540545031361	T	T	T
0.9406099943444133	0.0054327150181379	0.0365676919062707	F	F	F
0.9406099943444133	0.1308377264106326	0.1192775712302492	F	F	F
0.9391972729292933	0.2554897867788382	0.2019124169091558	T	T	T
0.9390491754831782	0.3803193152006276	0.2845551048902270	T	T	T
0.9397669193484751	0.0055481815078153	0.3669940915893917	T	T	T
0.9408182546351450	0.1318651954120064	0.4486400150483537	T	T	T
0.9403822919786237	0.2469327385255307	0.5301420360009905	T	T	T
0.4406099943444133	0.2388970992418606	0.0144891169119887	F	F	F
0.4406099943444133	0.3643021106343554	0.0971989962359672	F	F	F
0.4393894556536088	0.4892225096067966	0.1800390776730553	T	T	T
0.4391144990360890	0.1143846312240558	0.2627688844106209	T	T	T
0.4392381010707579	0.2394877519940506	0.3455941217935524	T	T	T
0.4396764398530591	0.3646661140894669	0.4285016975522144	T	T	T
0.4409484492000806	0.4952228395641085	0.5119700330088328	T	T	T
0.5593900056555867	0.0054327150181379	0.0365676919062707	F	F	F
0.5593900056555867	0.1308377264106326	0.1192775712302492	F	F	F
0.5605983516896523	0.2554606995262195	0.2019183090831644	T	T	T
0.5605090875410634	0.3802390274003806	0.2845878857962860	T	T	T
0.5606717860432039	0.0056589235416347	0.3678047296814345	T	T	T
0.5611671632119700	0.1325403178532494	0.4519742627148959	T	T	T

0.5831313729461995	0.2569600147853799	0.5366537119798076	T	T	T
0.0593900056555867	0.2388970992418606	0.0144891169119887	F	F	F
0.0593900056555867	0.3643021106343554	0.0971989962359672	F	F	F
0.0604616024128634	0.4892178595750881	0.1800432595157230	T	T	T
0.0604991201705210	0.1144647611310707	0.2627344664224215	T	T	T
0.0604381106135814	0.2400074294930454	0.3454314108958744	T	T	T
0.0608061060234166	0.3671168571890051	0.4281458229640309	T	T	T
0.0595620306395493	0.4949062055391552	0.5123869157721308	T	T	T
0.2500000000000000	0.5746099933052733	0.1245949913851589	F	F	F
0.2499157851364663	0.7001522051639114	0.2072044148474190	T	T	T
0.2499560099033442	0.8252074307297522	0.2898288318019636	T	T	T
0.2503002067920502	0.9501025240132731	0.3723064247208345	T	T	T
0.2500000000000000	0.9492049819127857	0.0418851120611805	F	F	F
0.2487969762564745	0.5766605337016287	0.4539787224747052	T	T	T
0.2494578659112638	0.6976063042870995	0.5352224923253017	T	T	T
0.7500000000000000	0.7951248323472200	0.0091716967570790	F	F	F
0.7500000000000000	0.9205298437397076	0.0918815760810574	F	F	F
0.7528260929051567	0.5474836255672624	0.5063817095100385	T	T	T
0.7498888933280035	0.5444284609210017	0.1744835388143854	T	T	T
0.7496105235021626	0.6690628649484561	0.2572659676554716	T	T	T
0.7490280427326240	0.7947548325376510	0.3399928382911824	T	T	T
0.7477890153713652	0.9213058015674614	0.4228681201035818	T	T	T
0.9406099943444133	0.5054327150181379	0.0365676919062707	F	F	F
0.9406099943444133	0.6308377264106326	0.1192775712302492	F	F	F
0.9392718950152391	0.7555990003723150	0.2019147900712571	T	T	T
0.9393057374275287	0.8804897363799326	0.2845484048862434	T	T	T
0.9389312621431054	0.5054283840547802	0.3670124490074386	T	T	T
0.9390006536591127	0.6316768682534348	0.4487809272700606	T	T	T
0.9385626597557792	0.7466535608735519	0.5307906337260402	T	T	T
0.4406099943444133	0.7388970992418606	0.0144891169119887	F	F	F
0.4406099943444133	0.8643021106343554	0.0971989962359672	F	F	F
0.4393428967918358	0.9893018306442599	0.1800318938814742	T	T	T
0.4392248142993375	0.6143440101579939	0.2627703915726477	T	T	T
0.4392284641681087	0.7401835094672298	0.3455633709417513	T	T	T
0.4394024991318607	0.8676080536541141	0.4286048406947784	T	T	T
0.4450822701252166	0.9894131523201662	0.5128431665539516	T	T	T
0.5593900056555867	0.5054327150181379	0.0365676919062707	F	F	F
0.5593900056555867	0.6308377264106326	0.1192775712302492	F	F	F
0.5605254811051276	0.7556160024354066	0.2019303079303013	T	T	T
0.5604432728695148	0.8805498121050265	0.2846952658457917	T	T	T
0.5604125273844541	0.5052698033260297	0.3670801276759583	T	T	T
0.5591926649681146	0.6310913041857696	0.4488590417146845	T	T	T
0.5624923781526558	0.7434080525653266	0.5311744941082629	T	T	T
0.0593900056555867	0.7388970992418606	0.0144891169119887	F	F	F
0.0593900056555867	0.8643021106343554	0.0971989962359672	F	F	F
0.0604905333918027	0.9893125806034192	0.1800284281718116	T	T	T
0.0603787535073306	0.6142427820624985	0.2627765093544172	T	T	T
0.0600242219273375	0.7396955500838099	0.3455043256059008	T	T	T
0.0594698140231998	0.8664784014344783	0.4282366697807728	T	T	T
0.0581695993064803	0.9899305626219783	0.5122107393301554	T	T	T

(9) [100]<sub>mol</sub>

100-water-mol

1.0000000000000000

10.3178596496581996 0.0000000000000000 0.0000000000000000

0.0000000000000000 10.3475399017334002 0.0000000000000000

0.0000000000000000 0.0000000000000000 26.7222900390625000

H N O Ta



## Selective dynamics

## Direct

0.2001257195433651	0.5043892648889057	0.4986017347446902	T T T
0.2276122097566558	0.6564838754212619	0.5050730628429745	T T T
0.2367299944162369	0.2500000000000000	0.0731099992990494	F F F
0.2349157690585635	0.2509603127818411	0.2192065409788348	T T T
0.2520380375935664	0.2495002472742305	0.3644561081353495	T T T
0.7367299795150757	0.2500000000000000	0.0000000000000000	F F F
0.7348844471086490	0.2503235619502018	0.1472019634483165	T T T
0.7364953678858768	0.2508502409808041	0.2936492130772394	T T T
0.7218169510022707	0.2532850808623737	0.4383101629423805	T T T
0.7632699608802795	0.7500000000000000	0.0731099992990494	F F F
0.7636788132617873	0.7509686190309075	0.2198257175820495	T T T
0.7567893505965017	0.7515628071138589	0.3649083988044167	T T T
0.2632699906826019	0.7500000000000000	0.0000000000000000	F F F
0.2654423239035198	0.7494665600761790	0.1473992834757289	T T T
0.2643417420854862	0.7493237792674304	0.2946428179468351	T T T
0.2734380303823161	0.7622726136476429	0.4403243903825644	T T T
0.9530599713325500	0.1194199994206429	0.0731099992990494	F F F
0.9529409024956031	0.1198037688175962	0.2201944644836719	T T T
0.9499489190797146	0.1184130972442649	0.3694443337019467	T T T
0.6913700103759766	0.0738499984145164	0.0731099992990494	F F F
0.6925623007365824	0.0736544008018305	0.2196205811969991	T T T
0.6838119542325553	0.0724801508144266	0.3655920761115583	T T T
0.4530600011348724	0.1194199994206429	0.0000000000000000	F F F
0.4535139708877628	0.1198326188850356	0.1466853796914321	T T T
0.4538524341180817	0.1197934719494758	0.2902292248527978	T T T
0.4578110386828252	0.1139108301295636	0.4514485765163229	T T T
0.1913699954748154	0.0738499984145164	0.0000000000000000	F F F
0.1925992148622557	0.0743414029331751	0.1470563556561353	T T T
0.1903223884608431	0.0760445008158748	0.2935465986848922	T T T
0.2009939644573311	0.0779802525682394	0.4391678696393648	T T T
0.0469399988651276	0.6194199919700623	0.0731099992990494	F F F
0.0477658221368143	0.6201144899117615	0.2207625873122605	T T T
0.0499840263294499	0.6173998800778506	0.3741688843810243	T T T
0.3086299896240234	0.5738499760627747	0.0731099992990494	F F F
0.3091323219609280	0.5731785261724619	0.2207200552034761	T T T
0.3129101256311134	0.5700413308143376	0.3692957743683625	T T T
0.5469399690628052	0.6194199919700623	0.0000000000000000	F F F
0.5463621798912520	0.6198942864025421	0.1466546585021443	T T T
0.5455684762381675	0.6205345351582953	0.2925855536915264	T T T
0.5438327957105218	0.6228554121345712	0.4477118195024216	T T T
0.8086299896240234	0.5738499760627747	0.0000000000000000	F F F
0.8082719274585364	0.5750043338247613	0.1473305612760853	T T T
0.8105638574087606	0.5758063336665041	0.2943124257265093	T T T
0.7944433270317869	0.5767957017391999	0.4402890054957904	T T T
0.9530599713325500	0.3805799782276154	0.0731099992990494	F F F
0.9532923096799326	0.3813455750984178	0.2210180276868867	T T T
0.9507350060731988	0.3819644209433825	0.3689187154902063	T T T
0.6913700103759766	0.4261499941349030	0.0731099992990494	F F F
0.6919812517914364	0.4276325110182094	0.2195593817721787	T T T
0.6848963806062656	0.4306379375549851	0.3650782725346271	T T T
0.4530600011348724	0.3805799782276154	0.0000000000000000	F F F
0.4533827146976728	0.3806206760953529	0.1467375904776809	T T T
0.4536906867092464	0.3814824970607867	0.2913969037997982	T T T
0.4577091419432681	0.3816863226394614	0.4411446529276697	T T T
0.1913699954748154	0.4261499941349030	0.0000000000000000	F F F

0.1923268934376517	0.4268327570138979	0.1473388298658347	T T T
0.1909682795482178	0.4260311502747574	0.2949025911798569	T T T
0.1921543882217187	0.4024144684448713	0.4427500181194401	T T T
0.0469399988651276	0.8805799484252930	0.0731099992990494	F F F
0.0474652639590716	0.8806327888683428	0.2206930626971235	T T T
0.0479117843487785	0.8812352114176214	0.3701021034383118	T T T
0.3086299896240234	0.9261499643325806	0.0731099992990494	F F F
0.3078294810300805	0.9263870872185680	0.2195756303989765	T T T
0.3116709259306621	0.9312100462878724	0.3645518694023037	T T T
0.5469399690628052	0.8805799484252930	0.0000000000000000	F F F
0.5467019404714856	0.8807093808853851	0.1465089413834293	T T T
0.5466929574589758	0.8812130216236467	0.2913791448249873	T T T
0.5422496934394486	0.8794686901817282	0.4314075047900124	T T T
0.8086299896240234	0.9261499643325806	0.0000000000000000	F F F
0.8082361633982504	0.9256895813473452	0.1472467488989953	T T T
0.8107672303808352	0.9265921832717008	0.2945401680040763	T T T
0.7940251283210622	0.9233221313831520	0.4424678902657191	T T T
0.2653269307746415	0.5699265647769021	0.5115822002069229	T T T
0.8021000027656555	0.2500000000000000	0.0731099992990494	F F F
0.8032129265232473	0.2505924268078128	0.2203626223280544	T T T
0.8017846712885403	0.2505164694200082	0.3685416826163169	T T T
0.3021000027656555	0.2500000000000000	0.0000000000000000	F F F
0.3015703883219508	0.2508106434078461	0.1465249795366796	T T T
0.3036999952074589	0.2515943581174152	0.2907083785817279	T T T
0.3049806387760816	0.2443823199089595	0.4335200436157413	T T T
0.1978999972343445	0.7500000000000000	0.0731099992990494	F F F
0.1984498350481624	0.7492499533646461	0.2211213199379139	T T T
0.1997356173894033	0.7478019616922678	0.3716487464570851	T T T
0.6978999972343445	0.7500000000000000	0.0000000000000000	F F F
0.6985418055599190	0.7500673302524031	0.1466215239902609	T T T
0.6971904163615892	0.7505469147976869	0.2912438702031053	T T T
0.6958146659958446	0.7541727920641352	0.4328837768009977	T T T
0.8665899634361267	0.5594399571418762	0.0731099992990494	F F F
0.8679418466856569	0.5599345060175989	0.2208617074070872	T T T
0.8680842331824982	0.5600503153361568	0.3703062006645774	T T T
0.3665899932384491	0.5594399571418762	0.0000000000000000	F F F
0.3655040349775269	0.5599476345241127	0.1475105389246408	T T T
0.3639472490548451	0.5605163941047446	0.2941676904487008	T T T
0.3748625899172442	0.5546562034882959	0.4402135854567837	T T T
0.1334099918603897	0.0594399981200695	0.0731099992990494	F F F
0.1330228616033012	0.0596190777506903	0.2204199361666414	T T T
0.1337365952545046	0.0593335206501191	0.3691362015941981	T T T
0.6334099769592285	0.0594399981200695	0.0000000000000000	F F F
0.6335503139934604	0.0594478337655406	0.1469470292167603	T T T
0.6333029242468941	0.0595157473005716	0.2913716443873010	T T T
0.6372498672640008	0.0567235898489121	0.4349522875939292	T T T
0.8665899634361267	0.9405599832534790	0.0731099992990494	F F F
0.8676391140736537	0.9406785213887868	0.2205858729611107	T T T
0.8668081947069439	0.9406638721700892	0.3696658284031402	T T T
0.3665899932384491	0.9405599832534790	0.0000000000000000	F F F
0.3664773567413563	0.9410795125739287	0.1468906176797003	T T T
0.3665175336361228	0.9415055614289880	0.2912967103950085	T T T
0.3595456693357635	0.9392373291122416	0.4338932974053530	T T T
0.1334099918603897	0.4405599832534790	0.0731099992990494	F F F
0.1342334092586104	0.4407405255973792	0.2213571974109549	T T T
0.1363198860479270	0.4379770112029810	0.3726995289590522	T T T
0.6334099769592285	0.4405599832534790	0.0000000000000000	F F F
0.6330719729097571	0.4414957122087783	0.1468687695234970	T T T

0.6324066582824779	0.4430180760731158	0.2910902719639566	T T T
0.6455885129132891	0.4362039057378778	0.4345438665181368	T T T

**(10) [100]<sub>dis</sub>**

100-water-dis

1.000000000000000			
10.3178596496581996	0.000000000000000	0.000000000000000	
0.000000000000000	10.3475399017334002	0.000000000000000	
0.000000000000000	0.000000000000000	26.7222900390625000	

H N O Ta

2 70 1 42

Selective dynamics

Direct

0.1286554224563521	0.4248702688095209	0.4726239111728857	T T T
0.3630008802520037	0.5916905554321323	0.5430097381663301	T T T
0.2367299944162369	0.250000000000000	0.0731099992990494	F F F
0.2350095621576267	0.2507261407129095	0.2190991993427237	T T T
0.2552727090826448	0.2513829203478330	0.3642848520690954	T T T
0.7367299795150757	0.250000000000000	0.000000000000000	F F F
0.7346632980795329	0.2499711825840084	0.1470904127922086	T T T
0.7364129677994224	0.2497913871625479	0.2933163240053530	T T T
0.7214503633334152	0.2527898627212777	0.4377632213793198	T T T
0.7632699608802795	0.750000000000000	0.0731099992990494	F F F
0.7635088925689643	0.7508444088797324	0.2195874379195143	T T T
0.7570169402237311	0.7511514927138230	0.3648058091047527	T T T
0.2632699906826019	0.750000000000000	0.000000000000000	F F F
0.2655414893499118	0.7489909429450432	0.1473778327134659	T T T
0.2651465356937250	0.7484550740845024	0.2943858401828688	T T T
0.2812595173011478	0.7589292193048726	0.4393620283281273	T T T
0.9530599713325500	0.1194199994206429	0.0731099992990494	F F F
0.9530707293472988	0.1192589748409333	0.2201394212255247	T T T
0.9505559352444994	0.1174369127013351	0.3694619969545651	T T T
0.6913700103759766	0.0738499984145164	0.0731099992990494	F F F
0.6927932779528355	0.0730055690037985	0.2193915218759249	T T T
0.6850278680116914	0.0711590773278536	0.3652221873206257	T T T
0.4530600011348724	0.1194199994206429	0.000000000000000	F F F
0.4534165344333700	0.1195537170990376	0.1467244477246223	T T T
0.4545676894646665	0.1190229488390499	0.2901223063136948	T T T
0.4596370647597406	0.1134107545645940	0.4510021996569019	T T T
0.1913699954748154	0.0738499984145164	0.000000000000000	F F F
0.1924758331484170	0.0740475404881635	0.1470718048727626	T T T
0.1910082709057277	0.0753850167629890	0.2935904984748259	T T T
0.2045256869595342	0.0758459789755881	0.4383534344379645	T T T
0.0469399988651276	0.6194199919700623	0.0731099992990494	F F F
0.0475047062491821	0.6197008221987421	0.2206813833466613	T T T
0.0489652169202215	0.6163603056953749	0.3740553688009686	T T T
0.3086299896240234	0.5738499760627747	0.0731099992990494	F F F
0.3084979115857341	0.5718286444225387	0.2209763237732143	T T T
0.3084515248891491	0.5679011907679424	0.3696879161175272	T T T
0.5469399690628052	0.6194199919700623	0.000000000000000	F F F
0.5460782294969341	0.6197117883228201	0.1468886782826941	T T T
0.5449388417731631	0.6201257232737717	0.2934904798681774	T T T
0.5471828444114490	0.6224170272361554	0.4520942051926191	T T T
0.8086299896240234	0.5738499760627747	0.000000000000000	F F F
0.8079191241056951	0.5748313181894370	0.1471837248771826	T T T
0.8095815225267853	0.5756619101924030	0.2937383475319872	T T T
0.7945863256317942	0.5757353415681580	0.439335552295615	T T T
0.9530599713325500	0.3805799782276154	0.0731099992990494	F F F

0.9531614625784331	0.3809095268297616	0.2203889679732609	T T T
0.9504899909765636	0.3812667596447519	0.3669890978730846	T T T
0.6913700103759766	0.4261499941349030	0.0731099992990494	F F F
0.6918149138330535	0.4269994727735220	0.2193854553674683	T T T
0.6860979989646906	0.4297551923496855	0.3644124647512810	T T T
0.4530600011348724	0.3805799782276154	0.0000000000000000	F F F
0.4531486795123785	0.3803875298358310	0.1466126494406339	T T T
0.4531130188435522	0.3813062436822388	0.2910293084639518	T T T
0.4562535024164744	0.3836418354615977	0.4361667029408723	T T T
0.1913699954748154	0.4261499941349030	0.0000000000000000	F F F
0.1920399516055952	0.4265336588259004	0.1472255086907736	T T T
0.1891202485199023	0.4244867425589816	0.2947953979939358	T T T
0.1853751768650272	0.3957559462985314	0.4433252939767159	T T T
0.0469399988651276	0.8805799484252930	0.0731099992990494	F F F
0.0478092866153326	0.8800755697844386	0.2205375469462106	T T T
0.0489909777129770	0.8799275929829018	0.3697030544002178	T T T
0.3086299896240234	0.9261499643325806	0.0731099992990494	F F F
0.3077507282370300	0.9256042033974768	0.2194499289487117	T T T
0.3121427194066518	0.9287761134200788	0.3640687123031917	T T T
0.5469399690628052	0.8805799484252930	0.0000000000000000	F F F
0.5465393412228535	0.8804876739541458	0.1462745620927575	T T T
0.5469516721789990	0.8804770460961910	0.2907046173666246	T T T
0.5439714869811126	0.8784854487856779	0.4306761717451998	T T T
0.8086299896240234	0.9261499643325806	0.0000000000000000	F F F
0.8081816484203946	0.9255112072274932	0.1470985420649304	T T T
0.8112587015358961	0.9257385309056186	0.2943021222191723	T T T
0.7953958929216203	0.9221565606392124	0.4425537131286375	T T T
0.3159393410980147	0.5488106286583403	0.5163090523484957	T T T
0.8021000027656555	0.2500000000000000	0.0731099992990494	F F F
0.8032377399377012	0.2501958799239695	0.2200865533832836	T T T
0.8015467206060028	0.2496398579718498	0.3678252461589829	T T T
0.3021000027656555	0.2500000000000000	0.0000000000000000	F F F
0.3017454462643693	0.2503972966685073	0.1464525736284796	T T T
0.3052963553906897	0.2502083226228640	0.2904138711338847	T T T
0.3114495065143398	0.2420032504881919	0.4324852624322735	T T T
0.1978999972343445	0.7500000000000000	0.0731099992990494	F F F
0.1989582006668064	0.7476266683556999	0.2210417964582290	T T T
0.2039831721267070	0.7434718708633796	0.3714913144634235	T T T
0.6978999972343445	0.7500000000000000	0.0000000000000000	F F F
0.6981913466530792	0.7499367275136055	0.1465280115255914	T T T
0.6971119560324828	0.7498454751865625	0.2911247862956749	T T T
0.6972316220994774	0.7537743583284575	0.4332919846140095	T T T
0.8665899634361267	0.5594399571418762	0.0731099992990494	F F F
0.8675746452194367	0.5594415687093125	0.2205688623542555	T T T
0.8657559449087870	0.5598136226669438	0.3699876338745348	T T T
0.3665899932384491	0.5594399571418762	0.0000000000000000	F F F
0.3652501671285019	0.5598544271091495	0.1478238232345644	T T T
0.3630344527447837	0.5604670523319532	0.2958278859584495	T T T
0.3757301229486218	0.5623819044676227	0.4470943213116664	T T T
0.1334099918603897	0.0594399981200695	0.0731099992990494	F F F
0.1330043026042874	0.0590239277095100	0.2203484818708003	T T T
0.1337968161441146	0.0570740506357740	0.3687904701761494	T T T
0.6334099769592285	0.0594399981200695	0.0000000000000000	F F F
0.6335101101778710	0.0591719638963610	0.1468193499969611	T T T
0.6341747118844751	0.0583471681844606	0.2910349855464224	T T T
0.6390568833596867	0.0542785599787173	0.4344438747332657	T T T
0.8665899634361267	0.9405599832534790	0.0731099992990494	F F F
0.8681448141319957	0.9397788459733024	0.2203167582846367	T T T

0.8683839095003003	0.9388948946436936	0.3691977873852826	T T T
0.3665899932384491	0.9405599832534790	0.0000000000000000	F F F
0.3663730119200070	0.9408625376333004	0.1468529027422853	T T T
0.3668458908635854	0.9407922835873672	0.2909756538853768	T T T
0.3597913440825012	0.9377326253574784	0.4333537829401470	T T T
0.1334099918603897	0.4405599832534790	0.0731099992990494	F F F
0.1342069242089253	0.4403852945692697	0.2208157868302568	T T T
0.1333606225304822	0.4401921402379410	0.3695954585109627	T T T
0.6334099769592285	0.4405599832534790	0.0000000000000000	F F F
0.6326918282560423	0.4413689221567947	0.1468052675073690	T T T
0.6315286169987264	0.4429525055769264	0.2908799208684800	T T T
0.6427190387734051	0.4335055422221576	0.4338436937634831	T T T

**(11) [100+O<sub>N3</sub>]<sub>mol</sub>**

100-on-water-mol

1.0000000000000000

10.3178596496581996	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.3475399017334002	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7222900390625000

H N O Ta

2 69 2 42

Selective dynamics

Direct

0.2168768645357723	0.6373887774233908	0.5204416392099079	T T T
0.2060538741935481	0.4920121829330274	0.4992450731112753	T T T
0.2367299944162369	0.2500000000000000	0.0731099992990494	F F F
0.2357600529867218	0.2501945847970599	0.2194983833041498	T T T
0.2497224448754904	0.2493744380506399	0.3647303118152984	T T T
0.7367299795150757	0.2500000000000000	0.0000000000000000	F F F
0.7349420791502047	0.2504262509830071	0.1475734658747251	T T T
0.7364888533549674	0.2510901294050459	0.2943598414476718	T T T
0.7210012972528315	0.2534835282906091	0.4394036737909678	T T T
0.7632699608802795	0.7500000000000000	0.0731099992990494	F F F
0.7637213232177660	0.7499352595606875	0.2199225393920711	T T T
0.7521212008740048	0.7515598545195498	0.3656703691441818	T T T
0.2632699906826019	0.7500000000000000	0.0000000000000000	F F F
0.2652591588321768	0.7497784805331489	0.1475554442118499	T T T
0.2638285316054416	0.7503380994915081	0.2945732119631748	T T T
0.2824275578580375	0.7568347044015791	0.4395917684829324	T T T
0.9530599713325500	0.1194199994206429	0.0731099992990494	F F F
0.9527837971773088	0.1197442260485879	0.2203603759607695	T T T
0.9515668436298006	0.1199493922714501	0.3699338299932818	T T T
0.6913700103759766	0.0738499984145164	0.0731099992990494	F F F
0.6929691315587236	0.0725946341499506	0.2198252342372454	T T T
0.6881643236604966	0.0704669489181273	0.3658599495162217	T T T
0.4530600011348724	0.1194199994206429	0.0000000000000000	F F F
0.4535694502674909	0.1197101924761545	0.1464632725676675	T T T
0.4546847189527244	0.1201288435381588	0.2905840116594088	T T T
0.4615751025379585	0.1247712538664016	0.4400646861394658	T T T
0.1913699954748154	0.0738499984145164	0.0000000000000000	F F F
0.1917888103060954	0.0749567821195617	0.1472020759000418	T T T
0.1893519593625501	0.0757735025481986	0.2943116898988816	T T T
0.2052567148899704	0.0801322302772201	0.4413398582425380	T T T
0.0469399988651276	0.6194199919700623	0.0731099992990494	F F F
0.0477382155650189	0.6198649896345192	0.2204671347988783	T T T
0.0495450798910245	0.6205880795613309	0.3723479559007907	T T T
0.3086299896240234	0.5738499760627747	0.0731099992990494	F F F
0.3085121482135203	0.5724684924487319	0.2204760147695464	T T T

0.3105471885744169	0.5700627078823596	0.3679262648127583	T T T
0.5469399690628052	0.6194199919700623	0.0000000000000000	F F F
0.5465506783159748	0.6196985491248930	0.1465319884129616	T T T
0.5457613898575111	0.6201881331781847	0.2921709602382735	T T T
0.5408160213940343	0.6203545409293976	0.4409128672897761	T T T
0.8086299896240234	0.5738499760627747	0.0000000000000000	F F F
0.8088016011992210	0.5750480868460603	0.1474207863652979	T T T
0.8121214261740680	0.5763992011378526	0.2951407539867369	T T T
0.7915398135350581	0.5774058726020703	0.4421361593507397	T T T
0.9530599713325500	0.3805799782276154	0.0731099992990494	F F F
0.9530270700164440	0.3811509623940161	0.2211108623839704	T T T
0.9503013919240773	0.3844045929654789	0.3702724513665642	T T T
0.6913700103759766	0.4261499941349030	0.0731099992990494	F F F
0.6924134747002754	0.4289800710450756	0.2199303306266528	T T T
0.6835533580404605	0.4322674053268264	0.3659398320520655	T T T
0.4530600011348724	0.3805799782276154	0.0000000000000000	F F F
0.4534296298530432	0.3805937541556628	0.1467371604173045	T T T
0.4537451006607068	0.3812671605638580	0.2915797681656162	T T T
0.1913699954748154	0.4261499941349030	0.0000000000000000	F F F
0.1917007666326275	0.4256804631531468	0.1474746145048584	T T T
0.1906674933606404	0.4247456022042333	0.2949243179109538	T T T
0.2024340790060902	0.4123824554958699	0.4413387510899879	T T T
0.0469399988651276	0.8805799484252930	0.0731099992990494	F F F
0.0475903558395724	0.8806268946981217	0.2203658505351195	T T T
0.0512423873646472	0.8834439584204363	0.3697802895697635	T T T
0.3086299896240234	0.9261499643325806	0.0731099992990494	F F F
0.3077718559652697	0.9277946142895592	0.2196703681736137	T T T
0.3167668270376341	0.9323067654925140	0.3651683988104035	T T T
0.5469399690628052	0.8805799484252930	0.0000000000000000	F F F
0.5468956165334040	0.8806765220094311	0.1466108592788711	T T T
0.5472860078855875	0.8814665589661591	0.2912541265407526	T T T
0.5446828312474457	0.8857974677463747	0.4454611409180844	T T T
0.8086299896240234	0.9261499643325806	0.0000000000000000	F F F
0.8085115087272505	0.9250208092796076	0.1473549249338936	T T T
0.8110269612916955	0.9250242141284032	0.2945649946050519	T T T
0.7991247230649314	0.9225677520039404	0.4409636760697411	T T T
0.4570495864801131	0.3896565171060334	0.4494312093295605	T T T
0.2665439206360642	0.5578825275018137	0.5156044121818837	T T T
0.8021000027656555	0.2500000000000000	0.0731099992990494	F F F
0.8029169264182995	0.2508852227922008	0.2203398878146892	T T T
0.8017590199449215	0.2519256336192864	0.3688669299168051	T T T
0.3021000027656555	0.2500000000000000	0.0000000000000000	F F F
0.3016729784816904	0.2505253175829425	0.1461935780153850	T T T
0.3035287182634313	0.2511315294750995	0.2903883949202019	T T T
0.3066505712387056	0.2430048764576486	0.4330004607897076	T T T
0.1978999972343445	0.7500000000000000	0.0731099992990494	F F F
0.1980747579391816	0.7498975515073312	0.2202670813907049	T T T
0.2006783199957428	0.7509644096232317	0.3687242065128507	T T T
0.6978999972343445	0.7500000000000000	0.0000000000000000	F F F
0.6985393047481993	0.7499431944987061	0.1463305466367187	T T T
0.6972428460531407	0.7508527199720593	0.2911108817888806	T T T
0.6940592184414746	0.7545977664259881	0.4339383539247318	T T T
0.8665899634361267	0.5594399571418762	0.0731099992990494	F F F
0.8673824077172242	0.5600103326442560	0.2205787109423337	T T T
0.8681364159001772	0.5615696551214235	0.3697269400439874	T T T
0.3665899932384491	0.5594399571418762	0.0000000000000000	F F F
0.3661592034273796	0.5600989336026738	0.1470641495756703	T T T
0.3645778922512137	0.5602575032279149	0.2928568675978028	T T T

0.3604726920563210	0.5743748847824210	0.4388086629211996	T T T
0.1334099918603897	0.0594399981200695	0.0731099992990494	F F F
0.1329914135311646	0.0593932235933664	0.2201102620758665	T T T
0.1339513510133248	0.0617878796008211	0.3686963863581115	T T T
0.6334099769592285	0.0594399981200695	0.0000000000000000	F F F
0.6337667979789163	0.0600481396586129	0.1467748568164355	T T T
0.6350425452661368	0.0606329014802037	0.2913534723619138	T T T
0.6443517856351566	0.0628665168911351	0.4351803907973343	T T T
0.8665899634361267	0.9405599832534790	0.0731099992990494	F F F
0.8671946393746258	0.9407189207821516	0.2203814472520016	T T T
0.8671682945325054	0.9402490340300552	0.3697916544683682	T T T
0.3665899932384491	0.9405599832534790	0.0000000000000000	F F F
0.3669963927117407	0.9406059724194812	0.1466536833932237	T T T
0.3682470467914968	0.9422116917387672	0.2909591369688709	T T T
0.3632374366036077	0.9443289472255338	0.4341120572476570	T T T
0.1334099918603897	0.4405599832534790	0.0731099992990494	F F F
0.1338936906957250	0.4409297400824899	0.2209052219828672	T T T
0.1374352427095935	0.4400243924199596	0.3716839927833859	T T T
0.6334099769592285	0.4405599832534790	0.0000000000000000	F F F
0.6334050627004040	0.4405712221362243	0.1467951664738709	T T T
0.6325842077124652	0.4423594135619854	0.2913313741952034	T T T
0.6457639350199520	0.4435043914326081	0.4351009961905124	T T T

**(12) [100+O<sub>N3</sub>]<sub>dis</sub>**

100-on-water-dis

1.0000000000000000

10.3178596496581996	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.3475399017334002	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7222900390625000

H N O Ta

2 69 2 42

Selective dynamics

Direct

0.3668930493249306	0.5967769507170699	0.5425939835008390	T T T
0.1343828969403688	0.4269986404923844	0.4720724252889210	T T T
0.2367299944162369	0.2500000000000000	0.0731099992990494	F F F
0.2357134348012800	0.2505572091077713	0.2193927052916003	T T T
0.2537523373617959	0.2508323318904651	0.3646392805187108	T T T
0.7367299795150757	0.2500000000000000	0.0000000000000000	F F F
0.7344436906036479	0.2501143482960470	0.1474658780949536	T T T
0.7358789743002602	0.2501999860703576	0.2938445625758946	T T T
0.7196901113739420	0.2531284500595346	0.4390798980287089	T T T
0.7632699608802795	0.7500000000000000	0.0731099992990494	F F F
0.7632867746847697	0.7500833795370822	0.2198129907230154	T T T
0.7531661783703599	0.7511724771304706	0.3655698592246563	T T T
0.2632699906826019	0.7500000000000000	0.0000000000000000	F F F
0.2651737904268616	0.7489828038608930	0.1476853713849968	T T T
0.2646632369645353	0.7492192803695356	0.2947415940560557	T T T
0.2844137961940914	0.7573276612042980	0.4391165133875977	T T T
0.9530599713325500	0.1194199994206429	0.0731099992990494	F F F
0.9526717711124896	0.1192046930376255	0.2201917984219866	T T T
0.9502808846122440	0.1179093334658446	0.3695519533267205	T T T
0.6913700103759766	0.0738499984145164	0.0731099992990494	F F F
0.6932033051923789	0.0714482598483752	0.2196036476191659	T T T
0.6869725720090947	0.0691715500758098	0.3657386383089031	T T T
0.4530600011348724	0.1194199994206429	0.0000000000000000	F F F
0.4533740141485382	0.1194133136021202	0.1466677371308462	T T T
0.4547881770141994	0.1194088912749995	0.2904467742771421	T T T

0.4610269071986646	0.1191739843607384	0.4455166090931346	T T T
0.1913699954748154	0.0738499984145164	0.0000000000000000	F F F
0.1917127975244027	0.0747401939753528	0.1472574720468035	T T T
0.1895505246985751	0.0757968778769966	0.2941304096809809	T T T
0.2038139201517355	0.0779959570271943	0.4398088521283323	T T T
0.0469399988651276	0.6194199919700623	0.0731099992990494	F F F
0.0475051269220506	0.6195340237690247	0.2206004535556189	T T T
0.0483853801867878	0.6186262364850947	0.3721470298310956	T T T
0.3086299896240234	0.5738499760627747	0.0731099992990494	F F F
0.3083541193857124	0.5714205059667712	0.2212184847950157	T T T
0.3070198469883168	0.5680585981465262	0.3696332121327491	T T T
0.5469399690628052	0.6194199919700623	0.0000000000000000	F F F
0.5461732802056112	0.6195614905549078	0.1467303230900661	T T T
0.5447915395528986	0.6199571925069199	0.2931461746905325	T T T
0.5434316141839713	0.6178400159402517	0.4494747249645374	T T T
0.8086299896240234	0.5738499760627747	0.0000000000000000	F F F
0.8084874582647767	0.5751286307802395	0.1472912634066963	T T T
0.8103861614339153	0.5759461448864271	0.2945405641894395	T T T
0.7923450082837474	0.5740252552778535	0.4403672581378203	T T T
0.9530599713325500	0.3805799782276154	0.0731099992990494	F F F
0.9528482697094284	0.3807788236645973	0.2204886745337839	T T T
0.9504061734330254	0.3822741395444589	0.3689313210852269	T T T
0.6913700103759766	0.4261499941349030	0.0731099992990494	F F F
0.6922361085484672	0.4286561553261932	0.2196137870489768	T T T
0.6844904202345710	0.4309014846949288	0.3649646197142188	T T T
0.4530600011348724	0.3805799782276154	0.0000000000000000	F F F
0.4530643793933903	0.3804001558950387	0.1466682646905421	T T T
0.4529705982313790	0.3812290660550635	0.2915139463471297	T T T
0.1913699954748154	0.4261499941349030	0.0000000000000000	F F F
0.1914545765283594	0.4259549383158168	0.1474341439974197	T T T
0.1884453290963045	0.4235851147778973	0.2951321066510624	T T T
0.1968575577799170	0.4063967549007308	0.4433856493041749	T T T
0.0469399988651276	0.8805799484252930	0.0731099992990494	F F F
0.0476917754480433	0.8801090952281259	0.2204927504184993	T T T
0.0502747523653643	0.8811911976799085	0.3694926815624588	T T T
0.3086299896240234	0.9261499643325806	0.0731099992990494	F F F
0.3075453211298131	0.9265897468354700	0.2196348151820448	T T T
0.3143863733266777	0.9303049611640049	0.3645047543400537	T T T
0.5469399690628052	0.8805799484252930	0.0000000000000000	F F F
0.5466254659574306	0.8804295681678532	0.1462922003347153	T T T
0.5471261732385748	0.8808029386366423	0.2906832075992438	T T T
0.5443248875645139	0.8806108785138002	0.4379986340958010	T T T
0.8086299896240234	0.9261499643325806	0.0000000000000000	F F F
0.8085406077028303	0.9247202371954580	0.1472288822759850	T T T
0.8111815512808410	0.9244900517834695	0.2945990567800302	T T T
0.7976855737440580	0.9213431095047177	0.4421303625172146	T T T
0.4561709626561927	0.3853801363602044	0.4388247750965830	T T T
0.3158954877202306	0.5537211578549633	0.5170085511708559	T T T
0.8021000027656555	0.2500000000000000	0.0731099992990494	F F F
0.8027918597161351	0.2501802736879398	0.2200538768117874	T T T
0.8004314752809768	0.2499511201700187	0.3681029163132425	T T T
0.3021000027656555	0.2500000000000000	0.0000000000000000	F F F
0.3018726081309132	0.2501525261416950	0.1461949074842713	T T T
0.3048256762671205	0.2496592882413109	0.2901728650098043	T T T
0.3089377490552418	0.2374606540056986	0.4324371241973843	T T T
0.1978999972343445	0.7500000000000000	0.0731099992990494	F F F
0.1986863204580857	0.7481458628874083	0.2204339059546608	T T T
0.2037172906478364	0.7455232092711243	0.3692849498753577	T T T



0.6978999972343445	0.7500000000000000	0.0000000000000000	F F F
0.6981938215154517	0.7498342839122092	0.1462004329784070	T T T
0.6967528385331876	0.7501683151885338	0.2909855790027097	T T T
0.6953587448114298	0.7541011136822828	0.4340300036574899	T T T
0.8665899634361267	0.5594399571418762	0.0731099992990494	F F F
0.8670085699566735	0.5594561453417871	0.2203085864781665	T T T
0.8659556446627374	0.5597216985672081	0.3694464919433261	T T T
0.3665899932384491	0.5594399571418762	0.0000000000000000	F F F
0.3658785170079155	0.5600464728350558	0.1474285839525362	T T T
0.3638034069514866	0.5600404796610142	0.2949151884221164	T T T
0.3643590263372041	0.5740591832044512	0.4465561105852480	T T T
0.1334099918603897	0.0594399981200695	0.0731099992990494	F F F
0.1326186246722698	0.0587220234150041	0.2200293060887473	T T T
0.1322944231727480	0.0585536538312097	0.3681965503893752	T T T
0.6334099769592285	0.0594399981200695	0.0000000000000000	F F F
0.6338155788578236	0.0598889936033669	0.1466744466518554	T T T
0.6352744837768186	0.0598864702277177	0.2910819831711322	T T T
0.6444122619569768	0.0584624950344498	0.4349702920082071	T T T
0.8665899634361267	0.9405599832534790	0.0731099992990494	F F F
0.8673144081421581	0.9397665089148750	0.2201281086546654	T T T
0.8674835485931692	0.9376740252319974	0.3691904310851905	T T T
0.3665899932384491	0.9405599832534790	0.0000000000000000	F F F
0.3668881730516950	0.9404551151835764	0.1466130530150137	T T T
0.3680253535624340	0.9412788030795658	0.2906931409461846	T T T
0.3618755988635410	0.9401229036226196	0.4332877363562246	T T T
0.1334099918603897	0.4405599832534790	0.0731099992990494	F F F
0.1338640456764510	0.4406001681672463	0.2204171457921202	T T T
0.1348321324756557	0.4419617325106443	0.3689165211309151	T T T
0.6334099769592285	0.4405599832534790	0.0000000000000000	F F F
0.6330228256364985	0.4403066716645010	0.1466437329273744	T T T
0.6318767233909426	0.4421592299558829	0.2908271928194586	T T T
0.6452580119618631	0.4385621563081582	0.4341037179259938	T T T