

Supporting Information

Redox-active Ligand Controlled Selectivity of Vanadium Oxidation on Au(100)

Christopher D. Tempas,^a Tobias W. Morris,^a David L. Wisman,^{a,b} Duy Le,^c Naseem U. Din,^c Christopher G. Williams,^a Miao Wang,^d Alexander V. Polezhaev,^a Talat S. Rahman,^{c,e} Kenneth G. Caulton,^{a,*} and Steven L. Tait^{a,d,*}

^a Department of Chemistry, Indiana University, Bloomington, IN 47401

^b NAVSEA Crane, Crane, IN 47522

^c Department of Physics, University of Central Florida, Orlando, FL

^d Department of Physics, Indiana University, Bloomington, IN 47401

^e Donostia International Physics Center (DIPC), 20018 San Sebastian, Spain

* E-mail: caulton@indiana.edu, tait@indiana.edu

Contents:

<i>S1. Experimental Procedures</i>	3
<i>S2. Computational details</i>	3
<i>S3. XPS Background Subtraction</i>	5
<i>S4. C and N 1s XPS Data for V-DPTZ + O₂</i>	6
Figure S1. N 1s XP spectra	6
Figure S2. N 1s XP spectra	6
<i>S5. Vanadium Deposited in an Oxygen Environment</i>	7
Figure S3. V 2p and O 1s XP spectrum	7
Figure S4. V 2p and O 1s XP spectrum	8
<i>S6. Alternative V 2p peak fitting for V-DPTZ + O₂</i>	9
Figure S5. V 2p XP spectrum	9
<i>S7. Alternative V 2p XPS Peak Fitting for V + O₂</i>	10
Figure S6. V 2p XP spectrum	10
<i>S8. V 2p_{3/2} Binding Energy Comparison</i>	11
Table S1. Binding energies and oxidation states of V species	11
<i>S9. 350 °C Anneal on V-DPTZ + O₂</i>	12
Figure S7. O 1s and V 2p XP spectrum	12
Figure S8. STM images	13

<i>S10. O₂ Exposures at Room Temperature</i>	13
Figure S9. O 1s and V 2p XP spectra and STM images	13
Figure S10. O 1s and V 2p XP spectra and STM images	14
<i>S11. Additional HREELS Data and Analysis</i>	15
Figure S11. HREELS of V + O ₂	15
Figure S12. HREELS of V-DPTZ	16
Figure S13. HREELS of V-DPTZ	16
<i>S12. References</i>	17
<i>S13. Coordinate of structures in Fig. 6</i>	19

Section S1. Experimental Procedures

All experiments were performed in a pristine ultra-high vacuum (UHV) system ($< 5 \times 10^{-10}$ Torr). One chamber contains the STM system (SPM UHV 750, RHK Technologies). A separate but connected chamber contains the ability to perform XPS (electron energy analyzer PHOIBOS 150 and Mg/Al dual anode X-ray source XR-50, SPECS GmbH). Due to the fact that the chambers are all interconnected, including the chamber for sample preparation, the sample remains free of contamination between preparation and each analysis step.

The gold (100) single crystal surface (Princeton Scientific) was prepared by repeated cycles of argon ion sputtering at a sample temperature of 200 °C and thermal annealing at 500 °C. This surface undergoes a spontaneous reconstruction, which is well characterized.¹⁻³ Vanadium (99.8% pure rod, Goodfellow) was vapor deposited onto the surface using an electron beam evaporator (QUAD-EV-S Mini e-beam Evaporator, Mantis Deposition Ltd.). Dipyrindyltetrazine (DPTZ, 96%) was purchased from Sigma-Aldrich. It was degassed for several hours in a quartz crucible in UHV at temperatures between 90-100 °C and was then vapor deposited from a Knudsen-type evaporator in UHV at 100 °C.

O₂ gas (Airgas, 99.8 % purity, zero grade) was leaked into the preparation chamber up to a maximum chamber pressure of 1.0×10^{-5} Torr. O₂ exposures are reported in units of Langmuir (L) and were in the range of 1 - 3000 L. After the O₂ exposure, the chamber took approximately 15 minutes to pump down to $\sim 2 \times 10^{-9}$ Torr. The sample was then transferred to the adjacent chambers to perform STM and XPS analyses. In some cases, as noted, the surface was heated at a temperature of 190 °C during O₂ exposure.

The STM images were all acquired at room temperature using tunneling currents between 0.1 and 0.3 nA and bias voltages of 1.0 to 1.5 V. The tungsten STM tips were prepared by electrochemical etching.⁴ The microscope was calibrated using images of terephthalic acid on Cu(100), which has been well characterized.^{5,6} Image analysis was performed using the WSxM software.⁷ Specifically, images were prepared using global plane subtractions and/or line-by-line linear flattening with no filtering.

All XPS data were calibrated in energy to the Au 4f_{7/2} peak (84.0 eV) and normalized to the height of that peak to account for variation in the photon intensity and analyzer sensitivity. The O 1s and V 2p peak features (530-500 eV BE) sit on the shoulder of the Au 4p_{3/2} feature (547 eV). Therefore, a careful background subtraction was made for those data based on a background recorded for clean Au. More information about this procedure can be found in the ESI.

All HREELS experiments were performed in a separate UHV system with a double-pass 127° angle cylindrical deflection electron spectrometer (LK Technologies, model LK 2000) operated at an initial beam energy of 5.5 eV and a peak width of 58 ± 7 cm⁻¹. This UHV system is equipped with the same deposition equipment described above. Each HREEL spectrum was normalized by the average intensity of a featureless background region to account for differences in initial

beam current. Full range scans ($150\text{-}3500\text{ cm}^{-1}$) were normalized by the average intensity of the flat background region from $3693\text{-}3723\text{ cm}^{-1}$. The higher resolution scans for the out-of-plane and in-plane ring modes ($550\text{-}2000\text{ cm}^{-1}$) and the V nanoparticle spectra ($200\text{-}2000\text{ cm}^{-1}$) were normalized to the $1920\text{-}1950\text{ cm}^{-1}$ region.

Section S2: Computational details

Spin-polarized density functional theory (DFT) simulations were performed for gas phase V-DPTZ metal-organic networks and for that on the hexagonal reconstructed Au(100) surface using the Vienna Ab-initio Simulation Package (VASP)⁸⁻⁹ employing the projector-augmented wave (PAW)¹⁰⁻¹¹ and plane wave basis set methods. We used DFT-D3¹² corrections for accounting the van der Waals interactions. Note that comparison between results obtained by DFT-D3 corrections and that by the more computationally expensive optB88-vdW¹³⁻¹⁴ functional does not show any significant difference for the V-DPTZ structure without the Au substrate. Inclusion of the Au substrate makes the system computationally challenging for application of optB88-vdW with spin-polarized simulations. Thus, we opt to use DFT-D3 correction for this work. We set the energy cutoff for plane-wave expansion at 500 eV. We model the reconstructed Au(100) surface with a 5-layer Au(100) slab with the top layer configured to resemble that of Au(111) to account for its (5×1) hexagonal reconstruction. Specifically, to construct reconstructed Au(100) slab, we first optimized the unreconstructed $(1\times 5\times 5)$ Au(100) slab on top of which we placed a $(1\times 6\times 1)$ Au(100) layer and a vacuum of $\sim 15\text{ \AA}$. The topmost of the relaxed structure of the resultant slab, referred herein as reconstructed $(1\times 5\times 5)$ Au(100) slab. For the system consisting of the DPTZ ligands and V adatoms on the Au(100) surface, our supercell consists of 3 V atoms, 3 DPTZ ligands, and reconstructed $(9\times 5\times 5)$ Au(100) slab. Because of the similarity between the experimental observation of Pt-DT on Au(100)¹⁵ and V-DPTZ on Au(100), we adapt the lowest energy structure of Pt-DT on Au(100)¹⁶ and replace Pt by V. All together, we thus have 360 atoms in the supercell. Given the large number of atoms in the supercell, we sampled the Brillouin Zone only at the Γ point, for computational feasibility. During relaxation, the bottom two Au layers are held fixed. All structures are relaxed until all component acting on each ion reach a threshold of $0.01\text{ eV/\AA}$.

For V-DPTZ chain on the hexagonal reconstructed Au(100) surface, because of the commensurateness between V-DPTZ chain and the Au(001) surface and of the computational feasibility, each supercell contains 3 V-DPTZ units, making the modeling of antiferromagnetic configuration of V atoms impossible. Thus, for simulating the V-DPTZ chain on Au(001) surface, antiferromagnetic configurations are assumed. It is worth noting that the difference in energy between antiferromagnetic and ferromagnetic configurations is small (see in the main text), suggesting that the outcome should not be affected by this magnetic constraint.

Section S3. XPS Background Subtraction

In order to obtain the correct peak intensities for oxygen and vanadium on the Au(100) surface, a background subtraction of the XPS data must be performed. This is due to the fact that the Au $4p_{3/2}$ (547 eV) peak is close enough to the O 1s and V 2p photoelectron peaks (542-505 eV) that the lower binding energy side of the Au $4p_{3/2}$ feature is the predominate background feature for both O 1s and V 2p. Using an XP spectrum for this region (542-505 eV) on clean Au(100), a background subtraction was performed such that the resulting spectra were flat on both sides of the region. Once this procedure was performed, the correct peak areas for O 1s and V 2p could be determined. Au 4f intensities were compared between experiments in case of detector intensity changes. XPS spectral analysis was performed using the SpecsLab2 and CasaXPS software packages.

Section S4. N 1s XPS Data for the V-DPTZ + O₂ Experiments

Here is the N 1s XPS data for two different oxygen exposure experiments that were performed, at room temperature (Figure S1) and at 190 °C (Figure S2), on the V-DPTZ/Au(100) surface. These results show that the interaction of O₂ with the V-DPTZ chains does not chemically alter the DPTZ ligand as the N 1s peak does not change.

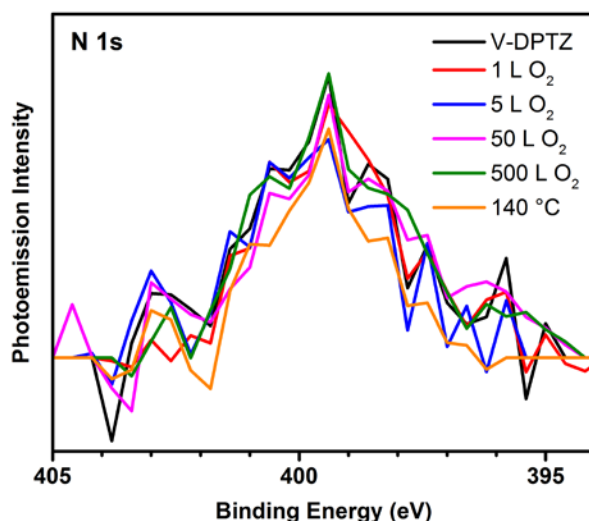


Figure S1. N 1s XP spectra from before and after a series of O₂ exposures performed while holding the surface at room temperature, as labeled on the graph. They show that the N 1s peak is unaffected by the reaction with O₂.

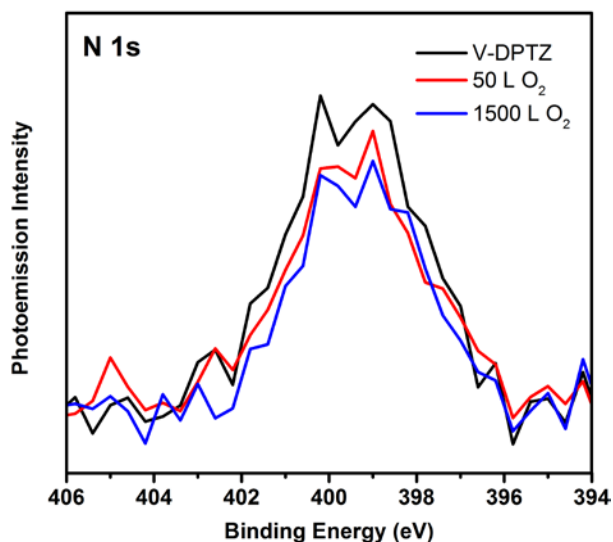


Figure S2. N 1s XP spectra from before and after oxygen exposures while holding the surface at 190 °C, as labeled in the graph. As with the room temperature exposures, the peak remains unchanged by exposure to O₂.

Section S5. Vanadium Deposited in an Oxygen Environment

In order to form an oxide on the Au(100) surface where the V is completely oxidized, an experiment was performed where V was deposited in an oxygen background. Oxygen was leaked into the chamber up to a pressure of 1.0×10^{-6} Torr and then the V was deposited. The surface was held at room temperature during this process. This resulted in the formation of an oxide on the surface. Based on atomic ratios from XPS, the O:V ratio was 1.7. This ratio, in combination with the V $2p_{3/2}$ peak position at 515.2 eV showing V^{III}, indicates that V₂O₃ was formed on the surface (Figure S4). After annealing at 350 °C for 20 minutes, the O:V ratio and V $2p_{3/2}$ peak position do not change significantly, being 1.6 and 514.9 eV respectively (Figure S5). This shows that V₂O₃ remains on the surface.

These results are in contrast with the sequential experiments, where V was deposited onto the surface first, which was then exposed to O₂. They show that when V has the opportunity to bond with itself in nanoislands, it becomes less reactive. They also verify the accuracy of the XPS atomic ratios presented in this paper, as 1.7 and 1.6 are close to the theoretical value of 1.5 for O:V in V₂O₃.

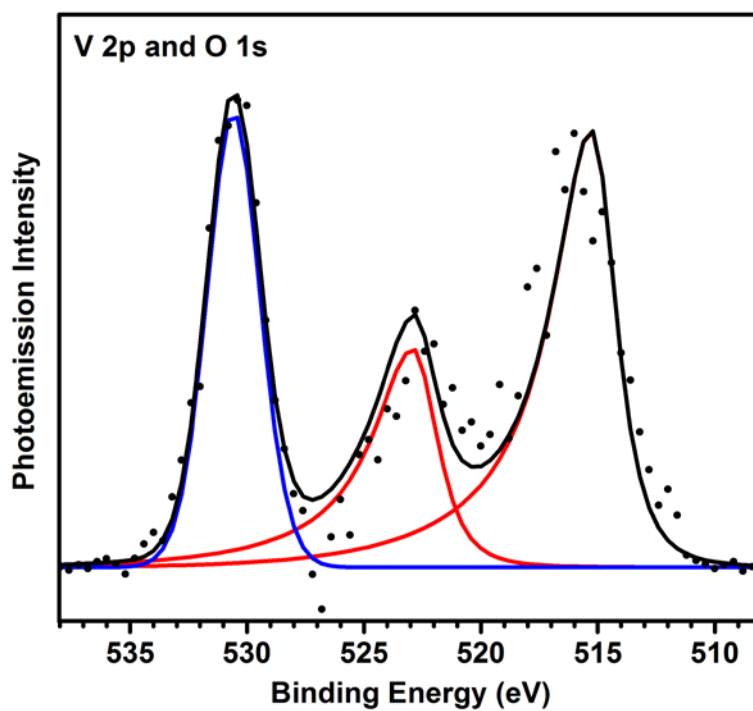


Figure S3. XP spectrum showing the V 2*p* and O 1*s* regions, where V 2*p* has been fit with a set of components representing V^{III}.

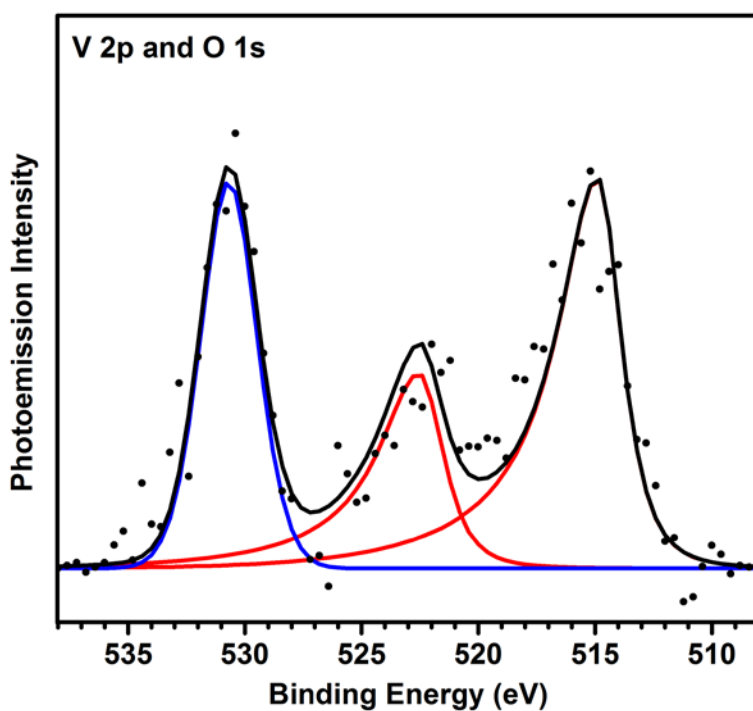


Figure S4. XP spectrum showing the V 2*p* and O 1*s* regions after annealing the surface at 350 °C.

Section S6. Alternative V 2p peak fitting for V-DPTZ + O₂

An additional set of components has been added to the data shown in Figures 3b and 3c of the main paper. These fits help to clarify that at the intermediate state of the oxidation reaction shown in Figures 3b and S5a, there is more than one oxidation state of V present. In Fig. 3b, this is represented as a wider component width in the fitting. In Figure S5a, the new components do not significantly improve the quality of the fit compared to Fig. 3b. In Figure S5b, the FWHM of the V 2p peaks is 3.0 eV, the same as the data before O₂ exposure (Figure 3a). The intensity of the added component is relatively insignificant and does not change the overall fit, indicating that at this point of the reaction, there is a single oxidation state of V.

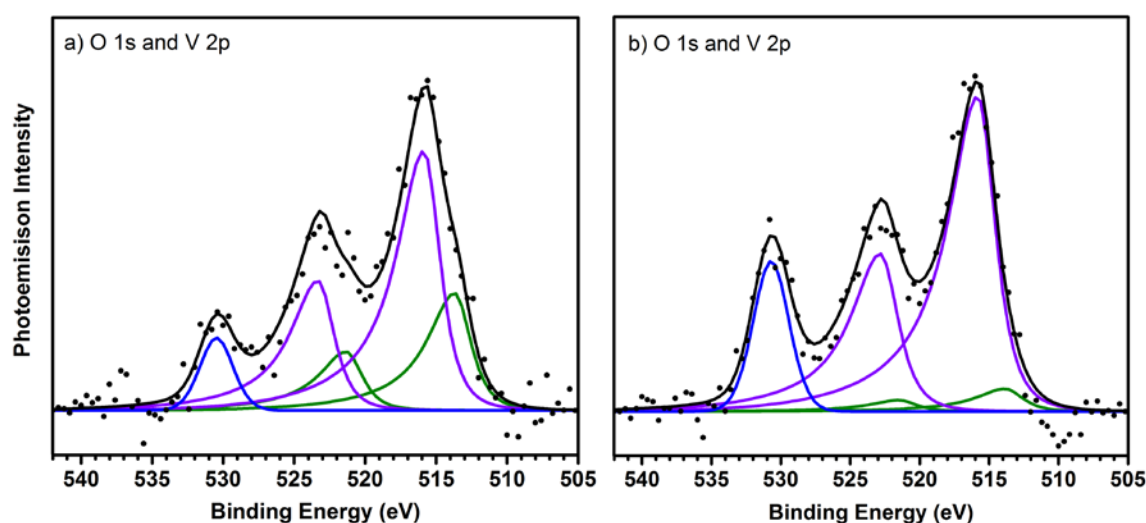


Figure S5. Alternative fit models for XP spectra showing the reaction of O₂ with V-DPTZ chains on Au(100) while holding the surface at 190 °C (Figures 3b and 3c). (a) Data from Figure 3b with a second set of components to represent an additional oxidation state of V. The peak widths here are comparable to the experiments before oxidation. Note that the overall fit quality is not better than in Fig. 3b, which has fewer components but at wider widths. (b) Data from Figure 3c with a second set of V 2p components, but these have such a small intensity that they do not impact the fitting in a significant way..

Section S7. Alternative V 2p Peak Fitting for V + O₂

Here, an additional set of components has been added to the XP spectrum presented in Figure 1c of the main paper. This illustrates the possibility of two oxidation states of V present on the surface, in this case V⁰ (512.8 eV) and V^{III} (515.0 eV). This graph shows that it is indeed likely that more than one oxidation state of V is present.

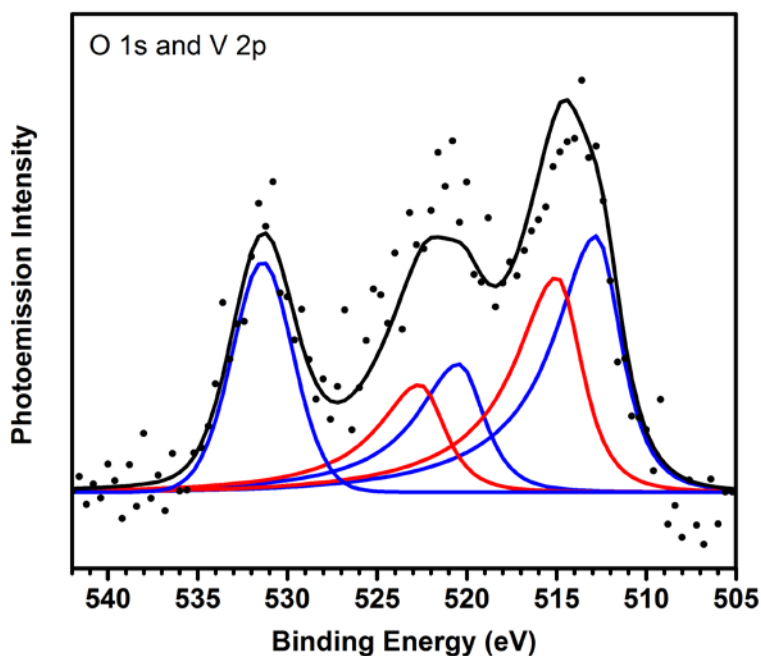


Figure S6. The O 1s and V 2p XP spectra shown here is the same data presented in Figure 1c with an additional set of components. The new fit shows V⁰ and V^{III} present. The fits for V⁰ and V^{III} are shown in blue and red respectively.

Section S8. V $2p_{3/2}$ Binding Energy Comparison

Table S1. Binding energies of V species and their oxidation states. The first five columns of binding energy data show reference data, while the sixth column is data collected for this paper.

V Oxidation State	Binding Energy (eV) ¹⁷	Binding Energy (eV) ¹⁸	Binding Energy (eV) ¹⁹	Binding Energy (eV) ²⁰	Binding Energy (eV) ²¹	Binding Energy (eV) (this work)
0	512.8	512.7	512.6	512.4	512.1	512.7
+2	N/A	513.8	N/A	513.7	N/A	513.8
+3	515.0	514.7	N/A	515.3	515.5	514.9-515.2
+4	516.4	N/A	516	515.8	516.1	515.8

In Table S1, we see the binding energy (BE) trends of V $2p_{3/2}$ as its oxidation state is increased. From this, we can see that the data presented in this paper is very consistent with data collected in previous papers. In most cases, V^{II} data is not available for comparison, but the BE values for V^{III} and V^{IV} are consistent with what we see, as well as the one V^{II} value that was available in addition to our previous work.²⁰ The BE shift from V^{III} to V^{IV} is not always consistent in magnitude, but the BE values are still generally consistent within a few tenths of an eV.

Section S9. Thermal Stability

A high temperature 350 °C annealing treatment was also performed to further test the thermal stability of the oxidized species. In these experiments, there was significant desorption of the ligand, resulting in a shift in the V 2p peaks to lower BE (514.6 eV), signifying a lower oxidation state (Figure S7). The FWHM of the V 2p peaks increases by nearly one eV, indicating that more than one oxidation state of V is present on the surface, *i.e.*, reduction of a significant fraction of the V. Between the beginning of the experiment and the final 350 °C annealing step, the carbon 1s and nitrogen 1s XPS peak areas both decrease by 60 %, showing that most, but not all, of the DPTZ ligand on the surface has either desorbed or decomposed. The oxygen intensity decreased by 30 %. The loss of some O₂ and much of the ligand explains the lower BE of the V, as there are less oxidants present on the surface. The loss of neutral DPTZ from the (DPTZ²⁻)V^{IV}O species is a redox process, where the departing DPTZ returns its two electrons to vanadium before leaving as a neutral molecule. STM experiments show that, after annealing at 350 °C, most of the 1D chains are gone from the surface and that nanoparticle features are now present (Figure S8), similar to those observed above after the same annealing step was performed after exposing just V on the surface to O₂. This provides microscopic and spectroscopic evidence for the formation of 3D metal-oxide nanoparticles.

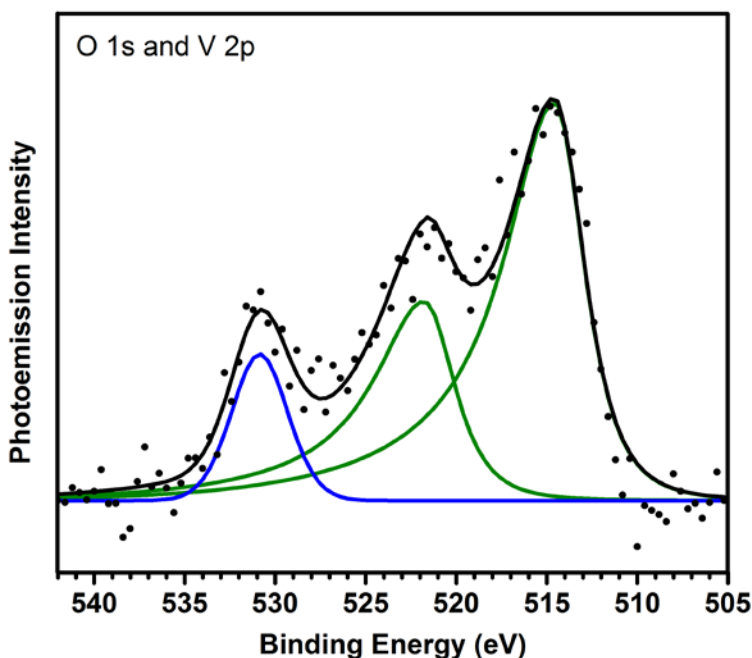


Figure S7. XP spectra of the V-DPTZ/Au(100) surface after being exposed to 1500 L O₂ with the surface held at 190 °C and then annealed at 350 °C for 20 minutes.

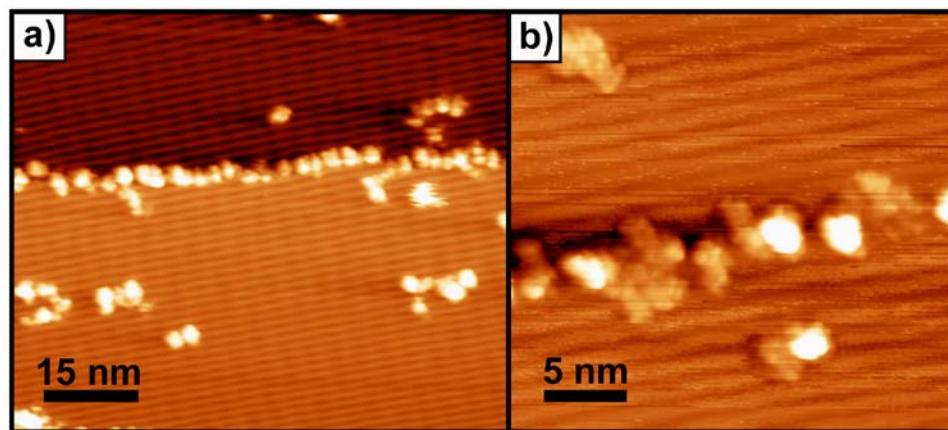


Figure S8. STM images showing the nanoparticles that form on the surface after annealing at 350 °C for 20 minutes.

After annealing the V + O₂ (room temperature) surface at 350 °C for 20 minutes, the FWHM of the V 2*p* peaks decreased to nearly the same peak width as metallic V, suggesting that the V on the surface is now mostly, if not all, in the same oxidation state (Figure S14d). The V 2*p*_{3/2} peak position shifted slightly to 513.5 eV, which is very similar to the peak position for V^{II} (513.8 eV),¹⁸ indicating the formation of VO_{*x*} particles, where *x* is close to 1. The average height of the particles also increases slightly through the annealing steps, and after the 350 °C annealing step the average height of the particles is 5.0 ± 0.7 Å (Figure S14g). This sintering is the expected behavior of nanoparticles after annealing.²²

Section S10. O₂ Exposures at Room Temperature

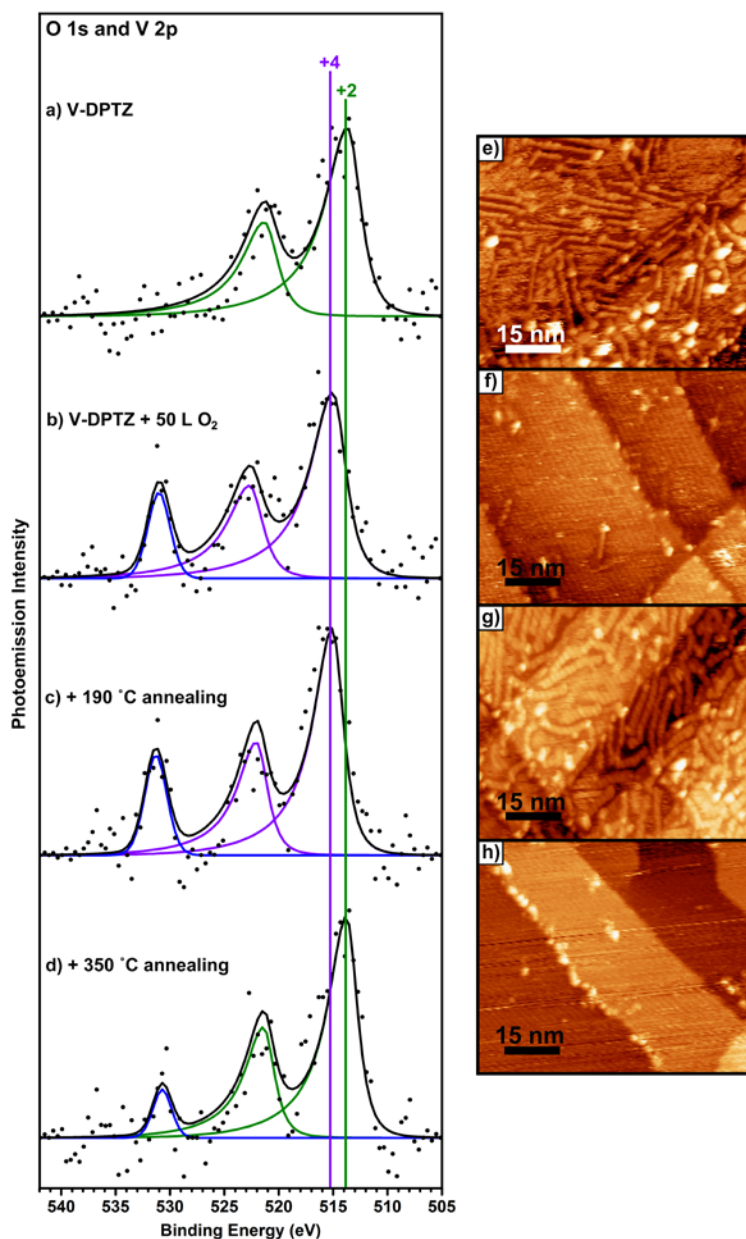


Figure S9. XP spectra and STM images showing the reaction of O₂ with V-DPTZ chains on Au(100) at room temperature. V oxidized to +2 is shown in (a) before the addition of O₂ with a typical STM image showing the 1D chains in (e). XPS of V 2p and O 1s after a 50 L O₂ exposure is shown in (b), with the corresponding STM image in (f). In (c), the surface was annealed for 20 minutes at 190 °C, with the corresponding STM image in (g). Further annealing at 350 °C for 20 minutes was performed with the XPS shown in (d) and the STM in (h). The vertical green and purple lines indicate the V 2p_{3/2} positions for the +2 and +4 oxidation states respectively.

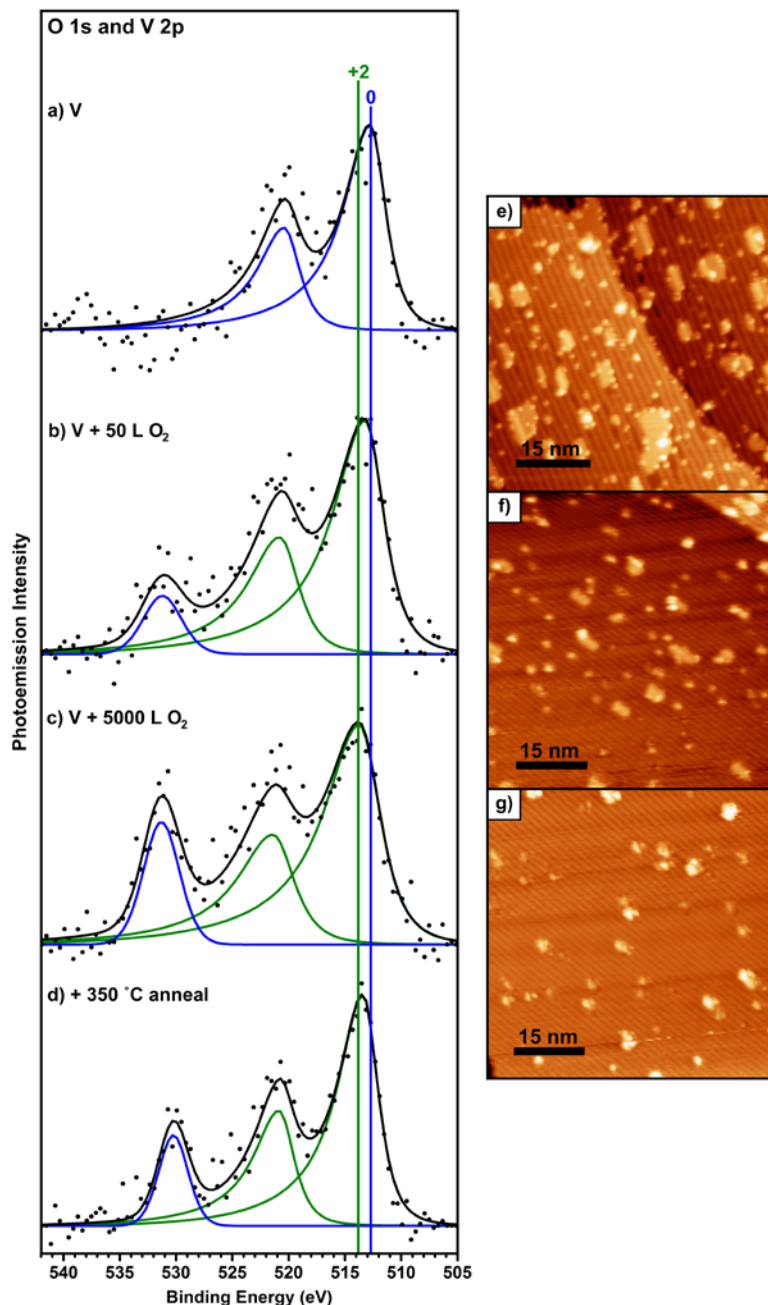


Figure S10. XP spectra and STM images showing the reaction of O_2 with V metal deposited on the Au(100) surface. (a) XPS of metallic V with (e) representative STM image of V islands. (b) After 50 L O_2 exposure (on a different V/Au(100) surface), an O 1s component is clearly observed along with a shift in the V peak position. (c) After 5000 L of O_2 , those changes continue and (f) corresponding STM images show oxidation at the edges of the V nanoislands. (d) After annealing at 350 °C, V XPS peaks sharpen, indicating a single oxidation state and (g) STM imaging shows fewer, but larger nanoparticles. The vertical blue and green lines drawn through the XPS data show the positions of the V oxidation states of 0 and +2, respectively.

Section S11. Additional HREELS Data and Analysis

To observe the difference in O₂ adsorption on different V species, O₂ was exposed to both the Au(100) surface with co-deposited DPTZ with equimolar V (Figure 4) and a Au(100) surface with only V deposited equal to the amount of V used in the V-DPTZ co-deposition experiment (Figures 2 and S16). For both experiments the O₂ exposure was done with the surface held at 190 °C to preserve the V-DPTZ chains. The initial deposition of DPTZ on Au(100) gave the expected peaks matching our previous paper²³ with the out-of-plane modes in the 300-900 cm⁻¹ region, the in-plane modes in the 900-2000 cm⁻¹ region, and the C-H stretching peaks located 2800-3300 cm⁻¹ (Figure S16). Metal complexation with V caused several peak shifts such as the pyridyl out-of-plane deformation peak from 589 to 640 cm⁻¹, the C-H bending mode from a doublet at 736 and 787 cm⁻¹ to a single peak at 758 cm⁻¹, and several peak shifts within the in-plane modes. It was also observed that the intensity of these peaks changed with the out-of-plane modes decreasing in intensity, the in-plane modes increasing in intensity (particularly the 1400-1600 cm⁻¹ region), and the C-H stretching mode increasing in intensity. All of these observed changes are expected for the redox formation of a metal DPTZ complex as previously observed.²³ These peak positions are unique from the Pt and Ag DPTZ complexes reported in that paper as the chemical identity of the metal and substrate utilized will produce unique spectra.

The V nanoparticles were exposed to very high exposures of O₂ to observe the saturation of the vanadium nanoparticles where the spectra no longer changed with increasing exposures (Figure S15). 3000 L was found to produce a spectra that not only had more discrete peak features, but did not change going to 4500 L of O₂. Annealing this spectra at 350 °C in the absence of oxygen was found to remove some of the oxygen yielding a spectra similar to the 1500 L O₂ exposure with the loss of the 369 cm⁻¹ and some peak position differences being the most notable differences between the two.

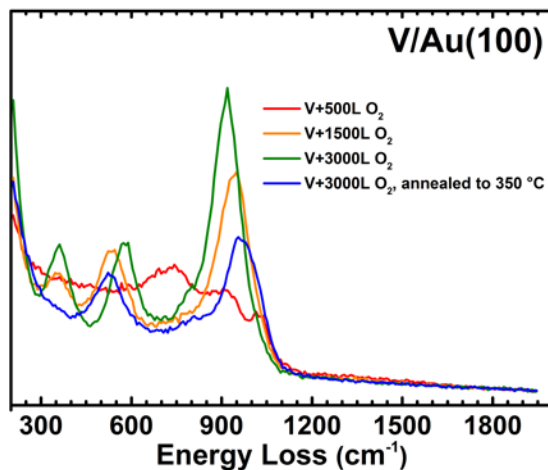


Figure S11. HREELS of V deposited onto Au(100). The V was exposed to high amounts of O₂ up to 3000L while the surface was held at 190 °C. HREELS was acquired after the annealing was allowed to cool to RT. The V-O peaks are seen to grow in sharpness and intensity until

it reaches a saturation point. This is where no more O_2 could be incorporated into the V nanoparticle through this experimental method noted by performing a 4500L exposure with no change from the 3000L exposure. The 3000L fully oxidized nanoparticle could then be annealed to 350 °C to remove some of the oxygen making it resemble the un-saturated 1500L O_2 exposure spectra.

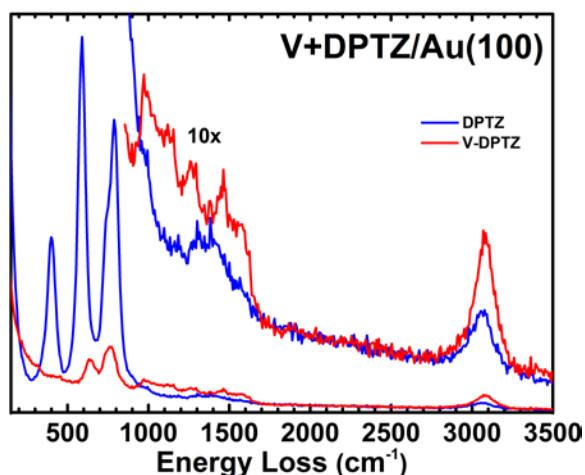


Figure S12. HREELS of DPTZ on the Au(100) surface. V was then deposited onto the DPTZ layer where multiple changes to the spectra were observed. There is a noted shift of the pyridyl peak at 589 to 640 cm^{-1} . A decrease to the out-of-plane modes, increase to the in-plane modes, and an increase to the C-H stretching peak can also be observed after deposition of the V. These changes correlate with the redox formation of a metal-organic complex.

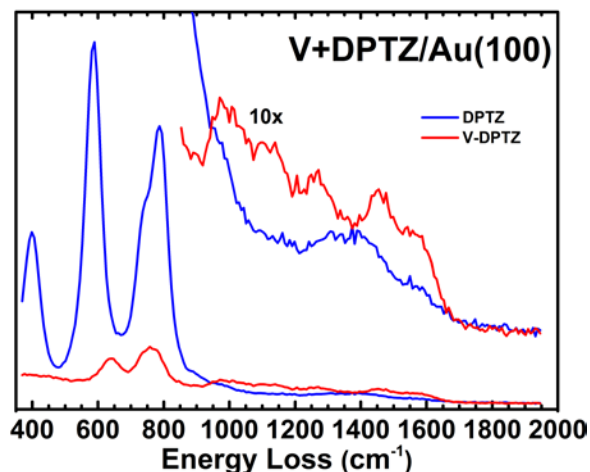


Figure S13. HREELS of DPTZ on the Au(100) showing the same data as Figure S16, but showing a higher resolution region between 400-2000 cm^{-1} .

Section S12. References

1. Vanhove, M. A.; Koestner, R. J.; Stair, P. C.; Bibérian, J. P.; Kesmodel, L. L.; Bartoš, I.; Somorjai, G. A., The Surface Reconstructions of the (100) Crystal Faces of Iridium, Platinum and Gold .1. Experimental-Observations and Possible Structural Models. *Surf. Sci.* **1981**, *103* (1), 189-217.
2. Tempas, C. D.; Skomski, D.; Tait, S. L., Lifting of the Au(100) surface reconstruction by Pt, Cr, Fe, and Cu adsorption. *Surf. Sci.* **2016**, *654*, 33-38.
3. Binnig, G. K.; Rohrer, H.; Gerber, C.; Stoll, E., Real-Space Observation of the Reconstruction of Au(100). *Surf. Sci.* **1984**, *144* (2-3), 321-335.
4. Ibe, J. P.; Bey, P. P.; Brandow, S. L.; Brizzolara, R. A.; Burnham, N. A.; Dilella, D. P.; Lee, K. P.; Marrian, C. R. K.; Colton, R. J., On the Electrochemical Etching of Tips for Scanning Tunneling Microscopy. *J. Vac. Sci. Technol. A* **1990**, *8* (4), 3570-3575.
5. Stepanow, S.; Strunskus, T.; Lingenfelder, M.; Dmitriev, A.; Spillmann, H.; Lin, N.; Barth, J. V.; Wöll, C.; Kern, K., Deprotonation-driven phase transformations in terephthalic acid self-assembly on Cu(100). *J. Phys. Chem. B* **2004**, *108* (50), 19392-19397.
6. Ge, Y.; Adler, H.; Theertham, A.; Kesmodel, L. L.; Tait, S. L., Adsorption and Bonding of First Layer and Bilayer Terephthalic Acid on the Cu(100) Surface by High-Resolution Electron Energy Loss Spectroscopy. *Langmuir* **2010**, *26* (21), 16325-16329.
7. Horcas, I.; Fernández, R.; Gómez-Rodríguez, J. M.; Colchero, J.; Gómez-Herrero, J.; Baro, A. M., WSXM: A software for scanning probe microscopy and a tool for nanotechnology. *Rev. Sci. Instrum.* **2007**, *78* (1).
8. Kresse, G.; Furthmüller, J., Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. *Comput. Mater. Sci.* **1996**, *6* (1), 15-50.
9. Kresse, G.; Hafner, J., Ab initio molecular dynamics for liquid metals. *Phys. Rev. B* **1993**, *47* (1), 558-561.
10. Kresse, G.; Joubert, D., From ultrasoft pseudopotentials to the projector augmented-wave method. *Phys. Rev. B* **1999**, *59* (3), 1758-1775.
11. Blöchl, P. E., Projector augmented-wave method. *Phys. Rev. B* **1994**, *50* (24), 17953-17979.
12. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H., A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **2010**, *132* (15), 154104.
13. Klimeš, J.; Bowler, D. R.; Michaelides, A., Van der Waals density functionals applied to solids. *Phys. Rev. B* **2011**, *83* (19), 195131.
14. Klimeš, J.; Bowler, D. R.; Michaelides, A., Chemical accuracy for the van der Waals density functional. *J. Phys. Condens. Matter* **2010**, *22* (2).
15. Skomski, D.; Tempas, C. D.; Smith, K. A.; Tait, S. L., Redox-Active On-Surface Assembly of Metal-Organic Chains with Single-Site Pt(II). *J. Am. Chem. Soc.* **2014**, *136* (28), 9862-9865.
16. Le, D.; Rahman, T. S., Pt-dipyridyl tetrazine metal-organic network on the Au(100) surface: insights from first principles calculations. *Faraday Discuss.* **2017**, *204*, 83-95.

17. Hoang, T. K. A.; Webb, M. I.; Mai, H. V.; Hamaed, A.; Walsby, C. J.; Trudeau, M.; Antonelli, D. M., Design and Synthesis of Vanadium Hydrazide Gels for Kubas-Type Hydrogen Adsorption: A New Class of Hydrogen Storage Materials. *J. Am. Chem. Soc.* **2010**, *132* (33), 11792-11798.
18. Skomski, D.; Tempas, C. D.; Cook, B. J.; Polezhaev, A. V.; Smith, K. A.; Caulton, K. G.; Tait, S. L., Two- and Three-Electron Oxidation of Single-Site Vanadium Centers at Surfaces by Ligand Design. *J. Am. Chem. Soc.* **2015**, *137* (24), 7898-7902.
19. Groenenb.Cj; Sawatzky, G.; Deliefde.Hj; Jellinek, F., Electron-Spectroscopy of Some Cyclopentadienylcycloheptatrienylmetal Compounds. *J. Organomet. Chem.* **1974**, *76* (1), C4-C6.
20. Silversmit, G.; Depla, D.; Poelman, H.; Marin, G. B.; De Gryse, R., Determination of the V2p XPS binding energies for different vanadium oxidation states (V5+ to V0+). *J. Electron Spectrosc. Relat. Phenom.* **2004**, *135* (2-3), 167-175.
21. Colton, R. J.; Guzman, A. M.; Rabalais, J. W., Electrochromism in Some Thin-Film Transition-Metal Oxides Characterized by X-Ray Electron-Spectroscopy. *J. Appl. Phys.* **1978**, *49* (1), 409-416.
22. Hansen, T. W.; Delariva, A. T.; Challa, S. R.; Datye, A. K., Sintering of Catalytic Nanoparticles: Particle Migration or Ostwald Ripening? *Acc. Chem. Res.* **2013**, *46* (8), 1720-1730.
23. Williams, C. G.; Wang, M.; Skomski, D.; Tempas, C. D.; Kesmodel, L. L.; Tait, S. L., Metal-Ligand Complexation through Redox Assembly at Surfaces Characterized by Vibrational Spectroscopy. *J. Phys. Chem. C* **2017**, *121* (24), 13183-13190.

Section S13: Coordinate of structures in Fig. 6

The following are the optimized coordinate of all structures in Fig. 6. Please refer to http://cms.mpi.univie.ac.at/vasp/vasp/POSCAR_file.html for the data format.

Fig. 6a

```
-----
Au C H N V
1.0000000000000000
26.0801187006857766 0.0000000000000000 0.0000000000000000
-14.4889548337143204 14.4889548337143204 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Au C H N V
279 36 24 18 3
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.1894422798390494 F F F
0.5555555555555571 0.2000000000000028 0.1894422798390494 F F F
0.4444444444444429 0.2000000000000028 0.1894422798390494 F F F
0.222222222222214 0.2000000000000028 0.1894422798390494 F F F
0.1111111111111143 0.2000000000000028 0.1894422798390494 F F F
0.7777777777777786 0.2000000000000028 0.1894422798390494 F F F
0.8888888888888857 0.0000000000000000 0.1894422798390494 F F F
0.6666666666666643 0.0000000000000000 0.1894422798390494 F F F
0.5555555555555571 0.0000000000000000 0.1894422798390494 F F F
0.4444444444444429 0.0000000000000000 0.1894422798390494 F F F
0.3333333333333357 0.0000000000000000 0.1894422798390494 F F F
0.222222222222214 0.0000000000000000 0.1894422798390494 F F F
0.1111111111111143 0.0000000000000000 0.1894422798390494 F F F
0.7777777777777786 0.0000000000000000 0.1894422798390494 F F F
0.8888888888888857 0.5000000000000000 0.2561864044279716 F F F
0.8888888888888857 0.2000000000000028 0.1894422798390494 F F F
0.222222222222214 0.3999999999999986 0.1894422798390494 F F F
0.8888888888888857 0.6000000000000014 0.1894422798390494 F F F
0.0000000000000000 0.3999999999999986 0.1894422798390494 F F F
0.3333333333333357 0.3999999999999986 0.1894422798390494 F F F
0.4444444444444429 0.3999999999999986 0.1894422798390494 F F F
0.5555555555555571 0.3999999999999986 0.1894422798390494 F F F
0.6666666666666643 0.3999999999999986 0.1894422798390494 F F F
0.7777777777777786 0.3999999999999986 0.1894422798390494 F F F
0.6666666666666671 0.2000000000000028 0.1894422798390494 F F F
0.8888888888888857 0.3999999999999986 0.1894422798390494 F F F
0.0000000000000000 0.2000000000000028 0.1894422798390494 F F F
0.3333333333333357 0.6000000000000014 0.1894422798390494 F F F
0.4444444444444429 0.6000000000000014 0.1894422798390494 F F F
0.5555555555555571 0.6000000000000014 0.1894422798390494 F F F
0.5544246947117385 0.0978279645378948 0.3895289825541366 T T T
0.7777777777777786 0.6000000000000014 0.1894422798390494 F F F
0.1111111111111107 0.3999999999999986 0.1894422798390494 F F F
0.0000000000000000 0.5000000000000000 0.2561864044279716 F F F
0.0000000000000000 0.6000000000000014 0.1894422798390494 F F F
0.222222222222214 0.6000000000000014 0.1894422798390494 F F F
0.6666666666666643 0.7999999999999972 0.1894422798390494 F F F
0.7777777777777786 0.7999999999999972 0.1894422798390494 F F F
0.8888888888888857 0.7999999999999972 0.1894422798390494 F F F
0.0000000000000000 0.7999999999999972 0.1894422798390494 F F F
```

0.1111111111111072	0.799999999999972	0.1894422798390494	F	F	F
0.222222222222214	0.799999999999972	0.1894422798390494	F	F	F
0.333333333333286	0.799999999999972	0.1894422798390494	F	F	F
0.111111111111143	0.100000000000014	0.2561864044279716	F	F	F
0.222222222222214	0.100000000000014	0.2561864044279716	F	F	F
0.333333333333357	0.100000000000014	0.2561864044279716	F	F	F
0.444444444444429	0.100000000000014	0.2561864044279716	F	F	F
0.555555555555571	0.100000000000014	0.2561864044279716	F	F	F
0.666666666666643	0.100000000000014	0.2561864044279716	F	F	F
0.777777777777786	0.100000000000014	0.2561864044279716	F	F	F
0.888888888888928	0.100000000000014	0.2561864044279716	F	F	F
0.000000000000000	0.100000000000014	0.2561864044279716	F	F	F
0.777777777777786	0.500000000000000	0.2561864044279716	F	F	F
0.888888888888857	0.299999999999972	0.2561864044279716	F	F	F
0.222222222222214	0.299999999999972	0.2561864044279716	F	F	F
0.333333333333286	0.299999999999972	0.2561864044279716	F	F	F
0.444444444444429	0.299999999999972	0.2561864044279716	F	F	F
0.555555555555571	0.299999999999972	0.2561864044279716	F	F	F
0.666666666666643	0.299999999999972	0.2561864044279716	F	F	F
0.111111111111143	0.600000000000014	0.1894422798390494	F	F	F
0.777777777777786	0.299999999999972	0.2561864044279716	F	F	F
0.444444444444429	0.799999999999972	0.1894422798390494	F	F	F
0.1111111111111072	0.299999999999972	0.2561864044279716	F	F	F
0.333333333333357	0.500000000000000	0.2561864044279716	F	F	F
0.444444444444429	0.500000000000000	0.2561864044279716	F	F	F
0.555555555555571	0.500000000000000	0.2561864044279716	F	F	F
0.666666666666643	0.500000000000000	0.2561864044279716	F	F	F
0.000000000000000	0.299999999999972	0.2561864044279716	F	F	F
0.555555555555571	0.799999999999972	0.1894422798390494	F	F	F
0.666666666666643	0.600000000000014	0.1894422798390494	F	F	F
0.9993960164625797	0.1987351969941716	0.3226671009522347	T	T	T
0.888888888888857	0.899999999999986	0.2561864044279716	F	F	F
0.777777777777786	0.899999999999986	0.2561864044279716	F	F	F
0.666666666666643	0.899999999999986	0.2561864044279716	F	F	F
0.555555555555571	0.899999999999986	0.2561864044279716	F	F	F
0.333333333333357	0.700000000000028	0.2561864044279716	F	F	F
0.1111111111111072	0.899999999999986	0.2561864044279716	F	F	F
0.222222222222214	0.700000000000028	0.2561864044279716	F	F	F
0.6665296283874225	0.1991036454730108	0.3223716410202495	T	T	T
0.8888888888888928	0.700000000000028	0.2561864044279716	F	F	F
0.777777777777786	0.700000000000028	0.2561864044279716	F	F	F
0.6666666666666714	0.700000000000028	0.2561864044279716	F	F	F
0.555555555555571	0.700000000000028	0.2561864044279716	F	F	F
0.444444444444429	0.700000000000028	0.2561864044279716	F	F	F
0.111111111111143	0.700000000000028	0.2561864044279716	F	F	F
0.222222222222214	0.899999999999986	0.2561864044279716	F	F	F
0.000000000000000	0.700000000000028	0.2561864044279716	F	F	F
0.444444444444429	0.899999999999986	0.2561864044279716	F	F	F
0.333333333333357	0.899999999999986	0.2561864044279716	F	F	F
0.1104346369185566	0.9992058796816683	0.3230552990141234	T	T	T
0.5551980017710180	0.9998939950742144	0.3225006257953550	T	T	T
0.6668955026331324	0.0001573768659305	0.3224151109276933	T	T	T
0.7785266483206893	0.0004085736913153	0.3225587780261225	T	T	T
0.8891330230117829	0.9998507703635193	0.3229395978252414	T	T	T
0.000000000000000	0.899999999999986	0.2561864044279716	F	F	F
0.9997047447611439	0.9995033079740505	0.3229826478000805	T	T	T

0.3320223991445659	0.9986887594166465	0.3227312224269205	T	T	T
0.4434651985743163	0.9990070634513624	0.3226258269328459	T	T	T
0.1103390788382653	0.1985707849144634	0.3226347391722219	T	T	T
0.2208333055080886	0.1979416294932248	0.3225325053650249	T	T	T
0.3318734966032307	0.1978262159483611	0.3223023928851724	T	T	T
0.4433929098655260	0.1982212910450344	0.3221435572164661	T	T	T
0.2211364754130681	0.9989183751903989	0.3229505330362835	T	T	T
0.2222222222222214	0.5000000000000000	0.2561864044279716	F	F	F
0.5548728424030477	0.1982332785706998	0.3222882040006878	T	T	T
0.7779713362426188	0.1994645664866900	0.3223780885065162	T	T	T
0.2222838126499932	0.4007590128250192	0.3225938979150174	T	T	T
0.3331392589072825	0.4005217085667017	0.3223778225565080	T	T	T
0.4445960145312804	0.4009076912405881	0.3223584065532615	T	T	T
0.5562902535668937	0.4018378591143277	0.3222738112907880	T	T	T
0.6677682089216180	0.4018437223261004	0.3221561421503939	T	T	T
0.7792662667286953	0.4021972574954929	0.3222985137479488	T	T	T
0.8902644288132570	0.4020490656554809	0.3225261477538485	T	T	T
0.1117178790912316	0.4012804259243157	0.3226638314819084	T	T	T
0.3326047051718601	0.5996154120723474	0.3225645440372508	T	T	T
0.4442148858608492	0.5998479877533671	0.3223960217965786	T	T	T
0.5559257809330844	0.6001094905573032	0.3224959021117204	T	T	T
0.6676948120142662	0.6010611137010463	0.3226375446504398	T	T	T
0.7791060619288939	0.6013323265977335	0.3227396138067382	T	T	T
0.8899754449971294	0.6010799664202807	0.3229609733841126	T	T	T
0.0006655152181636	0.6007847706207247	0.3230650199744728	T	T	T
0.1114020041353986	0.6005001448013805	0.3229851197303010	T	T	T
0.1111111111111143	0.5000000000000000	0.2561864044279716	F	F	F
0.0001206495008930	0.8000916473079100	0.3231430942084003	T	T	T
0.2219762387587181	0.6001407560570060	0.3229332875985358	T	T	T
0.4438881715908191	0.7996679611387230	0.3225596584163322	T	T	T
0.5555562346694073	0.7999957280880267	0.3225929073451263	T	T	T
0.6672514463267852	0.8003664840829713	0.3225703817439725	T	T	T
0.7787090059300045	0.8006624831450215	0.3227463786618084	T	T	T
0.0007853845515611	0.4014519079893209	0.3226381341746031	T	T	T
0.8895809697963453	0.8005517857546971	0.3230266586477686	T	T	T
0.8888240868455940	0.199262644429459	0.3226092705795520	T	T	T
0.2215340188890138	0.7994384386159582	0.3230293291425375	T	T	T
0.3324319003117052	0.7993651681541248	0.3227469353355969	T	T	T
0.1093781347936624	0.0973923938643212	0.3905088632243922	T	T	T
0.2202196908103408	0.0972056906149037	0.3902559102921425	T	T	T
0.3313206195395070	0.0971201965896013	0.3897359537326203	T	T	T
0.1109973990759676	0.7999102606772686	0.3231403197461170	T	T	T
0.4425167224745648	0.0973161487719105	0.3893839739510048	T	T	T
0.3333333333333357	0.2000000000000028	0.1894422798390494	F	F	F
0.6662743246064597	0.0986297074737239	0.3894208597068187	T	T	T
0.9991537795979339	0.0982338366481127	0.3904410169059428	T	T	T
0.2215309942641125	0.2994910556663757	0.3876857045067982	T	T	T
0.3322364552400991	0.2988478286067506	0.3871396083948793	T	T	T
0.4440570548626671	0.2995607010446362	0.3866494294955179	T	T	T
0.5555992267917887	0.3000714261108365	0.3864539148982030	T	T	T
0.6671411375538705	0.3005851663631378	0.3866638602861473	T	T	T
0.7788863154833743	0.3011752795177496	0.3871551296489373	T	T	T
0.8896092428672390	0.3006009482123123	0.3876821623991372	T	T	T
0.0003158080070233	0.3001999586655215	0.3878777216965029	T	T	T
0.1108392624902438	0.2998357759432073	0.3878857726639567	T	T	T
0.3335365013394100	0.5014250804916507	0.3897276998892562	T	T	T

0.4448362255638985	0.5013612849554332	0.3894014707052857	T	T	T
0.5567641974995946	0.5022691506210997	0.3895234019601614	T	T	T
0.6686636685506818	0.5027921652363520	0.3894076650315945	T	T	T
0.7798182260009172	0.5029348639436866	0.3897753395311771	T	T	T
0.8908808103636388	0.5028114365494643	0.3902915923940153	T	T	T
0.6676480204278039	0.9008403655134912	0.3887233052448935	T	T	T
0.7786831785224194	0.7008168370452672	0.3899312664036756	T	T	T
0.0017204314264138	0.5026304657417652	0.3905168446855694	T	T	T
0.1119785022660305	0.5018131761257036	0.3904367593453036	T	T	T
0.2227387429017508	0.5016408970482911	0.3903688916553381	T	T	T
0.4434882999084381	0.6991926820788594	0.3887232867444413	T	T	T
0.5551064950737968	0.6992743079462673	0.3887757107093853	T	T	T
0.8884007000262172	0.0984086215225044	0.3903714264080703	T	T	T
0.6672939595345655	0.7003757843571535	0.3891593894420694	T	T	T
0.8899066727540785	0.9005819015715568	0.3903316387385763	T	T	T
0.0001764211383989	0.7003767619828115	0.3906191096678288	T	T	T
0.1106262266782017	0.6998078355362809	0.3906950665871300	T	T	T
0.2212517985645350	0.6994485257478403	0.3903259189959334	T	T	T
0.3320667380623508	0.6992351450033411	0.3897572367933769	T	T	T
0.5559893042613651	0.9006927845897946	0.3887891306418503	T	T	T
0.8895110367871981	0.7006487387264203	0.3904069561557217	T	T	T
0.7790877310832207	0.9008174065676489	0.3897659348375352	T	T	T
0.0004937128612834	0.9001915456050866	0.3906927063815770	T	T	T
0.5554987563588351	0.5999977725856870	0.4566840155208916	T	T	T
0.3330159837304446	0.1995713257861325	0.4535302448531928	T	T	T
0.2214642818189751	0.2002237474348344	0.4538847189266738	T	T	T
0.1109328361120377	0.2008226051610220	0.4544941365057541	T	T	T
0.4448062045503562	0.0002005427333233	0.4566116182590030	T	T	T
0.3327166887951188	0.0000183733090563	0.4572784553283359	T	T	T
0.2213995166431648	0.9992992265663905	0.4581561503496587	T	T	T
0.4449841859307954	0.2017245777408892	0.4525324544120528	T	T	T
0.1110175955420276	0.9993898485914774	0.4587729993441146	T	T	T
0.8899065079338314	0.9996121920017101	0.4579447798101956	T	T	T
0.7785004362325935	0.9998780888864373	0.4574543073054132	T	T	T
0.6668649118094492	0.9989980002227982	0.4561457337938151	T	T	T
0.5555728603660132	0.9999613735175448	0.4566967030839303	T	T	T
0.3324860022913415	0.8992572908309352	0.3899057660050013	T	T	T
0.2216045224235922	0.8993728618592982	0.3903919571071347	T	T	T
0.0005178957658768	0.9998321710917188	0.4588104738369255	T	T	T
0.7775914486807129	0.0986034140549667	0.3897456962708252	T	T	T
0.5546239886908457	0.1991960478612923	0.4532652999589311	T	T	T
0.4441568368763770	0.6009302320477997	0.4561489624601736	T	T	T
0.5565833499358926	0.4009714844596374	0.4532550311627145	T	T	T
0.7779215105619641	0.2000656765800365	0.4534810486822374	T	T	T
0.4438722039332363	0.8997120027102780	0.3891465979153285	T	T	T
0.9998901900184032	0.2005608436366922	0.4546556118770568	T	T	T
0.2222859374384689	0.3996994047125661	0.4544732959778205	T	T	T
0.3332003666053155	0.3999269562771558	0.4534629602167605	T	T	T
0.6672301686740522	0.2018521279706885	0.4525192461581777	T	T	T
0.4439602230314671	0.3982563661621487	0.4525353478484609	T	T	T
0.1109479725521493	0.8996456537794341	0.3906122522324977	T	T	T
0.7781382106493357	0.4005120170803306	0.4535937851010720	T	T	T
0.8896468771254574	0.3997946235303308	0.4539139045313120	T	T	T
0.0002411030831041	0.3992392586216618	0.4544936918483188	T	T	T
0.1112660167483544	0.3995073304023259	0.4546458758965051	T	T	T
0.3326837250563719	0.6002088330505669	0.4574632463152933	T	T	T

0.6662149111799286	0.3984447049639786	0.4526087820125594	T	T	T
0.6664116084586121	0.6000232960048868	0.4566308070587991	T	T	T
0.8888766862334995	0.2004219164853286	0.4544492000249881	T	T	T
0.9265719103296959	0.4688314499896544	0.5376708332491845	T	T	T
0.1105780092147612	0.6001638699515001	0.4588050889274053	T	T	T
0.2212565787632937	0.6004686254206734	0.4579289103688328	T	T	T
0.4448557995058128	0.7998257299542801	0.4536004001785742	T	T	T
0.5555388998998931	0.7999557271272568	0.4546060633469629	T	T	T
0.6662637100423089	0.8002054856128460	0.4535733682456586	T	T	T
0.8890310169358269	0.8003375932937166	0.4563008852122078	T	T	T
0.0001939225624039	0.8002206688873326	0.4568076243181070	T	T	T
0.1109743673067857	0.7998174728858911	0.4568074335492485	T	T	T
0.2221134242390126	0.7996651363244379	0.4562589719957092	T	T	T
0.3336121018116176	0.8002298981969228	0.4556959741569959	T	T	T
0.1843770730951518	0.1310644369313508	0.5376257272602152	T	T	T
0.2951199606418043	0.1302975033256491	0.5373074561365466	T	T	T
0.4056953731820435	0.1300408311401439	0.5352683148350813	T	T	T
0.5185964880499209	0.1314980200459479	0.5379897713050195	T	T	T
0.6267379541529111	0.1287294697631569	0.5348742984390843	T	T	T
0.3722338078231834	0.4694137272262157	0.5370978514802844	T	T	T
0.1116157093531497	0.3004978169366922	0.5246736986369638	T	T	T
0.8896713172125973	0.6007941407795100	0.4582041294588884	T	T	T
0.4444009188496275	0.2996170792975663	0.5239224146574571	T	T	T
0.7388767601060905	0.1306704672029578	0.5371322985180000	T	T	T
0.8499026229984030	0.1310777216869309	0.5383316367268258	T	T	T
0.9619232607531325	0.1314767521887778	0.5384474689705642	T	T	T
0.0732501057119977	0.1312793241075302	0.5380290676661762	T	T	T
0.0000689266101443	0.6006573008684536	0.4587887568527187	T	T	T
0.2226309012786229	0.3001352340664969	0.5248847218540333	T	T	T
0.5554776987946950	0.2999649349014484	0.5214766340921534	T	T	T
0.5923484180803716	0.4684261400953459	0.5379647027561190	T	T	T
0.6665724442679446	0.3003138528656817	0.5239786635808442	T	T	T
0.7774642734460016	0.3000270258610119	0.5211623047544461	T	T	T
0.8884426011164455	0.2999011797206035	0.524854877778076	T	T	T
0.9995153776691390	0.2995581023520032	0.5246709610661030	T	T	T
0.3335455727925317	0.2999178363586034	0.5210982310905392	T	T	T
0.4842689287461613	0.4712506712252543	0.5349378098222758	T	T	T
0.7775991982420603	0.7999163051014793	0.4557174291403493	T	T	T
0.7784077179066435	0.6000785939980852	0.4573359262314965	T	T	T
0.6675178076766632	0.8004096041130170	0.5412010219408327	T	T	T
0.5555264752931404	0.8000431135200914	0.5437816154077227	T	T	T
0.2968282177930051	0.6348238510320097	0.5355584875323945	T	T	T
0.1860920096706734	0.6351299631228142	0.5377346010126056	T	T	T
0.0750779449481144	0.6356846495903042	0.5376891271917703	T	T	T
0.7051662948604311	0.4697647603276496	0.5354518908178185	T	T	T
0.7786970495056439	0.8013641734418210	0.5445911916601031	T	T	T
0.8537763594049769	0.6370162292923920	0.5365305473028806	T	T	T
0.6323619928180925	0.6372746922444631	0.5357278048450201	T	T	T
0.5206261507506648	0.6376220893423802	0.5335561402913047	T	T	T
0.4091073142865255	0.6361838828854453	0.5350735086835469	T	T	T
0.2612487298159382	0.4690081803214359	0.5383636901202066	T	T	T
0.1491716363351233	0.4685419181834042	0.5384358562084555	T	T	T
0.0377865034169164	0.4687015763334709	0.5380452898754577	T	T	T
0.7429191512413540	0.6375806423800388	0.5335438375855895	T	T	T
0.8893070922433983	0.8008424691612018	0.5450817560630410	T	T	T
0.9638940958141597	0.6356490575084961	0.5378402843759167	T	T	T

0.3679824558317693	0.9622022903714851	0.5334419775025685	T	T	T
0.4786648235435835	0.9627153961536173	0.5357058499437636	T	T	T
0.0000855431064793	0.8001186605313328	0.5455510033157271	T	T	T
0.1107972455892098	0.7996925340210620	0.5455531966695574	T	T	T
0.7020153791693634	0.9638953860237609	0.5349580925237372	T	T	T
0.3323323469146685	0.7985504104668084	0.5445545317564514	T	T	T
0.4436514384067317	0.7996934398010785	0.5412544973843803	T	T	T
0.2215891705248638	0.7989687705923632	0.5450296513857582	T	T	T
0.8143153341716420	0.9652149330856652	0.5355893008708462	T	T	T
0.8157478596244621	0.4695226501343779	0.5374147016163605	T	T	T
0.9249440395667011	0.9647906275279238	0.5377576403242595	T	T	T
0.0358706854527090	0.9641762755126310	0.5376747539561795	T	T	T
0.1469824612791374	0.9641673972225188	0.5378342558445636	T	T	T
0.2570732341021778	0.9627570203402489	0.5363875644923614	T	T	T
0.5905413980529639	0.9625363689823770	0.5336306451332931	T	T	T
0.3029821937208614	0.9803540000336498	0.6486429348767458	T	T	T
0.6782145596674495	0.1537624206079042	0.6391812158378392	T	T	T
0.6785925033281210	0.4858625709930458	0.6402945717644549	T	T	T
0.3886047746469313	0.6351409631430085	0.6406184098439662	T	T	T
0.4957457916999107	0.5451185053265190	0.6398779336995252	T	T	T
0.3024652638955550	0.3107756901222877	0.6403210503204985	T	T	T
0.3606688128231099	0.4061556274857744	0.6433269673705673	T	T	T
0.4312209712008253	0.4455949657680189	0.6391744681506075	T	T	T
0.6779329440703377	0.8187490348305541	0.6445996584313234	T	T	T
0.7484872190413129	0.8582462585728593	0.6490855660914217	T	T	T
0.8064382984072201	0.9538987740988247	0.6490536089056086	T	T	T
0.3168101408434651	0.2575405723521120	0.6334337523022051	T	T	T
0.7205186698846668	0.9640756119693984	0.6403547347937973	T	T	T
0.3882997412809474	0.3011301847628614	0.6291434162468075	T	T	T
0.7919288341807769	0.0075178396720426	0.6447746891801990	T	T	T
0.3611334297975626	0.0757840992641753	0.6464711392136384	T	T	T
0.6135472915785279	0.7192123429633613	0.6423181009024512	T	T	T
0.4310230281768862	0.1141028899104138	0.6400459094476588	T	T	T
0.8070054162711640	0.2885358823806093	0.6401731276324047	T	T	T
0.6141254219842873	0.3866987967830609	0.6369185409432357	T	T	T
0.3172167758563370	0.5918403252951967	0.6449612132118281	T	T	T
0.3608238927198598	0.7412224862980260	0.6491211968374595	T	T	T
0.3166795097351214	0.9258837049018823	0.6442545238472174	T	T	T
0.7926751069258314	0.3418558599828800	0.6336114085504353	T	T	T
0.4957562010852247	0.8801397829614563	0.6423652910734465	T	T	T
0.7487783107912269	0.1931410609404397	0.6431191067454731	T	T	T
0.3028048744641564	0.6455808572473339	0.6491003485083088	T	T	T
0.4313429477296321	0.7805890061914300	0.6446934845442900	T	T	T
0.6136257856848107	0.0542280384236360	0.6398671635325560	T	T	T
0.3874384181267548	0.9682600977216123	0.6375045934958063	T	T	T
0.4955649234352328	0.2132520972943560	0.6367883483121844	T	T	T
0.7220772057131543	0.6316482949019075	0.6378065934349597	T	T	T
0.7928362112147347	0.6741009103397007	0.6446446263867396	T	T	T
0.8065851105314771	0.6196899706095186	0.6490556066355824	T	T	T
0.7484871654913824	0.5242642731185925	0.6468191836492686	T	T	T
0.7211853422324890	0.2983320595520686	0.6294983856914501	T	T	T
0.2735027554961965	0.5167730120895130	0.6437176727911600	T	T	T
0.3528286171549810	0.4511808801212550	0.6482258104892524	T	T	T
0.7565629571200988	0.8130641308230470	0.6515780180291758	T	T	T
0.2468837364823551	0.2785973299819600	0.6422547483032313	T	T	T
0.2472660911572618	0.6134791174865406	0.6512086178382045	T	T	T

0.7566215998301385	0.1480711137626579	0.6477981262963075	T	T	T
0.3528517672509640	0.7865210304740637	0.6515247308670612	T	T	T
0.8619999488574380	0.9861104177699470	0.6512818707866195	T	T	T
0.7557779070619493	0.4782986961527399	0.6494884907654338	T	T	T
0.8625857248530787	0.3206664874934774	0.6419213083193718	T	T	T
0.2730704037893569	0.1828226692483400	0.6298640052861907	T	T	T
0.8355717166532394	0.0825810271168820	0.6434935195153398	T	T	T
0.7061390021701515	0.0024361126739783	0.6364318568591261	T	T	T
0.4022751043937250	0.2628690258911288	0.6229867249310230	T	T	T
0.3538762972920546	0.1217892873341188	0.6490909893045351	T	T	T
0.2478210767549694	0.9487977678967654	0.6526474620831050	T	T	T
0.8366853590332396	0.7492153898827973	0.6451045044970376	T	T	T
0.2728050308161740	0.8507700151520703	0.6446734491986983	T	T	T
0.8617472643422955	0.6512820288736468	0.6531136243499249	T	T	T
0.7085414114960558	0.6708625790892485	0.6336171398142726	T	T	T
0.4028918270922871	0.5966538044511993	0.6367931026115146	T	T	T
0.7072168663662730	0.3366767513541404	0.6235854068793061	T	T	T
0.8364143444094144	0.4166024316532684	0.6301397983766180	T	T	T
0.4009524415127076	0.9290104433487585	0.6333640000498796	T	T	T
0.6642160254675543	0.2057271375086167	0.6319711174075946	T	T	T
0.6637863128984525	0.8711726568676208	0.6402552931342865	T	T	T
0.6214338748453381	0.6627003742612400	0.6412951177477906	T	T	T
0.5485390953047657	0.6952005938529384	0.6391976359879601	T	T	T
0.4878583575367073	0.6015853277015126	0.6414475406679563	T	T	T
0.4879316355634712	0.9367205052534271	0.6414054421834862	T	T	T
0.5484184414901465	0.0297268538632784	0.6363474920127047	T	T	T
0.6214488365568419	0.9976952678729161	0.6413686492047302	T	T	T
0.4453926338041297	0.7280482740494780	0.6404200630697340	T	T	T
0.4444362622282025	0.0610076865987937	0.6355183750813266	T	T	T
0.4452649988081591	0.3937323073427775	0.6317406211106553	T	T	T
0.5609775875174630	0.5697025714632867	0.6362620747789495	T	T	T
0.5602232398721705	0.2363743617861280	0.6331296579008726	T	T	T
0.6651331467634845	0.5388975908290916	0.6357029173269392	T	T	T
0.6213009704012751	0.3295525656296993	0.6367110782379343	T	T	T
0.5494791507116256	0.3635584395125264	0.6330278618692530	T	T	T
0.4883853690818212	0.2703897947469150	0.6364837851216137	T	T	T
0.5607283349977301	0.9040890190876707	0.6391612597000629	T	T	T
0.5532332787687165	0.1319678231603211	0.6204350540394206	T	T	T
0.5545813758659340	0.7995819329796602	0.6274054441274902	T	T	T
0.5563533308997382	0.4677647788058820	0.6202204114689677	T	T	T

Fig. 6b

Au C H N V O

1.000000000000000

26.0801187006857766 0.0000000000000000 0.0000000000000000

-14.4889548337143204 14.4889548337143204 0.0000000000000000

0.0000000000000000 0.0000000000000000 31.0000000000000000

Au C H N V O

279 36 24 18 3 2

Selective dynamics

Direct

0.0000000000000000 0.0000000000000000 0.1894422798390494 F F F

0.5555555555555571 0.2000000000000028 0.1894422798390494 F F F

0.4444444444444429 0.2000000000000028 0.1894422798390494 F F F

0.2222222222222214 0.2000000000000028 0.1894422798390494 F F F

0.1111111111111143	0.2000000000000028	0.1894422798390494	F	F	F
0.777777777777786	0.2000000000000028	0.1894422798390494	F	F	F
0.888888888888857	0.0000000000000000	0.1894422798390494	F	F	F
0.666666666666643	0.0000000000000000	0.1894422798390494	F	F	F
0.555555555555571	0.0000000000000000	0.1894422798390494	F	F	F
0.444444444444429	0.0000000000000000	0.1894422798390494	F	F	F
0.333333333333357	0.0000000000000000	0.1894422798390494	F	F	F
0.222222222222214	0.0000000000000000	0.1894422798390494	F	F	F
0.111111111111143	0.0000000000000000	0.1894422798390494	F	F	F
0.777777777777786	0.0000000000000000	0.1894422798390494	F	F	F
0.888888888888857	0.5000000000000000	0.2561864044279716	F	F	F
0.8888888888888928	0.2000000000000028	0.1894422798390494	F	F	F
0.222222222222214	0.3999999999999986	0.1894422798390494	F	F	F
0.8888888888888928	0.6000000000000014	0.1894422798390494	F	F	F
0.0000000000000000	0.3999999999999986	0.1894422798390494	F	F	F
0.333333333333357	0.3999999999999986	0.1894422798390494	F	F	F
0.444444444444429	0.3999999999999986	0.1894422798390494	F	F	F
0.555555555555571	0.3999999999999986	0.1894422798390494	F	F	F
0.666666666666643	0.3999999999999986	0.1894422798390494	F	F	F
0.777777777777786	0.3999999999999986	0.1894422798390494	F	F	F
0.6666666666666714	0.2000000000000028	0.1894422798390494	F	F	F
0.888888888888857	0.3999999999999986	0.1894422798390494	F	F	F
0.0000000000000000	0.2000000000000028	0.1894422798390494	F	F	F
0.333333333333357	0.6000000000000014	0.1894422798390494	F	F	F
0.444444444444429	0.6000000000000014	0.1894422798390494	F	F	F
0.555555555555571	0.6000000000000014	0.1894422798390494	F	F	F
0.5544488876149091	0.0975497407710905	0.3894571685165162	T	T	T
0.777777777777786	0.6000000000000014	0.1894422798390494	F	F	F
0.1111111111111072	0.3999999999999986	0.1894422798390494	F	F	F
0.0000000000000000	0.5000000000000000	0.2561864044279716	F	F	F
0.0000000000000000	0.6000000000000014	0.1894422798390494	F	F	F
0.222222222222214	0.6000000000000014	0.1894422798390494	F	F	F
0.666666666666643	0.7999999999999972	0.1894422798390494	F	F	F
0.777777777777786	0.7999999999999972	0.1894422798390494	F	F	F
0.888888888888857	0.7999999999999972	0.1894422798390494	F	F	F
0.0000000000000000	0.7999999999999972	0.1894422798390494	F	F	F
0.1111111111111072	0.7999999999999972	0.1894422798390494	F	F	F
0.222222222222214	0.7999999999999972	0.1894422798390494	F	F	F
0.3333333333333286	0.7999999999999972	0.1894422798390494	F	F	F
0.111111111111143	0.1000000000000014	0.2561864044279716	F	F	F
0.222222222222214	0.1000000000000014	0.2561864044279716	F	F	F
0.333333333333357	0.1000000000000014	0.2561864044279716	F	F	F
0.444444444444429	0.1000000000000014	0.2561864044279716	F	F	F
0.555555555555571	0.1000000000000014	0.2561864044279716	F	F	F
0.666666666666643	0.1000000000000014	0.2561864044279716	F	F	F
0.777777777777786	0.1000000000000014	0.2561864044279716	F	F	F
0.8888888888888928	0.1000000000000014	0.2561864044279716	F	F	F
0.0000000000000000	0.1000000000000014	0.2561864044279716	F	F	F
0.777777777777786	0.5000000000000000	0.2561864044279716	F	F	F
0.888888888888857	0.2999999999999972	0.2561864044279716	F	F	F
0.222222222222214	0.2999999999999972	0.2561864044279716	F	F	F
0.3333333333333286	0.2999999999999972	0.2561864044279716	F	F	F
0.444444444444429	0.2999999999999972	0.2561864044279716	F	F	F
0.555555555555571	0.2999999999999972	0.2561864044279716	F	F	F
0.666666666666643	0.2999999999999972	0.2561864044279716	F	F	F
0.111111111111143	0.6000000000000014	0.1894422798390494	F	F	F

0.7777777777777786	0.2999999999999972	0.2561864044279716	F	F	F
0.4444444444444429	0.7999999999999972	0.1894422798390494	F	F	F
0.11111111111111072	0.2999999999999972	0.2561864044279716	F	F	F
0.3333333333333357	0.5000000000000000	0.2561864044279716	F	F	F
0.4444444444444429	0.5000000000000000	0.2561864044279716	F	F	F
0.5555555555555571	0.5000000000000000	0.2561864044279716	F	F	F
0.6666666666666643	0.5000000000000000	0.2561864044279716	F	F	F
0.0000000000000000	0.2999999999999972	0.2561864044279716	F	F	F
0.5555555555555571	0.7999999999999972	0.1894422798390494	F	F	F
0.6666666666666643	0.6000000000000014	0.1894422798390494	F	F	F
0.9994552006888584	0.1987653113797848	0.3226782049633251	T	T	T
0.8888888888888857	0.8999999999999986	0.2561864044279716	F	F	F
0.7777777777777786	0.8999999999999986	0.2561864044279716	F	F	F
0.6666666666666643	0.8999999999999986	0.2561864044279716	F	F	F
0.5555555555555571	0.8999999999999986	0.2561864044279716	F	F	F
0.3333333333333357	0.7000000000000028	0.2561864044279716	F	F	F
0.11111111111111072	0.8999999999999986	0.2561864044279716	F	F	F
0.2222222222222214	0.7000000000000028	0.2561864044279716	F	F	F
0.6663928691006765	0.1990368983656481	0.3223297934215122	T	T	T
0.88888888888888928	0.7000000000000028	0.2561864044279716	F	F	F
0.7777777777777786	0.7000000000000028	0.2561864044279716	F	F	F
0.66666666666666714	0.7000000000000028	0.2561864044279716	F	F	F
0.5555555555555571	0.7000000000000028	0.2561864044279716	F	F	F
0.4444444444444429	0.7000000000000028	0.2561864044279716	F	F	F
0.11111111111111143	0.7000000000000028	0.2561864044279716	F	F	F
0.2222222222222214	0.8999999999999986	0.2561864044279716	F	F	F
0.0000000000000000	0.7000000000000028	0.2561864044279716	F	F	F
0.4444444444444429	0.8999999999999986	0.2561864044279716	F	F	F
0.3333333333333357	0.8999999999999986	0.2561864044279716	F	F	F
0.1104463646230041	0.9992067199024735	0.3230160858754976	T	T	T
0.5551650400487246	0.9997876946425609	0.3224186948347384	T	T	T
0.6668482123569434	0.0001028446506416	0.3224063448448439	T	T	T
0.7785084798331131	0.0003840636608701	0.3225386667645608	T	T	T
0.8891062552991480	0.9997989509383114	0.3229133900839278	T	T	T
0.0000000000000000	0.8999999999999986	0.2561864044279716	F	F	F
0.9998237600212722	0.9995333812382575	0.3229934747413932	T	T	T
0.3322466206636996	0.9990641785347847	0.3227598902815407	T	T	T
0.4436035706780868	0.9992362291872934	0.3226435538034761	T	T	T
0.1104093706360662	0.1985150950877969	0.3226349670526896	T	T	T
0.2211564957370966	0.1981077638200569	0.3225969969053386	T	T	T
0.3323089606912969	0.1982884634868332	0.3225118776990856	T	T	T
0.4436426742301910	0.1988501779687267	0.3223847042218069	T	T	T
0.2213730733380914	0.9992511129472961	0.3229670965295726	T	T	T
0.2222222222222214	0.5000000000000000	0.2561864044279716	F	F	F
0.5547860852037438	0.1986250674973708	0.3224824188799898	T	T	T
0.7779124711591529	0.1994107147590309	0.3223916987056701	T	T	T
0.2223542539330158	0.4007060701576906	0.3225924268390691	T	T	T
0.3332991453999410	0.4004929938709286	0.3224485749894312	T	T	T
0.4446611395714525	0.4008065176143888	0.3224464825646329	T	T	T
0.5562394964684851	0.4019559753978693	0.3223155597420217	T	T	T
0.6675522559095668	0.4018278297257293	0.3222642774745371	T	T	T
0.7791413944032900	0.4020931149014909	0.3223099044700947	T	T	T
0.8902382624868821	0.4019919414931568	0.3225676124134791	T	T	T
0.1117443937976068	0.4013022052474316	0.3226716573863758	T	T	T
0.3326054511175892	0.5995392029895600	0.3225933923859162	T	T	T
0.4442293280259840	0.5996836650385281	0.3225034130783256	T	T	T

0.5559024398885389	0.5998252490454183	0.3225564774385370	T	T	T
0.6675697665399964	0.6008836103417026	0.3227316164862013	T	T	T
0.7787982992095394	0.6011020109273302	0.3228157134444590	T	T	T
0.8898437835263346	0.6010403155884121	0.3229515474984574	T	T	T
0.0006772455939247	0.6008115643118962	0.3230436768955361	T	T	T
0.1114623844758114	0.6005904044131166	0.3230132816293337	T	T	T
0.1111111111111143	0.5000000000000000	0.2561864044279716	F	F	F
0.0001743375508511	0.8001723279379431	0.3230950903903589	T	T	T
0.2220320622980574	0.6002108723514468	0.3229633862371803	T	T	T
0.4438001478020299	0.7995665573290279	0.3225624870747030	T	T	T
0.5554242455084055	0.7998301937525318	0.3226357642867444	T	T	T
0.6671414356884552	0.8001647071563519	0.3226125169661223	T	T	T
0.7785471197385996	0.8004589664212252	0.3228119790240759	T	T	T
0.0008667158211942	0.4015510904295267	0.3226546119762661	T	T	T
0.8893984088084609	0.8003548193383350	0.3230322175372768	T	T	T
0.8888774753093286	0.1993199813308205	0.3226198421868738	T	T	T
0.2216470252116741	0.7996086257084941	0.3230326103429498	T	T	T
0.3325089077334613	0.7994907058789853	0.3227760055555028	T	T	T
0.1096043310204259	0.0974618963647394	0.3905583794348945	T	T	T
0.2204518862131165	0.0974673602100899	0.3902781243406952	T	T	T
0.3317839767917269	0.0978209482434961	0.3898744806754225	T	T	T
0.1111228542999011	0.8000838932289911	0.3231427122035589	T	T	T
0.4427542853633872	0.0978191248834626	0.3894061181742756	T	T	T
0.3333333333333357	0.2000000000000028	0.1894422798390494	F	F	F
0.6662661276070196	0.0984416670872688	0.3894834506735123	T	T	T
0.9992540347297331	0.0981779658409133	0.3903539764834513	T	T	T
0.2216535623766790	0.2994039205380550	0.3876903479048211	T	T	T
0.3327904116925430	0.2992194815530501	0.3875236095439398	T	T	T
0.4447628571367981	0.3007364162204524	0.3874470458571778	T	T	T
0.5557988921478164	0.3013335145386140	0.3869961138124001	T	T	T
0.6670500969959596	0.3005851915285161	0.3865969560975823	T	T	T
0.7787081878422443	0.3008730637062518	0.3871255883846805	T	T	T
0.8896296689119746	0.3005912799263668	0.3877056506742608	T	T	T
0.0003747602200732	0.3003393825978652	0.3879394855718003	T	T	T
0.1109410694660058	0.2999226920708966	0.3878602310847175	T	T	T
0.3335922815912835	0.5012499643780988	0.3897489811091979	T	T	T
0.4451067938230795	0.5012111135907770	0.3896502885963052	T	T	T
0.5568072144195148	0.5020674672091665	0.3899779945421704	T	T	T
0.6681716607057023	0.5026319920514420	0.3898934086230575	T	T	T
0.7795845059505383	0.5028831599687476	0.3897676532066632	T	T	T
0.8907706496117828	0.5027738276537407	0.3901953500496536	T	T	T
0.6676827185340211	0.9009147031413335	0.3886148696707298	T	T	T
0.7784575722762603	0.7006666345171407	0.3900680524548052	T	T	T
0.0017557495588826	0.5026923431436839	0.3905263050093581	T	T	T
0.1120544894963599	0.5018964663932881	0.3905029933072354	T	T	T
0.2227642453169664	0.5016221799612276	0.3903801646150218	T	T	T
0.4432721564301109	0.6989879894138965	0.3887043920239771	T	T	T
0.5550867866940777	0.6990463340995270	0.3887932597677929	T	T	T
0.8884602452307908	0.0984526425024752	0.3903334089066508	T	T	T
0.6672322863711687	0.7003583892023657	0.3893139253629467	T	T	T
0.8897889947989597	0.9004062560755821	0.3902782864742227	T	T	T
0.0002596197006255	0.7004419266203047	0.3904964405070925	T	T	T
0.1107512018736829	0.6999919014234696	0.3906833012542460	T	T	T
0.2213422609076045	0.6996230732357643	0.3903790057940293	T	T	T
0.3319986313274338	0.6991800015440465	0.3898163516372700	T	T	T
0.5558761493128799	0.9006673972720615	0.3887775077838719	T	T	T

0.8894126909677227	0.7005516836584553	0.3903489810940646	T	T	T
0.7790349035723446	0.9008145512792179	0.3897367548045327	T	T	T
0.0004274731497186	0.9000999638131306	0.3906730443608047	T	T	T
0.5561017616427455	0.6001285021720194	0.4569349439597086	T	T	T
0.3331865996801285	0.1997018516220204	0.4538890649281663	T	T	T
0.2217068494431294	0.2001670568284282	0.4540254087497156	T	T	T
0.1109909690715302	0.2007304814510374	0.4544287338103481	T	T	T
0.4453416991723373	0.0006733089681864	0.4565932741839179	T	T	T
0.3331619817664272	0.0005968736078191	0.4572556415033522	T	T	T
0.2216271793928697	0.9996681578688333	0.4581415287646918	T	T	T
0.4456084002896361	0.2028678685043549	0.4528151896326845	T	T	T
0.1110212518146819	0.9993483127593128	0.4587590295881251	T	T	T
0.8901770183336692	0.9999130543410296	0.4578709791565517	T	T	T
0.7787080458209761	0.9999431706071573	0.4574843272429235	T	T	T
0.6669545501828879	0.9987100430734024	0.4562791601452232	T	T	T
0.5558000312459026	0.9996705985147936	0.4568929237976530	T	T	T
0.3327143752525897	0.8996327417408677	0.3898764424919480	T	T	T
0.2218528282739020	0.8998037843073698	0.3903824391663480	T	T	T
0.0004516082334910	0.9996168070718127	0.4587511028036818	T	T	T
0.7776338270458194	0.0985948251551101	0.3897456048884444	T	T	T
0.5551115307023454	0.1999161292966869	0.4528351216690176	T	T	T
0.4444570371525403	0.6009687374314758	0.4561776215462583	T	T	T
0.5574844279370242	0.4033032569022060	0.4552838497938376	T	T	T
0.7779308027328073	0.1999225980564275	0.4535502223247970	T	T	T
0.4438777525679677	0.8996725327768414	0.3892108074506366	T	T	T
0.0000219142260052	0.2006458224397314	0.4545838777957324	T	T	T
0.2223294441580804	0.3997052733331115	0.4544393147658509	T	T	T
0.3332078515903854	0.3996384078844120	0.4535085101653964	T	T	T
0.6670088667543924	0.2013084115566880	0.4525426522147385	T	T	T
0.4443271721679555	0.3988991376489168	0.4536544389472483	T	T	T
0.1110318017691533	0.8998235236794186	0.3905819496212674	T	T	T
0.7777938686510714	0.3998842692587073	0.4534253367764908	T	T	T
0.8895526212084962	0.3997790109921233	0.4538303550838180	T	T	T
0.0002768865753492	0.3994663459029314	0.4546203901741238	T	T	T
0.1112917405155430	0.3995727214064151	0.4547250742878857	T	T	T
0.3328571601869318	0.6001877335534593	0.4574620575552196	T	T	T
0.6663783074229281	0.3988029310777956	0.4528297768245214	T	T	T
0.6672278997200737	0.6015469881617266	0.4571354085195447	T	T	T
0.8890198209727058	0.2005688352746778	0.4544628815603220	T	T	T
0.9265297231468477	0.4682135848504388	0.5376635798344281	T	T	T
0.1108047118778344	0.6003293943565604	0.4588096095527874	T	T	T
0.2214330674134512	0.6005617510232207	0.4580329410517125	T	T	T
0.4446056015349062	0.7997630406482098	0.4537399746699324	T	T	T
0.5552669007323593	0.7998686975195840	0.4542420640960128	T	T	T
0.6660789853696217	0.8002915628108441	0.4537052143398378	T	T	T
0.8887827755928728	0.8000872155449792	0.4562581800719441	T	T	T
0.0000502753463398	0.8000707976753412	0.4567012529950347	T	T	T
0.1109616873007059	0.7999825406865961	0.4567470797177778	T	T	T
0.2221544481109522	0.7999523949140546	0.4561986329301572	T	T	T
0.3336140325674951	0.8004554375433606	0.4557218059360398	T	T	T
0.1837947880668654	0.1300553080380719	0.5376055562898309	T	T	T
0.2944230073362488	0.1292595995509458	0.5376742110971969	T	T	T
0.4050260978699644	0.1288224743056594	0.5351729090016510	T	T	T
0.5181210273912586	0.1302231368141385	0.5369669178120263	T	T	T
0.6267061393334841	0.1276034910627848	0.5349116848811927	T	T	T
0.3721000962532225	0.4684188600052238	0.5369889788347604	T	T	T

0.1114041165383756	0.2999197325952996	0.5245881499245478	T	T	T
0.8895258392263282	0.6005176411305024	0.4579527399417688	T	T	T
0.4437271525093366	0.2982627262985920	0.5250687936546191	T	T	T
0.7388071642620196	0.1296752049421166	0.5371422093639464	T	T	T
0.8495839245556159	0.1299464138577282	0.5381297481554222	T	T	T
0.9615508312408179	0.1306208561579491	0.5382322785190696	T	T	T
0.0727609970400548	0.1304023141041280	0.5379091030144429	T	T	T
0.0001485237914033	0.6006094677142794	0.4587156840665622	T	T	T
0.2222819151160520	0.2993241905678614	0.5246360553533639	T	T	T
0.5549938182729346	0.2989301201592134	0.5216332533990458	T	T	T
0.5914708984621373	0.4658469342210771	0.5414955039609636	T	T	T
0.6663950210011501	0.2993746102459758	0.5238115281819097	T	T	T
0.7773558175675056	0.2993380558952192	0.5211534177322750	T	T	T
0.8882804841240128	0.2992152902709956	0.5249450812670009	T	T	T
0.9993576624989260	0.2990114686246872	0.5247968524923285	T	T	T
0.3334752148648863	0.2992762567598043	0.5218472251859817	T	T	T
0.4842636494624875	0.4689765978821054	0.5368445241068730	T	T	T
0.7777207555904893	0.8005048661238000	0.4559105380357831	T	T	T
0.7781120790163516	0.6002073679753512	0.4574429890070731	T	T	T
0.6674344891981931	0.7985835968074307	0.5414379473783014	T	T	T
0.5553449468835394	0.7981403442952728	0.5431485792393912	T	T	T
0.2966593172530210	0.6338607377410843	0.5357235883401364	T	T	T
0.1858789813037457	0.6343167669837642	0.5378676738293944	T	T	T
0.0748917610450919	0.6349259984048289	0.5377453332890840	T	T	T
0.7043371670544932	0.4683653930176340	0.5359142860321804	T	T	T
0.7778976096057576	0.7993878453477121	0.5448907384898252	T	T	T
0.8532176662127210	0.6359817176138493	0.5360888450710218	T	T	T
0.6312333914108109	0.6343474400637756	0.5368584872365025	T	T	T
0.5203139178544267	0.6354142904510290	0.5335068866677586	T	T	T
0.4089825275394107	0.6351041685922661	0.5351820162896009	T	T	T
0.2611041740217278	0.4682239369382526	0.5384652020992950	T	T	T
0.1489445255500721	0.4678327326611889	0.5386365128377635	T	T	T
0.0375547510371793	0.4679240002041485	0.5384312552536867	T	T	T
0.7415200834445085	0.6352166029254634	0.5346618507918433	T	T	T
0.8884891652745229	0.7994815824738959	0.5449864733326752	T	T	T
0.9634790472545716	0.6347986439345278	0.5376419256711980	T	T	T
0.3676374124754395	0.9610466683266646	0.5331444230873745	T	T	T
0.4785776592367108	0.9615093763948095	0.5355929560728193	T	T	T
0.9995470181596173	0.7991646019842732	0.5454869436429581	T	T	T
0.1103004074880333	0.7986362700405389	0.5455194936221344	T	T	T
0.7016148772821731	0.9623383894496402	0.5349443049378122	T	T	T
0.3322594863914797	0.7976079266639255	0.5445814765764831	T	T	T
0.4435282749639413	0.7984996508484441	0.5414785613964653	T	T	T
0.2213839890011053	0.7981173786090566	0.5449467357506096	T	T	T
0.8138565021005645	0.9638017569618387	0.5354857642577902	T	T	T
0.8154212309257005	0.4686839388786193	0.5371485487469946	T	T	T
0.9243256446906206	0.9636457871998740	0.5376662106541636	T	T	T
0.0351961259831438	0.9631330010582093	0.5376037566885412	T	T	T
0.1463326233119495	0.9630176385878938	0.5377794841502668	T	T	T
0.2565473447972236	0.9616496846404894	0.5361099325659683	T	T	T
0.5904452379030777	0.9612513124474793	0.5338932702720357	T	T	T
0.3037035737366103	0.9788918028851763	0.6485274818375600	T	T	T
0.6786295663356673	0.1547083322264571	0.6396338104423924	T	T	T
0.6794272773772226	0.4847404232961725	0.6403683536329575	T	T	T
0.3885856406440712	0.6366890099970762	0.6409682724008101	T	T	T
0.4952089128991434	0.5483798016104628	0.6399634867714580	T	T	T

0.3020382144573198	0.3131439297286076	0.6361517465587357	T	T	T
0.3596839158446523	0.4087428251574894	0.6386891485392137	T	T	T
0.4305923097050069	0.4484676903938546	0.6394627221106015	T	T	T
0.6774825897221309	0.8215534479755489	0.6447597724521180	T	T	T
0.7481805093213824	0.8613997614241388	0.6493393642303482	T	T	T
0.8058953120182323	0.9569573104660574	0.6491257548139449	T	T	T
0.3169351000000451	0.2597820110466610	0.6341448065704808	T	T	T
0.7198073320607357	0.9667760759047375	0.6399822162177389	T	T	T
0.3887316711262052	0.3035104034453837	0.6350689649435074	T	T	T
0.7912001391551572	0.0103826001784171	0.6444326717092729	T	T	T
0.3616124928726838	0.0742699196654881	0.6463426053563229	T	T	T
0.6133283660442778	0.7224852153536651	0.6426639924490629	T	T	T
0.4316215114018778	0.1129437569059678	0.6396105817179725	T	T	T
0.8074182364114957	0.2891969924873156	0.6408802895136329	T	T	T
0.6147181768975040	0.3853445319599036	0.6365976707819327	T	T	T
0.3172909148649733	0.5934941081245320	0.6456474724305226	T	T	T
0.3611792327452396	0.7429402101550688	0.6505104769141156	T	T	T
0.3175908833178006	0.9246467403250176	0.6436918844501311	T	T	T
0.7932874678815839	0.3425494148052973	0.6335796289193735	T	T	T
0.4959806474454829	0.8815363311634071	0.6428102436956551	T	T	T
0.7490716587924927	0.1939124167019971	0.6440919998215286	T	T	T
0.3030738147115108	0.6473442561549488	0.6503609189629858	T	T	T
0.4315716433776969	0.7821806431980123	0.6455373983337644	T	T	T
0.6140409947978406	0.0553506990149394	0.6401595006732270	T	T	T
0.3883185018661806	0.9672552217596030	0.6366472810399209	T	T	T
0.4959287313870087	0.2117185826682986	0.6364398881090518	T	T	T
0.7218376064252239	0.6301109123455353	0.6432518454430803	T	T	T
0.7934819982156375	0.6733273797545417	0.6450146476335492	T	T	T
0.8079536667690460	0.6193989096752425	0.6448518793696343	T	T	T
0.7501223471041689	0.5238875988016596	0.6422709791748109	T	T	T
0.7219028541486324	0.2991352773258172	0.6290110291746883	T	T	T
0.2735205459398140	0.5184436330533057	0.6443702854684973	T	T	T
0.3510190660302980	0.4534158762358505	0.6395671198742787	T	T	T
0.7563781483315805	0.8163582960476840	0.6519779373221459	T	T	T
0.2463881824013821	0.2808364552796163	0.6345191282443322	T	T	T
0.2476058930636579	0.6153519907457904	0.6529073605327890	T	T	T
0.7566774264707505	0.1487454220890744	0.6494182267883712	T	T	T
0.3533578436588619	0.7883247123391166	0.6534611985986025	T	T	T
0.8615126378303879	0.9894064562901360	0.6515328754113311	T	T	T
0.7584132843414133	0.4788354604545646	0.6412472010297952	T	T	T
0.8629346791934995	0.3212262671282546	0.6430459615908699	T	T	T
0.2736200729904425	0.1849656684623362	0.6308595763834184	T	T	T
0.8347628116557421	0.0854469428406308	0.6429729022791804	T	T	T
0.7052274846678326	0.0048797723260905	0.6359837575222564	T	T	T
0.4037876841272618	0.2656193987347579	0.6331930820557945	T	T	T
0.3541287773109711	0.1200027431935925	0.6492354214685361	T	T	T
0.2485341697192729	0.9470931706517089	0.6529250265953601	T	T	T
0.8371573424703755	0.7484192716841163	0.6457821156807247	T	T	T
0.2738624803270917	0.8495233456534256	0.6441350887328300	T	T	T
0.8635587820811376	0.6514696120127661	0.6456431311045432	T	T	T
0.7071285654799579	0.6684700845064416	0.6431394641522263	T	T	T
0.4029264151882752	0.5983254890077919	0.6368594421983381	T	T	T
0.7080131373038235	0.3373743726673248	0.6225337408428191	T	T	T
0.8371230342726791	0.4172308962667505	0.6299057333091863	T	T	T
0.4020241014829313	0.9282752569610520	0.6323572431200059	T	T	T
0.6647634113139762	0.2065958286886127	0.6317245610634719	T	T	T

0.6630835960574240	0.8737258009164268	0.6402213768216298	T	T	T
0.6205266308357144	0.6652747753174459	0.6438039194015316	T	T	T
0.5483158920077629	0.6984967472953706	0.6376814018483474	T	T	T
0.4870866195743327	0.6047178327754080	0.6395278982728039	T	T	T
0.4883400058059412	0.9381436400532354	0.6418912971296067	T	T	T
0.5489370465093105	0.0309701937440689	0.6361044307914439	T	T	T
0.6216581585740628	0.9987834792232688	0.6416601267523451	T	T	T
0.4454743208342219	0.7295757782216392	0.6408222121827302	T	T	T
0.4452700072288907	0.0601072288220867	0.6348490534196504	T	T	T
0.4447651793190231	0.3959989585254124	0.6379235418467255	T	T	T
0.5602311219554663	0.5732109626253226	0.6396277592797449	T	T	T
0.5607012447235243	0.2352564366318338	0.6311347963578017	T	T	T
0.6655755822406642	0.5375479172504602	0.6413499616708370	T	T	T
0.6220740106034747	0.3283224725369785	0.6346212106660195	T	T	T
0.5501146011026408	0.3615740610336962	0.6352893795817719	T	T	T
0.4893375865312984	0.2694355450678988	0.6381063712880292	T	T	T
0.5607629620299509	0.9052282260614387	0.6388719368897786	T	T	T
0.5535823889264853	0.1316464321561434	0.6186045766443986	T	T	T
0.5544692831938454	0.8015876314425960	0.6260245631427667	T	T	T
0.5549867314239124	0.4664960292299198	0.6455126519648318	T	T	T
0.5528257095106276	0.4534666511529873	0.7416533107137339	T	T	T
0.5526673869891345	0.4609071089611517	0.7004113164405216	T	T	T

Fig. 6c

Au C H N V O

1.000000000000000

26.0801187006857766 0.0000000000000000 0.0000000000000000

-14.4889548337143204 14.4889548337143204 0.0000000000000000

0.0000000000000000 0.0000000000000000 31.0000000000000000

Au C H N V O

279 36 24 18 3 2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.1894422798390494	F	F	F
0.5555555555555571	0.2000000000000028	0.1894422798390494	F	F	F
0.4444444444444429	0.2000000000000028	0.1894422798390494	F	F	F
0.222222222222214	0.2000000000000028	0.1894422798390494	F	F	F
0.1111111111111143	0.2000000000000028	0.1894422798390494	F	F	F
0.7777777777777786	0.2000000000000028	0.1894422798390494	F	F	F
0.8888888888888857	0.0000000000000000	0.1894422798390494	F	F	F
0.6666666666666643	0.0000000000000000	0.1894422798390494	F	F	F
0.5555555555555571	0.0000000000000000	0.1894422798390494	F	F	F
0.4444444444444429	0.0000000000000000	0.1894422798390494	F	F	F
0.3333333333333357	0.0000000000000000	0.1894422798390494	F	F	F
0.222222222222214	0.0000000000000000	0.1894422798390494	F	F	F
0.1111111111111143	0.0000000000000000	0.1894422798390494	F	F	F
0.7777777777777786	0.0000000000000000	0.1894422798390494	F	F	F
0.8888888888888857	0.5000000000000000	0.2561864044279716	F	F	F
0.8888888888888928	0.2000000000000028	0.1894422798390494	F	F	F
0.222222222222214	0.3999999999999986	0.1894422798390494	F	F	F
0.8888888888888928	0.6000000000000014	0.1894422798390494	F	F	F
0.0000000000000000	0.3999999999999986	0.1894422798390494	F	F	F
0.3333333333333357	0.3999999999999986	0.1894422798390494	F	F	F
0.4444444444444429	0.3999999999999986	0.1894422798390494	F	F	F
0.5555555555555571	0.3999999999999986	0.1894422798390494	F	F	F

0.6666666666666643	0.3999999999999986	0.1894422798390494	F	F	F
0.7777777777777786	0.3999999999999986	0.1894422798390494	F	F	F
0.6666666666666714	0.2000000000000028	0.1894422798390494	F	F	F
0.8888888888888857	0.3999999999999986	0.1894422798390494	F	F	F
0.0000000000000000	0.2000000000000028	0.1894422798390494	F	F	F
0.3333333333333357	0.6000000000000014	0.1894422798390494	F	F	F
0.4444444444444429	0.6000000000000014	0.1894422798390494	F	F	F
0.5555555555555571	0.6000000000000014	0.1894422798390494	F	F	F
0.5543536845942768	0.0974277665578405	0.3894204074060312	T	T	T
0.7777777777777786	0.6000000000000014	0.1894422798390494	F	F	F
0.11111111111111072	0.3999999999999986	0.1894422798390494	F	F	F
0.0000000000000000	0.5000000000000000	0.2561864044279716	F	F	F
0.0000000000000000	0.6000000000000014	0.1894422798390494	F	F	F
0.2222222222222214	0.6000000000000014	0.1894422798390494	F	F	F
0.6666666666666643	0.7999999999999972	0.1894422798390494	F	F	F
0.7777777777777786	0.7999999999999972	0.1894422798390494	F	F	F
0.8888888888888857	0.7999999999999972	0.1894422798390494	F	F	F
0.0000000000000000	0.7999999999999972	0.1894422798390494	F	F	F
0.11111111111111072	0.7999999999999972	0.1894422798390494	F	F	F
0.2222222222222214	0.7999999999999972	0.1894422798390494	F	F	F
0.3333333333333286	0.7999999999999972	0.1894422798390494	F	F	F
0.1111111111111143	0.1000000000000014	0.2561864044279716	F	F	F
0.2222222222222214	0.1000000000000014	0.2561864044279716	F	F	F
0.3333333333333357	0.1000000000000014	0.2561864044279716	F	F	F
0.4444444444444429	0.1000000000000014	0.2561864044279716	F	F	F
0.5555555555555571	0.1000000000000014	0.2561864044279716	F	F	F
0.6666666666666643	0.1000000000000014	0.2561864044279716	F	F	F
0.7777777777777786	0.1000000000000014	0.2561864044279716	F	F	F
0.88888888888888928	0.1000000000000014	0.2561864044279716	F	F	F
0.0000000000000000	0.1000000000000014	0.2561864044279716	F	F	F
0.7777777777777786	0.5000000000000000	0.2561864044279716	F	F	F
0.8888888888888857	0.2999999999999972	0.2561864044279716	F	F	F
0.2222222222222214	0.2999999999999972	0.2561864044279716	F	F	F
0.3333333333333286	0.2999999999999972	0.2561864044279716	F	F	F
0.4444444444444429	0.2999999999999972	0.2561864044279716	F	F	F
0.5555555555555571	0.2999999999999972	0.2561864044279716	F	F	F
0.6666666666666643	0.2999999999999972	0.2561864044279716	F	F	F
0.1111111111111143	0.6000000000000014	0.1894422798390494	F	F	F
0.7777777777777786	0.2999999999999972	0.2561864044279716	F	F	F
0.4444444444444429	0.7999999999999972	0.1894422798390494	F	F	F
0.11111111111111072	0.2999999999999972	0.2561864044279716	F	F	F
0.3333333333333357	0.5000000000000000	0.2561864044279716	F	F	F
0.4444444444444429	0.5000000000000000	0.2561864044279716	F	F	F
0.5555555555555571	0.5000000000000000	0.2561864044279716	F	F	F
0.6666666666666643	0.5000000000000000	0.2561864044279716	F	F	F
0.0000000000000000	0.2999999999999972	0.2561864044279716	F	F	F
0.5555555555555571	0.7999999999999972	0.1894422798390494	F	F	F
0.6666666666666643	0.6000000000000014	0.1894422798390494	F	F	F
0.9994200450431739	0.1986879682943767	0.3226696486008397	T	T	T
0.8888888888888857	0.8999999999999986	0.2561864044279716	F	F	F
0.7777777777777786	0.8999999999999986	0.2561864044279716	F	F	F
0.6666666666666643	0.8999999999999986	0.2561864044279716	F	F	F
0.5555555555555571	0.8999999999999986	0.2561864044279716	F	F	F
0.3333333333333357	0.7000000000000028	0.2561864044279716	F	F	F
0.11111111111111072	0.8999999999999986	0.2561864044279716	F	F	F
0.2222222222222214	0.7000000000000028	0.2561864044279716	F	F	F

0.6663220984553229	0.1989600879449689	0.3223193816883299	T	T	T
0.8888888888888928	0.7000000000000028	0.2561864044279716	F	F	F
0.7777777777777786	0.7000000000000028	0.2561864044279716	F	F	F
0.6666666666666714	0.7000000000000028	0.2561864044279716	F	F	F
0.5555555555555571	0.7000000000000028	0.2561864044279716	F	F	F
0.4444444444444429	0.7000000000000028	0.2561864044279716	F	F	F
0.1111111111111143	0.7000000000000028	0.2561864044279716	F	F	F
0.2222222222222214	0.8999999999999986	0.2561864044279716	F	F	F
0.0000000000000000	0.7000000000000028	0.2561864044279716	F	F	F
0.4444444444444429	0.8999999999999986	0.2561864044279716	F	F	F
0.3333333333333357	0.8999999999999986	0.2561864044279716	F	F	F
0.1103718011697095	0.9990914593832849	0.3230135208780283	T	T	T
0.5551293273011330	0.9996928351724264	0.3224129299653348	T	T	T
0.6667792943939365	-0.0000104093391771	0.3224138557724360	T	T	T
0.7784266503045465	0.0002571397087981	0.3225383004462473	T	T	T
0.8890357669735958	0.9996884245476827	0.3229083028947191	T	T	T
0.0000000000000000	0.8999999999999986	0.2561864044279716	F	F	F
0.9997721203227299	0.9994238483415477	0.3229998867118935	T	T	T
0.3322478330499342	0.9990710937226203	0.3227577443001415	T	T	T
0.4436024373875906	0.9992228482260171	0.3226324462387504	T	T	T
0.1103524740710947	0.1983927947493367	0.3226272012706650	T	T	T
0.2211415718987809	0.1980176042778318	0.3225968258485108	T	T	T
0.3323056244297884	0.1982285989382780	0.3225154929124227	T	T	T
0.4436458183389825	0.1988896907466747	0.3224219288870724	T	T	T
0.2213396152550545	0.9992050333324580	0.3229649284054805	T	T	T
0.2222222222222214	0.5000000000000000	0.2561864044279716	F	F	F
0.5547561887859715	0.1986636159156057	0.3225005133869314	T	T	T
0.7778403233852831	0.1993009747786094	0.3223878942655736	T	T	T
0.2223582559075423	0.4006248816774020	0.3225705518834993	T	T	T
0.3333058677204795	0.4003877917435890	0.3224748126182689	T	T	T
0.4446417151000256	0.4007236340569031	0.3224504395002635	T	T	T
0.5562086196873894	0.4019167259010792	0.3223245830004894	T	T	T
0.6674898949647168	0.4018041999934911	0.3222914379064115	T	T	T
0.7790636587438442	0.4020234571997392	0.3222962725593046	T	T	T
0.8901811772730022	0.4019201787538583	0.3225476332763366	T	T	T
0.1117487612585590	0.4012583625496331	0.3226434831646576	T	T	T
0.3326114625463459	0.5994768334144469	0.3225802991771557	T	T	T
0.4442153955228725	0.5995713641833583	0.3225185956045633	T	T	T
0.5558867738148312	0.5997350269764242	0.3225716101201936	T	T	T
0.6675215304215310	0.6008041492416388	0.3227586840265533	T	T	T
0.7786932446370121	0.6010214965831340	0.3228472941214064	T	T	T
0.8897388710145486	0.6009684652048769	0.3229503435870177	T	T	T
0.0006047397242372	0.6007509649752111	0.3230260134546628	T	T	T
0.1114220047351278	0.6005443423619530	0.3229952523983864	T	T	T
0.1111111111111143	0.5000000000000000	0.2561864044279716	F	F	F
0.0000762276749220	0.8000796891461875	0.3230938753670687	T	T	T
0.2220280939324904	0.6001780485728296	0.3229336268682070	T	T	T
0.4438172047781387	0.7995121882102751	0.3225535398826498	T	T	T
0.5553961374246166	0.7997279077141565	0.3226526872668700	T	T	T
0.6670748780450712	0.8000248137329588	0.3226446601039138	T	T	T
0.7784655262506472	0.8003448543994306	0.3228323498460728	T	T	T
0.0008431492142776	0.4014947083811691	0.3226309403283193	T	T	T
0.8892790537643944	0.8002260134204179	0.3230581639827852	T	T	T
0.8888313487923359	0.1992258389399557	0.3226105555993351	T	T	T
0.2216442574477504	0.7996084954571376	0.3230169218181765	T	T	T
0.3325366814983283	0.7994982342740173	0.3227585293371902	T	T	T

0.1095315052890979	0.0972525781113985	0.3905648276540757	T	T	T
0.2203330684677466	0.0972625452540457	0.3903057270876096	T	T	T
0.3317079287524883	0.0977439179696122	0.3898986399765028	T	T	T
0.1110732993264954	0.8000422792818185	0.3231320209394968	T	T	T
0.4426957560144026	0.0977885974076838	0.3893852201640636	T	T	T
0.3333333333333357	0.2000000000000028	0.1894422798390494	F	F	F
0.6661582037428315	0.0982842924524381	0.3894744455426548	T	T	T
0.9991879379675893	0.0980072566741639	0.3903196430299501	T	T	T
0.2215585575437999	0.2991730637193886	0.3876585580567707	T	T	T
0.3327100983547525	0.2989042610971252	0.3875696695030890	T	T	T
0.4447334177937038	0.3007203762175021	0.3875316953481577	T	T	T
0.5557688689829181	0.3014116130350514	0.3870958864384166	T	T	T
0.6669793643807018	0.3005327350574044	0.3865845626901724	T	T	T
0.7786284353996652	0.3007721787733917	0.3870894309067509	T	T	T
0.8895821518578485	0.3005272116148269	0.3876625430428489	T	T	T
0.0003865965339037	0.3003366401106307	0.3878927097786506	T	T	T
0.1109404577626045	0.2998789948397746	0.3878227667713590	T	T	T
0.3335272035152572	0.5010658467447837	0.3897275781051067	T	T	T
0.4450774312134958	0.5009861941147653	0.3896834600411586	T	T	T
0.5567431241859376	0.5018968690842930	0.3900520902053554	T	T	T
0.6680163148064915	0.5024936944166440	0.3900090102484837	T	T	T
0.7794712199272952	0.5028123523489825	0.3897887399577159	T	T	T
0.8906586328300000	0.5026316335519843	0.3901700401465065	T	T	T
0.6675990349383428	0.9007619935497934	0.3886455541038076	T	T	T
0.7783329811427692	0.7005289728406462	0.3901690098255258	T	T	T
0.0016803745258205	0.5025667104790842	0.3904870886727957	T	T	T
0.1120233772748054	0.5018118889537047	0.3904615814937570	T	T	T
0.2227253672199858	0.5015087993965965	0.3903460541855214	T	T	T
0.4432364471820181	0.6988404787432451	0.3886910484779970	T	T	T
0.5550048555933440	0.6988256545467342	0.3888274100666569	T	T	T
0.8883925596872250	0.0983032693473123	0.3903037752607618	T	T	T
0.6671494877928820	0.7001282050127658	0.3894028383473692	T	T	T
0.8896494293656164	0.9002048310211778	0.3903188575788586	T	T	T
0.0001249092929517	0.7002882725033568	0.3904538827666335	T	T	T
0.1106787738702439	0.6998920635903514	0.3906337816170251	T	T	T
0.2212999207271663	0.6995565095598937	0.3903140659222980	T	T	T
0.3319582415964839	0.6990903689552551	0.3897536688001828	T	T	T
0.5558404871246825	0.9005216314230468	0.3888112615609232	T	T	T
0.8892498500145934	0.7004127974834828	0.3904005107028419	T	T	T
0.7789512226752451	0.9006516266298512	0.3897565351014021	T	T	T
0.0002639859985589	0.8999063437897136	0.3906897580639626	T	T	T
0.5559396985165571	0.5997091212919562	0.4569696564631650	T	T	T
0.3329188604019077	0.1992968818322245	0.4540552121926674	T	T	T
0.2215792166541139	0.1998432025702762	0.4540978009571129	T	T	T
0.1109111489583704	0.2005501624218613	0.4543557259434239	T	T	T
0.4452014191276388	0.0005104289630257	0.4565671077304758	T	T	T
0.3330954734024832	0.0004180884694800	0.4572341449541384	T	T	T
0.2215024160278800	0.9994299317053293	0.4581545792107972	T	T	T
0.4455376826109162	0.2029353189482388	0.4527826992404578	T	T	T
0.1108825967419119	0.9990505992333828	0.4587901474280989	T	T	T
0.8901999870351542	0.9998756818646896	0.4578584813868498	T	T	T
0.7786446057690095	0.9998373735444651	0.4574785906264586	T	T	T
0.6668983252720041	0.9986065176629401	0.4562861581439689	T	T	T
0.5556953147429216	0.9995423371717596	0.4568695015898636	T	T	T
0.3326822034505921	0.8995584037492634	0.3898572211389066	T	T	T
0.2217879827206028	0.8997196259808522	0.3903669075332827	T	T	T

0.0003792576727498	0.9994239813985665	0.4587581392468004	T	T	T
0.7775501576403581	0.0984396146245834	0.3897226435377478	T	T	T
0.5550249546632050	0.1997441416288808	0.4527886053318935	T	T	T
0.4442850188162292	0.6006708386745938	0.4561402407179229	T	T	T
0.5573474633218105	0.4033871720127308	0.4555561775566677	T	T	T
0.7778786093078468	0.1998593197632048	0.4534785814000667	T	T	T
0.4438460322230072	0.8995761098094387	0.3892042906006681	T	T	T
0.0000258555137856	0.2006177643906688	0.4544820481978705	T	T	T
0.2222971610631470	0.3995858587778442	0.4544240582943180	T	T	T
0.3329914322677644	0.3991044079710107	0.4534035157100476	T	T	T
0.6669244171399220	0.2012098491992109	0.4524856694392735	T	T	T
0.4440580120458694	0.3984665326392375	0.4537989514773689	T	T	T
0.1108950079846396	0.8996530983750872	0.3905777892002095	T	T	T
0.7777194746338906	0.3997143728433550	0.4534179969533871	T	T	T
0.8894764409070250	0.3996424125288109	0.4538317925225860	T	T	T
0.0002676952912473	0.3994308825756001	0.4546166588310659	T	T	T
0.1113069199733945	0.3995719015123621	0.4547228959467145	T	T	T
0.3327372255483951	0.6000524402006312	0.4573936278990241	T	T	T
0.6663644028334231	0.3987337045589522	0.4528762212895940	T	T	T
0.6674759566070085	0.6016117173169760	0.4573160839973426	T	T	T
0.8890356352291252	0.2005690738260570	0.4543383912901419	T	T	T
0.9261579384354262	0.4673706835351802	0.5377826056561033	T	T	T
0.1107437049193651	0.6001983348605925	0.4587348461420517	T	T	T
0.2213566959933069	0.6004766265807130	0.4579702880981403	T	T	T
0.4445252110195388	0.7995763077983555	0.4536718781348735	T	T	T
0.5551316321255056	0.7995835802000674	0.4543196846509978	T	T	T
0.6659387212453768	0.8000635551313440	0.4536731862691544	T	T	T
0.8885973239327928	0.7998893246515802	0.4563768162095126	T	T	T
0.9998404478436909	0.7998183845112994	0.4566989566774499	T	T	T
0.1107650587643431	0.7997396812902017	0.4567096335897993	T	T	T
0.2220324799644859	0.7997795191290331	0.4561440200912500	T	T	T
0.3335043479336326	0.8002356970743795	0.4556952016721431	T	T	T
0.1833456104399950	0.1292366189920116	0.5376385100810961	T	T	T
0.2941167355683013	0.1287550906306708	0.5379136135601755	T	T	T
0.4046744447384687	0.1281326880349898	0.5348739249045638	T	T	T
0.5178763330929974	0.1295378783053434	0.5368520280189161	T	T	T
0.6263789226724024	0.1268271489880543	0.5347391741411160	T	T	T
0.3716161466799043	0.4677601585986660	0.5367709931834904	T	T	T
0.1109101885871262	0.2991071959893250	0.5245075661391445	T	T	T
0.8893694921520895	0.6002844986911842	0.4579153716584992	T	T	T
0.4433826722143508	0.2977014945324758	0.5254144005535273	T	T	T
0.7382654600825190	0.1286489763266552	0.5369240453102923	T	T	T
0.8489487072667231	0.1287916478059064	0.5378004301613564	T	T	T
0.9609548244780304	0.1295731916367256	0.5379730962618352	T	T	T
0.0722235392228889	0.1294403300551801	0.5377408570304620	T	T	T
0.0000316356084425	0.6003751059851791	0.4586558604116799	T	T	T
0.2218014732893815	0.2985124819878696	0.5244961029423422	T	T	T
0.5547627442146292	0.2983713006402812	0.5214071843176794	T	T	T
0.5914073639766171	0.4651863585362721	0.5417324495799507	T	T	T
0.6661648317720376	0.2987820562821853	0.5238769243713408	T	T	T
0.7770512592115377	0.2986723971082931	0.5212065588703965	T	T	T
0.8878373246570522	0.2983593722316817	0.5248788467439949	T	T	T
0.9988629680800847	0.2981399733588209	0.5247508186097966	T	T	T
0.3330761734001604	0.2985956787710414	0.5222735554090666	T	T	T
0.4835234229822507	0.4678970865932674	0.5370534953693566	T	T	T
0.7776615505762857	0.8004807208262527	0.4560491134518426	T	T	T

0.7779486601999324	0.6001423326825267	0.4576141672278413	T	T	T
0.6668170582779650	0.7975148002981274	0.5413645887657331	T	T	T
0.5546456653617419	0.7971390017133981	0.5432474299537511	T	T	T
0.2960003718368596	0.6328594508279061	0.5357274829853940	T	T	T
0.1853377297406203	0.6334049715988889	0.5378930296368934	T	T	T
0.0744817469537116	0.6340670891056182	0.5377121687726359	T	T	T
0.7041016645717033	0.4676120860045921	0.5360991301677458	T	T	T
0.7773559130495595	0.7982015646779568	0.5450653630764252	T	T	T
0.8529125524152750	0.6352392965845064	0.5360648088398680	T	T	T
0.6307034061829142	0.6333328754812033	0.5366590608125388	T	T	T
0.5197854955004659	0.6344901765340937	0.5334941229403383	T	T	T
0.4083186024605295	0.6341287125541853	0.5351698546888690	T	T	T
0.2604307074796532	0.4672476585495046	0.5386054136951218	T	T	T
0.1483281329558384	0.4668568465396263	0.5387978500129971	T	T	T
0.0370518155035041	0.4669858088780684	0.5385780698603447	T	T	T
0.7409059075808659	0.6340123959398367	0.5354849927759450	T	T	T
0.8879649867845101	0.7984811483537215	0.5451336303636263	T	T	T
0.9631620693912899	0.6339981443628663	0.5376247985300063	T	T	T
0.3672885973123529	0.9603432045270315	0.5331374629446272	T	T	T
0.4780769873682756	0.9606787144253506	0.5354711377796909	T	T	T
0.9991992413208877	0.7983177363663932	0.5454938302934955	T	T	T
0.1099957995977571	0.7978767608539011	0.5454775710180308	T	T	T
0.7009330391686315	0.9611725190770891	0.5348762724747143	T	T	T
0.3316910038714370	0.7967603522012998	0.5445682902024341	T	T	T
0.4428444598039949	0.7975225620928621	0.5413566967534020	T	T	T
0.2210125971588141	0.7973913446471276	0.5449027528494191	T	T	T
0.8131889297751507	0.9625287598255362	0.5353126362247177	T	T	T
0.8151344823078138	0.4679197816953764	0.5372396172077982	T	T	T
0.9237694963460831	0.9625980575530622	0.5376065376406977	T	T	T
0.0347005106461419	0.9621591316396493	0.5375696844871682	T	T	T
0.1459871637530913	0.9622639256610612	0.5377845211417345	T	T	T
0.2561952284509569	0.9609866466303930	0.5359986731272651	T	T	T
0.5898032838403415	0.9602235494790790	0.5337661059294545	T	T	T
0.3042072584448303	0.9811026318177473	0.6478460861809557	T	T	T
0.6785626063343725	0.1550429538012080	0.6394084026913550	T	T	T
0.6797102896573305	0.4858246100389478	0.6419767332460031	T	T	T
0.3894804641422818	0.6369576790231829	0.6411867262491777	T	T	T
0.4967157485607305	0.5488384678220772	0.6400397138468359	T	T	T
0.3041384263482390	0.3135114098181980	0.6347478032567708	T	T	T
0.3616376527652381	0.4091645178413773	0.6369458065637092	T	T	T
0.4324077682763502	0.4490368537553125	0.6406019255995723	T	T	T
0.6785661899967711	0.8223685714044181	0.6445896396958819	T	T	T
0.7493217847397798	0.8623280015612189	0.6489270955806661	T	T	T
0.8069579908276017	0.9579104328489058	0.6487620506582240	T	T	T
0.3191166096710070	0.2601841567035804	0.6362085086884545	T	T	T
0.7206193941807439	0.9673986517221078	0.6399776220037207	T	T	T
0.3905999457964693	0.3038244849543721	0.6404799144043607	T	T	T
0.7920864379919863	0.0111565033544847	0.6442941894741563	T	T	T
0.3621051943789177	0.0764301700148225	0.6451712920334112	T	T	T
0.6144942757470236	0.7231323038656702	0.6423816169340303	T	T	T
0.4321699264581854	0.1150544465400926	0.6387835698457315	T	T	T
0.8073319670834738	0.2896522361352734	0.6408670942444291	T	T	T
0.6152105725479312	0.3870057775981672	0.6368173753502302	T	T	T
0.3180664132935269	0.5933714181495054	0.6457798485392180	T	T	T
0.3612369889277778	0.7425006595191203	0.6496994287901117	T	T	T
0.3181081800479053	0.9267819620410992	0.6436728105842665	T	T	T

0.7931673123853448	0.3430575639936412	0.6339465433091644	T	T	T
0.4960722895594074	0.8816239448805883	0.6422507931296438	T	T	T
0.7490181859672616	0.1943084501136823	0.6438064139273415	T	T	T
0.3034033155367035	0.6468351558997316	0.6499630263648669	T	T	T
0.4318058348688373	0.7821703280004209	0.6449652510345523	T	T	T
0.6139903895038208	0.0555995654398823	0.6398018250797313	T	T	T
0.3888305513194390	0.9692334773534431	0.6368800978930267	T	T	T
0.4965687180007264	0.2137601370929910	0.6353078132447953	T	T	T
0.7216962140845303	0.6306986684486487	0.6482719238076677	T	T	T
0.7934381919671045	0.6744053049247046	0.6475307470216208	T	T	T
0.8083448699152774	0.6210729421843877	0.6442902643874154	T	T	T
0.7506671019489328	0.5256400892130759	0.6412347483964624	T	T	T
0.7217572284357601	0.2996198797982559	0.6294538615606059	T	T	T
0.2745182046096413	0.5182690371361802	0.6448454500958916	T	T	T
0.3530624019514478	0.4538910957534883	0.6351040014105123	T	T	T
0.7576784827984506	0.8174119708016278	0.6511915953579756	T	T	T
0.2487657456760225	0.2812074495135574	0.6305930384690277	T	T	T
0.2478224850590962	0.6144798384528583	0.6524354536402465	T	T	T
0.7567012204241068	0.1491622149893737	0.6488479577453914	T	T	T
0.3530652335903256	0.7875727061363080	0.6522612971886939	T	T	T
0.8626238249464835	0.9904507651343397	0.6509212584427320	T	T	T
0.7592444495098193	0.4811628504409344	0.6374881982462359	T	T	T
0.8628609710372852	0.3217017189687059	0.6429878520495875	T	T	T
0.2760199194608141	0.1852990604453458	0.6332450116189128	T	T	T
0.8355859061358551	0.0862178648435815	0.6428143918505211	T	T	T
0.7059286739331659	0.0053874105107303	0.6360389949005910	T	T	T
0.4058534653903850	0.2661215619755669	0.6413413087206706	T	T	T
0.3544597226272402	0.1220540682342062	0.6474541624310917	T	T	T
0.2490456171746896	0.9494314056511861	0.6520499274101973	T	T	T
0.8368976872681431	0.7494682126896940	0.6486878814543569	T	T	T
0.2743567553220153	0.8516772932061466	0.6443580351330532	T	T	T
0.8640542200954324	0.6536064321645634	0.6428112522469284	T	T	T
0.7066335064624416	0.6685724092603900	0.6502029984160779	T	T	T
0.4040776535315418	0.5988100458425655	0.6374967282608360	T	T	T
0.7078126897003473	0.3379012936389774	0.6233553784144906	T	T	T
0.8369854257141723	0.4178095115293126	0.6305487447552984	T	T	T
0.4025167232918462	0.9301277995775628	0.6330275720752583	T	T	T
0.6646832397638998	0.2070132459949906	0.6318356687610622	T	T	T
0.6640371869575735	0.8743850641155180	0.6401887012507662	T	T	T
0.6220561356710511	0.6663020657838896	0.6433715329961597	T	T	T
0.5493524962170684	0.6987179125571987	0.6374980757551728	T	T	T
0.4884722729504893	0.6050469494836632	0.6399314741918001	T	T	T
0.4882769784527757	0.9381089193193389	0.6412454695565489	T	T	T
0.5488565428915152	0.0311086861968653	0.6356901573938519	T	T	T
0.6217858169317947	0.9991799629053678	0.6413816728483726	T	T	T
0.4460883799225551	0.7298901834974486	0.6406774243019245	T	T	T
0.4457710381564315	0.0620350774574023	0.6346842787549215	T	T	T
0.4465738687091184	0.3964771188719776	0.6427945807995937	T	T	T
0.5620547145202824	0.5741920125532579	0.6383762134464360	T	T	T
0.5612605502226985	0.2370323116439804	0.6304856624811402	T	T	T
0.6655553038249850	0.538028977729902	0.6459319171743511	T	T	T
0.6223981240158820	0.3297552845523157	0.6349691812577067	T	T	T
0.5509205761826448	0.3637449310614427	0.6333304980645545	T	T	T
0.4902512506313715	0.2718221391708349	0.6362365272041126	T	T	T
0.5609966655165363	0.9055390766612229	0.6385817757274498	T	T	T
0.5538056594222146	0.1325651869382985	0.6186189665991612	T	T	T

0.5551346932668149	0.8020042813373831	0.6262375598009750	T	T	T
0.5565161683369840	0.4692390480858620	0.6517996778790707	T	T	T
0.5457977513244667	0.4206513455430654	0.7077139287345887	T	T	T
0.5624096833859179	0.5024131269188756	0.7069649388521114	T	T	T

Fig. 6d

```

-----
Au C H N V O
1.000000000000000
26.0801187006857766 0.000000000000000 0.000000000000000
-14.4889548337143204 14.4889548337143204 0.000000000000000
0.000000000000000 0.000000000000000 31.000000000000000
Au C H N V O
279 36 24 18 3 2
Selective dynamics
Direct
0.000000000000000 0.000000000000000 0.1894422798390494 F F F
0.5555555555555571 0.2000000000000028 0.1894422798390494 F F F
0.4444444444444429 0.2000000000000028 0.1894422798390494 F F F
0.2222222222222214 0.2000000000000028 0.1894422798390494 F F F
0.1111111111111143 0.2000000000000028 0.1894422798390494 F F F
0.7777777777777786 0.2000000000000028 0.1894422798390494 F F F
0.8888888888888857 0.0000000000000000 0.1894422798390494 F F F
0.6666666666666643 0.0000000000000000 0.1894422798390494 F F F
0.5555555555555571 0.0000000000000000 0.1894422798390494 F F F
0.4444444444444429 0.0000000000000000 0.1894422798390494 F F F
0.3333333333333357 0.0000000000000000 0.1894422798390494 F F F
0.2222222222222214 0.0000000000000000 0.1894422798390494 F F F
0.1111111111111143 0.0000000000000000 0.1894422798390494 F F F
0.7777777777777786 0.0000000000000000 0.1894422798390494 F F F
0.8888888888888857 0.5000000000000000 0.2561864044279716 F F F
0.8888888888888828 0.2000000000000028 0.1894422798390494 F F F
0.2222222222222214 0.3999999999999986 0.1894422798390494 F F F
0.8888888888888828 0.6000000000000014 0.1894422798390494 F F F
0.0000000000000000 0.3999999999999986 0.1894422798390494 F F F
0.3333333333333357 0.3999999999999986 0.1894422798390494 F F F
0.4444444444444429 0.3999999999999986 0.1894422798390494 F F F
0.5555555555555571 0.3999999999999986 0.1894422798390494 F F F
0.6666666666666643 0.3999999999999986 0.1894422798390494 F F F
0.7777777777777786 0.3999999999999986 0.1894422798390494 F F F
0.66666666666666714 0.2000000000000028 0.1894422798390494 F F F
0.8888888888888857 0.3999999999999986 0.1894422798390494 F F F
0.0000000000000000 0.2000000000000028 0.1894422798390494 F F F
0.3333333333333357 0.6000000000000014 0.1894422798390494 F F F
0.4444444444444429 0.6000000000000014 0.1894422798390494 F F F
0.5555555555555571 0.6000000000000014 0.1894422798390494 F F F
0.5546779298792380 0.0979128714569980 0.3893326662258524 T T T
0.7777777777777786 0.6000000000000014 0.1894422798390494 F F F
0.11111111111111072 0.3999999999999986 0.1894422798390494 F F F
0.0000000000000000 0.5000000000000000 0.2561864044279716 F F F
0.0000000000000000 0.6000000000000014 0.1894422798390494 F F F
0.2222222222222214 0.6000000000000014 0.1894422798390494 F F F
0.6666666666666643 0.7999999999999972 0.1894422798390494 F F F
0.7777777777777786 0.7999999999999972 0.1894422798390494 F F F
0.8888888888888857 0.7999999999999972 0.1894422798390494 F F F
0.0000000000000000 0.7999999999999972 0.1894422798390494 F F F

```

0.1111111111111072	0.7999999999999972	0.1894422798390494	F	F	F
0.222222222222214	0.7999999999999972	0.1894422798390494	F	F	F
0.3333333333333286	0.7999999999999972	0.1894422798390494	F	F	F
0.1111111111111143	0.1000000000000014	0.2561864044279716	F	F	F
0.222222222222214	0.1000000000000014	0.2561864044279716	F	F	F
0.3333333333333357	0.1000000000000014	0.2561864044279716	F	F	F
0.4444444444444429	0.1000000000000014	0.2561864044279716	F	F	F
0.5555555555555571	0.1000000000000014	0.2561864044279716	F	F	F
0.6666666666666643	0.1000000000000014	0.2561864044279716	F	F	F
0.7777777777777786	0.1000000000000014	0.2561864044279716	F	F	F
0.8888888888888928	0.1000000000000014	0.2561864044279716	F	F	F
0.0000000000000000	0.1000000000000014	0.2561864044279716	F	F	F
0.7777777777777786	0.5000000000000000	0.2561864044279716	F	F	F
0.8888888888888857	0.2999999999999972	0.2561864044279716	F	F	F
0.222222222222214	0.2999999999999972	0.2561864044279716	F	F	F
0.3333333333333286	0.2999999999999972	0.2561864044279716	F	F	F
0.4444444444444429	0.2999999999999972	0.2561864044279716	F	F	F
0.5555555555555571	0.2999999999999972	0.2561864044279716	F	F	F
0.6666666666666643	0.2999999999999972	0.2561864044279716	F	F	F
0.1111111111111143	0.6000000000000014	0.1894422798390494	F	F	F
0.7777777777777786	0.2999999999999972	0.2561864044279716	F	F	F
0.4444444444444429	0.7999999999999972	0.1894422798390494	F	F	F
0.1111111111111072	0.2999999999999972	0.2561864044279716	F	F	F
0.3333333333333357	0.5000000000000000	0.2561864044279716	F	F	F
0.4444444444444429	0.5000000000000000	0.2561864044279716	F	F	F
0.5555555555555571	0.5000000000000000	0.2561864044279716	F	F	F
0.6666666666666643	0.5000000000000000	0.2561864044279716	F	F	F
0.0000000000000000	0.2999999999999972	0.2561864044279716	F	F	F
0.5555555555555571	0.7999999999999972	0.1894422798390494	F	F	F
0.6666666666666643	0.6000000000000014	0.1894422798390494	F	F	F
0.9994835857700148	0.1987278010502339	0.3226734273246179	T	T	T
0.8888888888888857	0.8999999999999986	0.2561864044279716	F	F	F
0.7777777777777786	0.8999999999999986	0.2561864044279716	F	F	F
0.6666666666666643	0.8999999999999986	0.2561864044279716	F	F	F
0.5555555555555571	0.8999999999999986	0.2561864044279716	F	F	F
0.3333333333333357	0.7000000000000028	0.2561864044279716	F	F	F
0.1111111111111072	0.8999999999999986	0.2561864044279716	F	F	F
0.222222222222214	0.7000000000000028	0.2561864044279716	F	F	F
0.6664254483765917	0.1991519184024803	0.3223050353545850	T	T	T
0.8888888888888928	0.7000000000000028	0.2561864044279716	F	F	F
0.7777777777777786	0.7000000000000028	0.2561864044279716	F	F	F
0.6666666666666714	0.7000000000000028	0.2561864044279716	F	F	F
0.5555555555555571	0.7000000000000028	0.2561864044279716	F	F	F
0.4444444444444429	0.7000000000000028	0.2561864044279716	F	F	F
0.1111111111111143	0.7000000000000028	0.2561864044279716	F	F	F
0.222222222222214	0.8999999999999986	0.2561864044279716	F	F	F
0.0000000000000000	0.7000000000000028	0.2561864044279716	F	F	F
0.4444444444444429	0.8999999999999986	0.2561864044279716	F	F	F
0.3333333333333357	0.8999999999999986	0.2561864044279716	F	F	F
0.1104008856539632	0.9991576022725579	0.3230345444189144	T	T	T
0.5552619472240589	0.9998540645347296	0.3223669231810759	T	T	T
0.6668406226416809	0.9999779413594656	0.3223818071421110	T	T	T
0.7785127345999594	0.0002810713537318	0.3225091834694888	T	T	T
0.8890981948651384	0.9996805913127238	0.3229029519826057	T	T	T
0.0000000000000000	0.8999999999999986	0.2561864044279716	F	F	F
0.9997743669730241	0.9993920419617188	0.3230073815786920	T	T	T

0.3323493804911281	0.9993910000584412	0.3226873586384733	T	T	T
0.4437753895644582	0.9994788340611207	0.3225875477123896	T	T	T
0.1103861798079448	0.1983532832512580	0.3226225226733805	T	T	T
0.2211658661990274	0.1979708341927173	0.3225928553842550	T	T	T
0.3324021723942432	0.1983550896284176	0.3225019029484800	T	T	T
0.4438032185807204	0.1992255883767938	0.3224072391209928	T	T	T
0.2213554725152189	0.9993893850591467	0.3229383844909384	T	T	T
0.2222222222222214	0.5000000000000000	0.2561864044279716	F	F	F
0.5549113221134651	0.1989478036923545	0.3224783273666521	T	T	T
0.7779147379982475	0.1993672060760471	0.3223560742532036	T	T	T
0.2224122852061237	0.4005080987831950	0.3225756154862862	T	T	T
0.3333187713955177	0.4002272748887802	0.3225257635339274	T	T	T
0.4446794589260645	0.4007270133411230	0.3224976334946324	T	T	T
0.5562541800951268	0.4020752329399557	0.3223784185028430	T	T	T
0.6675847043763821	0.4020197587059952	0.3222616422814637	T	T	T
0.7790801869993709	0.4020710469256698	0.3223115656447588	T	T	T
0.8902191682084535	0.4019724640946450	0.3225269354567114	T	T	T
0.1118171584103269	0.4012579046935303	0.3226178744926604	T	T	T
0.3325592187252437	0.5993105416409016	0.3225607360563492	T	T	T
0.4442017242212352	0.5993864228858156	0.3225155236937030	T	T	T
0.5559482940182371	0.5996509731574994	0.3225918162828584	T	T	T
0.6675373971839687	0.6008083096817823	0.3227962604453847	T	T	T
0.7786982510713425	0.6010927462203426	0.3228756646537951	T	T	T
0.8896601731242959	0.6009482610928826	0.3229465471887387	T	T	T
0.0005545849355544	0.6007459574377394	0.3230064600117208	T	T	T
0.1114413489961842	0.6005784419225351	0.3229531342998129	T	T	T
0.1111111111111143	0.5000000000000000	0.2561864044279716	F	F	F
0.9999937635439561	0.8000878885308155	0.3230660391462194	T	T	T
0.2220501769838864	0.6001512590449541	0.3229128268421653	T	T	T
0.4438146075151416	0.7994032464610447	0.3224980243266176	T	T	T
0.5554087627219848	0.7995995636479327	0.3226436433696817	T	T	T
0.6671305195499186	0.7999606029403361	0.3226540796125732	T	T	T
0.7784982389109543	0.8003784033150877	0.3228416142886502	T	T	T
0.0009210308543895	0.4015681934776862	0.3226056994321684	T	T	T
0.8892471721712726	0.8002456290252827	0.3230726830241620	T	T	T
0.8889153971477274	0.1993194097503275	0.3226266284862487	T	T	T
0.2216529246474744	0.7996935593380263	0.3229484203095944	T	T	T
0.3326002130515613	0.7995514384583374	0.3227069601440781	T	T	T
0.1096088720780478	0.0971607304097847	0.3906345028609144	T	T	T
0.2205178025481912	0.0974531932982365	0.3904241267077143	T	T	T
0.3319683145253735	0.0984421540979034	0.3898752588002952	T	T	T
0.1110082632465269	0.8000966823394096	0.3230660868292279	T	T	T
0.4429443883145137	0.0984225087954286	0.3892634625294061	T	T	T
0.3333333333333357	0.2000000000000028	0.1894422798390494	F	F	F
0.6663352042353972	0.0984218156517844	0.3893663148336923	T	T	T
0.9993217102362463	0.0979896554490949	0.3902900462463552	T	T	T
0.2215089533535237	0.2988113263747149	0.3876681793658657	T	T	T
0.3327760768527150	0.2985789820165327	0.3876750112845297	T	T	T
0.4447322209963670	0.3008118343621691	0.3877500035309349	T	T	T
0.5560055843001742	0.3018351992925793	0.3870906335425579	T	T	T
0.6670806974915127	0.3008612895367384	0.3866662878257833	T	T	T
0.7786410989361768	0.3007434017720558	0.3870601804507623	T	T	T
0.8897625742224112	0.3008152852947222	0.3876268228390741	T	T	T
0.0006393753740466	0.3006684305880069	0.3878520797569073	T	T	T
0.1110596982276756	0.2999412526372111	0.3878283378276997	T	T	T
0.3336270252494191	0.5008209463546693	0.3897610634872020	T	T	T

0.4451471781698944	0.5006787785399569	0.3897967652436362	T	T	T
0.5567516370810910	0.5018311043483309	0.3902240403981001	T	T	T
0.6681365821299740	0.5027132846344712	0.3901380585957424	T	T	T
0.7793523561945763	0.5027183330007579	0.3898657793161955	T	T	T
0.8906395495890295	0.5025819877792284	0.3901463553105120	T	T	T
0.6678089729614093	0.9008242253077599	0.3885884775674102	T	T	T
0.7782862229119729	0.7005817901363277	0.3902501596895009	T	T	T
0.0017707027074808	0.5026507347840976	0.3904732335997694	T	T	T
0.1121444469970607	0.5019155179828548	0.3904639049223050	T	T	T
0.2227645753816094	0.5014091037393036	0.3902887645166366	T	T	T
0.4430607241312840	0.6984637657499828	0.3885948381267200	T	T	T
0.5550625941767690	0.6984852866297212	0.3887239704814511	T	T	T
0.8885499338874967	0.0983653340641638	0.3902005298093898	T	T	T
0.6672656255766390	0.7000811356178416	0.3895078285244118	T	T	T
0.8896015232818038	0.9001791748403154	0.3903950057567551	T	T	T
0.0000501427169996	0.7002740459156325	0.3904040803766034	T	T	T
0.1106219312108006	0.6999506696482677	0.3904968092578784	T	T	T
0.2213184279249220	0.6995525371574827	0.3901297061273893	T	T	T
0.3320229830226173	0.6990862469534643	0.3896644420477063	T	T	T
0.5558504796252269	0.9004574569389069	0.3886120080955739	T	T	T
0.8891482854798770	0.7003394437129891	0.3903816186371335	T	T	T
0.7789959389885107	0.9006182842270358	0.3898005235000214	T	T	T
0.0001571258072190	0.8998468461562289	0.3907003268712013	T	T	T
0.5562541796554338	0.5996826888469732	0.4571291210113866	T	T	T
0.3332335054355405	0.1995360794154316	0.4546166395254935	T	T	T
0.2216171732134839	0.1992959407848672	0.4544066906609547	T	T	T
0.1110232957169568	0.2004352466080915	0.4543127590501376	T	T	T
0.4460570997368991	0.0011906886276130	0.4559804888914669	T	T	T
0.3332133166660594	0.0011865944597987	0.4566759785488218	T	T	T
0.2215696660610953	0.9997405781393536	0.4580976840138691	T	T	T
0.4457559045482189	0.2032880085728805	0.4532193726794778	T	T	T
0.1107279195870460	0.9987613078902107	0.4588643787528364	T	T	T
0.8904353203625888	0.0000184011962287	0.4578296707790757	T	T	T
0.7789001457653421	0.0000807499245990	0.4573142491427006	T	T	T
0.6667757265276999	0.9986084741580127	0.4562031027480316	T	T	T
0.5559589800939281	0.9992090189684401	0.4567514525637222	T	T	T
0.3329468635248956	0.9000259794379361	0.3895072274284204	T	T	T
0.2217895760806430	0.9000747776911945	0.3900820579510768	T	T	T
0.0004232847457469	0.9993001906342760	0.4588280100153218	T	T	T
0.7776587601949024	0.0985152967736854	0.3896581114521687	T	T	T
0.5551812135136001	0.2007300866391124	0.4526486931757595	T	T	T
0.4444934937515665	0.6003250173699174	0.4561357896607665	T	T	T
0.5569320120000962	0.4023428399284407	0.4553907897719949	T	T	T
0.7780224282626241	0.1998633834699780	0.4534057172120654	T	T	T
0.4441122171185737	0.8996795991916514	0.3890129067871859	T	T	T
0.0002210148792686	0.2008239130478877	0.4543395026665691	T	T	T
0.2224175518463624	0.3995016603842159	0.4543697002531382	T	T	T
0.3327235455919199	0.3980246599552109	0.4532012549708643	T	T	T
0.6667547755657238	0.2008187062511156	0.4524650885002549	T	T	T
0.4442409957437923	0.3985223704738768	0.4543813872770170	T	T	T
0.1107991582400391	0.8997355214346440	0.3905334972594010	T	T	T
0.7776272423717131	0.3994171337611502	0.4532993075266983	T	T	T
0.8895745706601157	0.3996706065623997	0.4538783375707501	T	T	T
0.0005504467630416	0.3998452124836767	0.4546884940509680	T	T	T
0.1115543284603329	0.3998727950507185	0.4547716680349375	T	T	T
0.3327107467275750	0.5999903365525567	0.4571942475201606	T	T	T

0.6665074821943917	0.3993801682365582	0.4533696863315048	T	T	T
0.6673935646931920	0.6014589828090707	0.4576618298565691	T	T	T
0.8894159429782195	0.2010723875738026	0.4540834609668738	T	T	T
0.9253652208310065	0.4661235759860563	0.5380009771228444	T	T	T
0.1110362756248543	0.6005785310134054	0.4586169214406706	T	T	T
0.2216952610229883	0.6008225963758106	0.4579382760259277	T	T	T
0.4444688071273896	0.7994410695985820	0.4537196873261372	T	T	T
0.5549828657369422	0.7992542835058978	0.4536225502299575	T	T	T
0.6658721439091247	0.7999489827859729	0.4537724447653557	T	T	T
0.8884887122911982	0.7997775520123167	0.4564060199549113	T	T	T
0.9996503939242212	0.7996082452315005	0.4566660685519205	T	T	T
0.1108037099072696	0.7999518012097659	0.4565392817012943	T	T	T
0.2221957251026686	0.8002567507986079	0.4555552615503085	T	T	T
0.3336699162549878	0.8006806083838321	0.4551952568229783	T	T	T
0.1835139698062572	0.1288120624800428	0.5380674567398129	T	T	T
0.2942440800977080	0.1282345531753702	0.5384355133116900	T	T	T
0.4043819933968127	0.1266169241518484	0.5349735377569684	T	T	T
0.5170832031899204	0.1277912827529145	0.5360799871690730	T	T	T
0.6255885079739019	0.1253128157608143	0.5346623578362188	T	T	T
0.3715321412369972	0.4671200768505255	0.5360918003071931	T	T	T
0.1104673412230621	0.2981873201617289	0.5243873577596374	T	T	T
0.8892831795808676	0.6001187784566465	0.4578303463199532	T	T	T
0.4436607901717051	0.2972246525247949	0.5265853495738543	T	T	T
0.7374964477724757	0.1275526905846702	0.5367469911257651	T	T	T
0.8483059369357187	0.1276698789355829	0.5371192498626570	T	T	T
0.9604532778765468	0.1286060830190032	0.5376382394581267	T	T	T
0.0720089008069953	0.1287178466242214	0.5376000199885413	T	T	T
0.0000956604207536	0.6004147115262556	0.4585491726483118	T	T	T
0.2215838285938553	0.2976609391718821	0.5243454946356626	T	T	T
0.5543414700607529	0.2972951891401535	0.5232770116066401	T	T	T
0.5920845841383816	0.4647162325151638	0.5410182620103057	T	T	T
0.6655479610604768	0.2977863578117740	0.5230876921191074	T	T	T
0.7765624720595719	0.2977928466992315	0.5211144997868793	T	T	T
0.8872008566225187	0.2973071827639541	0.5249813709025619	T	T	T
0.9983557427942661	0.2972465259372860	0.5247314867715043	T	T	T
0.3331405848907718	0.2979413068724721	0.5233371588669862	T	T	T
0.4830151151626904	0.4664760572224893	0.5381378647148980	T	T	T
0.7775778643768143	0.8003891547955708	0.4562191156806821	T	T	T
0.7779293034260214	0.6001875139138707	0.4577083367983700	T	T	T
0.6663846079391974	0.7962687941293537	0.5415824080941556	T	T	T
0.5539221310217309	0.7955802463186962	0.5422551876090214	T	T	T
0.2952010610830769	0.6309607807063266	0.5360656772737369	T	T	T
0.1845141229582765	0.6317737447287184	0.5379241555178469	T	T	T
0.0735218751640887	0.6324766606653409	0.5377425540974791	T	T	T
0.7037265667240507	0.4664684159448160	0.5371529583119580	T	T	T
0.7769576776375137	0.7973149484259762	0.5452659793633871	T	T	T
0.8526238193032998	0.6345626137000334	0.5360269773400647	T	T	T
0.6300773356055682	0.6319629433879916	0.5375717013681869	T	T	T
0.5195027357503970	0.6331297122182167	0.5337710155528661	T	T	T
0.4076364582960473	0.6328215113084945	0.5347989040677469	T	T	T
0.2597516719526720	0.4657946904290740	0.5387455199497522	T	T	T
0.1475531646361125	0.4654309043954047	0.5390935509485921	T	T	T
0.0362419752116377	0.4656591337274049	0.5388857324617310	T	T	T
0.7408606243372504	0.6334349187886602	0.5358326630354129	T	T	T
0.8879427402251751	0.7980092481720464	0.5451579552641070	T	T	T
0.9627625910194469	0.6330932584144131	0.5375792335691038	T	T	T

0.3659491045538408	0.9577345938530092	0.5312632403467128	T	T	T
0.4773515785002843	0.9589068404145702	0.5350783658027277	T	T	T
0.9989936968950551	0.7976233004017288	0.5454464273847353	T	T	T
0.1095743091853320	0.7968788837732457	0.5452805947762592	T	T	T
0.7001890956490945	0.9597247409747846	0.5341439707333534	T	T	T
0.3309778133592217	0.7946026274406776	0.5439062524980857	T	T	T
0.4422120645202203	0.7960361192933910	0.5416333281355118	T	T	T
0.2198567120950179	0.7954817828709864	0.5440703612541673	T	T	T
0.8126515099409886	0.9613480267565474	0.5350389948083438	T	T	T
0.8147372170787148	0.4672791826967222	0.5370181317463274	T	T	T
0.9234833873053829	0.9618115632097803	0.5375623775209711	T	T	T
0.0347060159448202	0.9616806461333497	0.5376390701240237	T	T	T
0.1458720513002258	0.9616172366981369	0.5377150454476112	T	T	T
0.2558143645698873	0.9600110595992085	0.5356729010732412	T	T	T
0.5891672233718609	0.9589040183972435	0.5342238095505658	T	T	T
0.2971357324920964	0.9597216755905135	0.6469218638694331	T	T	T
0.6802540293908026	0.1595516315163849	0.6399275424076946	T	T	T
0.6678387548930602	0.4744130521871741	0.6463277532629665	T	T	T
0.3926584700977388	0.6415436111384122	0.6401386461645072	T	T	T
0.5004895422172042	0.5597541618328816	0.6429362416940924	T	T	T
0.3098554745425511	0.3221244510570977	0.6350696705097059	T	T	T
0.3660284848108700	0.4181051627638248	0.6355107099304653	T	T	T
0.4362057720431855	0.4602209418815000	0.6451566228353403	T	T	T
0.6835228240728310	0.8326522406125277	0.6451016936845526	T	T	T
0.7540349917203542	0.8722769683220697	0.6504309964724215	T	T	T
0.8119864596394221	0.9677236890947470	0.6489280667924141	T	T	T
0.3255086484387917	0.2711987563545680	0.6448865005090397	T	T	T
0.7261997906233837	0.9774214842320742	0.6370693427471541	T	T	T
0.3960905596777169	0.3174187029748167	0.6559400544501642	T	T	T
0.7975209231267236	0.0209965637539165	0.6421951642829264	T	T	T
0.3536659974910905	0.0554255570337155	0.6457602300220547	T	T	T
0.6193351346103363	0.7336498793295616	0.6443168079600007	T	T	T
0.4243718229759489	0.0966806610382664	0.6388791093016151	T	T	T
0.8081553042367671	0.2968799366910115	0.6425736250600220	T	T	T
0.6045065079175806	0.3739920238099630	0.6438040490863114	T	T	T
0.3214293886440666	0.5978753665117807	0.6460929776124635	T	T	T
0.3651288763485709	0.7467212773173125	0.6538127644264291	T	T	T
0.3133379233937372	0.9084039832157138	0.6405059103763776	T	T	T
0.7920700007961369	0.3476550793934344	0.6336513238754328	T	T	T
0.4993768627024486	0.8856795982626683	0.6444639801803906	T	T	T
0.7512133289538743	0.2013554158185444	0.6457926280844118	T	T	T
0.3071022343858767	0.6511371863335100	0.6529685945236262	T	T	T
0.4353639842913584	0.7862777352033402	0.6472866659696159	T	T	T
0.6167972799639512	0.0599172606221259	0.6408184532419908	T	T	T
0.3847276567626592	0.9540363579461338	0.6326679819200515	T	T	T
0.4871666359401258	0.1966416190912170	0.6387116533937037	T	T	T
0.7160861429705013	0.6235735792074447	0.6496037423815522	T	T	T
0.7865669052276418	0.6640041461325085	0.6453703161045413	T	T	T
0.7978626607730602	0.6069214056404723	0.6423439420845553	T	T	T
0.7380406464015532	0.5118843591869126	0.6422769574293744	T	T	T
0.7201872593895341	0.3015058996149556	0.6276388577241192	T	T	T
0.2777920994201455	0.5228702529145179	0.6441603302158916	T	T	T
0.3568790716973446	0.4608730325369740	0.6273427989481557	T	T	T
0.7617431495722810	0.8269611135953597	0.6546657427602780	T	T	T
0.2551625405447674	0.2877265053915884	0.6259614656854343	T	T	T
0.2516642732688668	0.6187681408620846	0.6567275651854049	T	T	T

0.7603109701612903	0.1580400246208807	0.6523753931802667	T	T	T
0.3573793121845892	0.7918218119795660	0.6587642670513090	T	T	T
0.8675290182434898	0.0001115571647461	0.6518590677356791	T	T	T
0.7442036758726305	0.4649821419529512	0.6386996943224309	T	T	T
0.8641601526152557	0.3311202294522682	0.6460146033077017	T	T	T
0.2836206621542687	0.1960564726939137	0.6436703461920554	T	T	T
0.8411933557861693	0.0959176861123850	0.6396541109264939	T	T	T
0.7120168144489563	0.0156340190869603	0.6317145350623611	T	T	T
0.4106722528006965	0.2806956576160861	0.6644425136029498	T	T	T
0.3449255078979401	0.0997352243256529	0.6496551816885895	T	T	T
0.2413965910352687	0.9256732488764980	0.6517084718217815	T	T	T
0.8314116233456387	0.7388888781357276	0.6439570577621475	T	T	T
0.2709120348616684	0.8331961085685414	0.6400190257314387	T	T	T
0.8523448366394035	0.6360525024646083	0.6386717285130766	T	T	T
0.7042781830290533	0.6650772080705893	0.6519510141845303	T	T	T
0.4070574970495979	0.6035946869907115	0.6347274002124447	T	T	T
0.7048103976076521	0.3375562115841623	0.6198028282932907	T	T	T
0.8348239822699985	0.4224113261399816	0.6299132233705449	T	T	T
0.3999329280442678	0.9172173409294589	0.6268854776521980	T	T	T
0.6644471869938019	0.2088297262559403	0.6305162853608569	T	T	T
0.6692394802346421	0.8845241331710196	0.6385626909350528	T	T	T
0.6259943417049314	0.6762979128801548	0.6485429829340321	T	T	T
0.5546124509649775	0.7095522779327992	0.6375297876209668	T	T	T
0.4928976654114329	0.6161173699645913	0.6392719052771818	T	T	T
0.4910624643916335	0.9414568108293278	0.6439846237583755	T	T	T
0.5509676947950642	0.0337479577441109	0.6367249522735462	T	T	T
0.6251919428010881	0.0042755092311378	0.6425323281314567	T	T	T
0.4494843480314327	0.7344118627034865	0.6405658917508131	T	T	T
0.4403336160672050	0.0470594915073715	0.6321983993794088	T	T	T
0.4508267027161473	0.4103988675335052	0.6560000915830837	T	T	T
0.5651281945469723	0.5841994461147423	0.6458092951289112	T	T	T
0.5540267358011375	0.2262653359897589	0.6332419803153071	T	T	T
0.6576274051122196	0.5310777264882562	0.6510112751566058	T	T	T
0.6133419156814847	0.3196633248129306	0.6371978925494149	T	T	T
0.5355707757781191	0.3424708795850159	0.6457674428810793	T	T	T
0.4755810591560639	0.2482381562681837	0.6441549003336673	T	T	T
0.5644733469992331	0.9106294243617030	0.6393990903631094	T	T	T
0.5519514217869788	0.1283254753950955	0.6175700608686169	T	T	T
0.5596040412339417	0.8099058940624900	0.6246806215963013	T	T	T
0.5612081484437410	0.4889456024770174	0.6730453944486479	T	T	T
0.5298573031505495	0.3743850224650306	0.6843336385392764	T	T	T
0.5811704460042046	0.5308314718303559	0.7211396401818764	T	T	T

Fig. 6e

```

-----
Au C H N V O
1.000000000000000
26.0801187006857766 0.0000000000000000 0.0000000000000000
-14.4889548337143204 14.4889548337143204 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Au C H N V O
279 36 24 18 3 2
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.1894422798390494 F F F
0.5555555555555571 0.2000000000000028 0.1894422798390494 F F F

```

0.444444444444429	0.2000000000000028	0.1894422798390494	F	F	F
0.222222222222214	0.2000000000000028	0.1894422798390494	F	F	F
0.111111111111143	0.2000000000000028	0.1894422798390494	F	F	F
0.777777777777786	0.2000000000000028	0.1894422798390494	F	F	F
0.888888888888857	0.0000000000000000	0.1894422798390494	F	F	F
0.666666666666643	0.0000000000000000	0.1894422798390494	F	F	F
0.555555555555571	0.0000000000000000	0.1894422798390494	F	F	F
0.444444444444429	0.0000000000000000	0.1894422798390494	F	F	F
0.333333333333357	0.0000000000000000	0.1894422798390494	F	F	F
0.222222222222214	0.0000000000000000	0.1894422798390494	F	F	F
0.111111111111143	0.0000000000000000	0.1894422798390494	F	F	F
0.777777777777786	0.0000000000000000	0.1894422798390494	F	F	F
0.888888888888857	0.5000000000000000	0.2561864044279716	F	F	F
0.8888888888888928	0.2000000000000028	0.1894422798390494	F	F	F
0.222222222222214	0.3999999999999986	0.1894422798390494	F	F	F
0.8888888888888928	0.6000000000000014	0.1894422798390494	F	F	F
0.0000000000000000	0.3999999999999986	0.1894422798390494	F	F	F
0.333333333333357	0.3999999999999986	0.1894422798390494	F	F	F
0.444444444444429	0.3999999999999986	0.1894422798390494	F	F	F
0.555555555555571	0.3999999999999986	0.1894422798390494	F	F	F
0.666666666666643	0.3999999999999986	0.1894422798390494	F	F	F
0.777777777777786	0.3999999999999986	0.1894422798390494	F	F	F
0.6666666666666714	0.2000000000000028	0.1894422798390494	F	F	F
0.888888888888857	0.3999999999999986	0.1894422798390494	F	F	F
0.0000000000000000	0.2000000000000028	0.1894422798390494	F	F	F
0.333333333333357	0.6000000000000014	0.1894422798390494	F	F	F
0.444444444444429	0.6000000000000014	0.1894422798390494	F	F	F
0.555555555555571	0.6000000000000014	0.1894422798390494	F	F	F
0.5544875599046162	0.0971290396854245	0.3894750954196732	T	T	T
0.777777777777786	0.6000000000000014	0.1894422798390494	F	F	F
0.1111111111111072	0.3999999999999986	0.1894422798390494	F	F	F
0.0000000000000000	0.5000000000000000	0.2561864044279716	F	F	F
0.0000000000000000	0.6000000000000014	0.1894422798390494	F	F	F
0.222222222222214	0.6000000000000014	0.1894422798390494	F	F	F
0.666666666666643	0.7999999999999972	0.1894422798390494	F	F	F
0.777777777777786	0.7999999999999972	0.1894422798390494	F	F	F
0.888888888888857	0.7999999999999972	0.1894422798390494	F	F	F
0.0000000000000000	0.7999999999999972	0.1894422798390494	F	F	F
0.1111111111111072	0.7999999999999972	0.1894422798390494	F	F	F
0.222222222222214	0.7999999999999972	0.1894422798390494	F	F	F
0.333333333333286	0.7999999999999972	0.1894422798390494	F	F	F
0.111111111111143	0.1000000000000014	0.2561864044279716	F	F	F
0.222222222222214	0.1000000000000014	0.2561864044279716	F	F	F
0.333333333333357	0.1000000000000014	0.2561864044279716	F	F	F
0.444444444444429	0.1000000000000014	0.2561864044279716	F	F	F
0.555555555555571	0.1000000000000014	0.2561864044279716	F	F	F
0.666666666666643	0.1000000000000014	0.2561864044279716	F	F	F
0.777777777777786	0.1000000000000014	0.2561864044279716	F	F	F
0.8888888888888928	0.1000000000000014	0.2561864044279716	F	F	F
0.0000000000000000	0.1000000000000014	0.2561864044279716	F	F	F
0.777777777777786	0.5000000000000000	0.2561864044279716	F	F	F
0.888888888888857	0.2999999999999972	0.2561864044279716	F	F	F
0.222222222222214	0.2999999999999972	0.2561864044279716	F	F	F
0.333333333333286	0.2999999999999972	0.2561864044279716	F	F	F
0.444444444444429	0.2999999999999972	0.2561864044279716	F	F	F
0.555555555555571	0.2999999999999972	0.2561864044279716	F	F	F

0.6666666666666643	0.2999999999999972	0.2561864044279716	F	F	F
0.1111111111111143	0.6000000000000014	0.1894422798390494	F	F	F
0.7777777777777786	0.2999999999999972	0.2561864044279716	F	F	F
0.4444444444444429	0.7999999999999972	0.1894422798390494	F	F	F
0.11111111111111072	0.2999999999999972	0.2561864044279716	F	F	F
0.3333333333333357	0.5000000000000000	0.2561864044279716	F	F	F
0.4444444444444429	0.5000000000000000	0.2561864044279716	F	F	F
0.5555555555555571	0.5000000000000000	0.2561864044279716	F	F	F
0.6666666666666643	0.5000000000000000	0.2561864044279716	F	F	F
0.0000000000000000	0.2999999999999972	0.2561864044279716	F	F	F
0.5555555555555571	0.7999999999999972	0.1894422798390494	F	F	F
0.6666666666666643	0.6000000000000014	0.1894422798390494	F	F	F
0.9993080473190583	0.1985363474936202	0.3226905835465693	T	T	T
0.8888888888888857	0.8999999999999986	0.2561864044279716	F	F	F
0.7777777777777786	0.8999999999999986	0.2561864044279716	F	F	F
0.6666666666666643	0.8999999999999986	0.2561864044279716	F	F	F
0.5555555555555571	0.8999999999999986	0.2561864044279716	F	F	F
0.3333333333333357	0.7000000000000028	0.2561864044279716	F	F	F
0.11111111111111072	0.8999999999999986	0.2561864044279716	F	F	F
0.2222222222222214	0.7000000000000028	0.2561864044279716	F	F	F
0.6663955682902530	0.1988350034964828	0.3223034905406423	T	T	T
0.88888888888888928	0.7000000000000028	0.2561864044279716	F	F	F
0.7777777777777786	0.7000000000000028	0.2561864044279716	F	F	F
0.66666666666666714	0.7000000000000028	0.2561864044279716	F	F	F
0.5555555555555571	0.7000000000000028	0.2561864044279716	F	F	F
0.4444444444444429	0.7000000000000028	0.2561864044279716	F	F	F
0.1111111111111143	0.7000000000000028	0.2561864044279716	F	F	F
0.2222222222222214	0.8999999999999986	0.2561864044279716	F	F	F
0.0000000000000000	0.7000000000000028	0.2561864044279716	F	F	F
0.4444444444444429	0.8999999999999986	0.2561864044279716	F	F	F
0.3333333333333357	0.8999999999999986	0.2561864044279716	F	F	F
0.1102570902709744	0.9991466334940657	0.3230309539104713	T	T	T
0.5552267021746188	0.9996091737733372	0.3223709338683402	T	T	T
0.6667665209714898	0.9998328388499491	0.3224710539703855	T	T	T
0.7783114357338088	0.0000555818980044	0.3225915035154851	T	T	T
0.8888866799339052	0.9995085973192485	0.3229609645680873	T	T	T
0.0000000000000000	0.8999999999999986	0.2561864044279716	F	F	F
0.9995833195428604	0.9993063252882926	0.3230581697895615	T	T	T
0.3320616640611226	0.9988495168521734	0.3226771673227017	T	T	T
0.4436893114131748	0.9991215403644841	0.3225995557660672	T	T	T
0.1102501184426271	0.1983405438150968	0.3226186370347711	T	T	T
0.2210402474237211	0.1980724820136105	0.3225986817934146	T	T	T
0.3320285116284123	0.1980904189522232	0.3224409022570477	T	T	T
0.4433820591757039	0.1984369700957208	0.3222372649980313	T	T	T
0.2211411667462750	0.9991081083663544	0.3229170406552854	T	T	T
0.2222222222222214	0.5000000000000000	0.2561864044279716	F	F	F
0.5548233152188544	0.1983969892899213	0.3223936842042642	T	T	T
0.7778178680820351	0.1991574172199993	0.3223580508022431	T	T	T
0.2224081142022489	0.4005697728685492	0.3226002163324786	T	T	T
0.3333715410248996	0.4004533709379402	0.3225088178260176	T	T	T
0.4445864825617081	0.4007674249999916	0.3224951315733651	T	T	T
0.5561062935070723	0.4018111032626709	0.3224001796927257	T	T	T
0.6675835314691049	0.4018143611280709	0.3222584286308394	T	T	T
0.7790418934062526	0.4019218775382964	0.3223473317490950	T	T	T
0.8900490149057573	0.4017609537003167	0.3225565300392876	T	T	T
0.1116952539774351	0.4011284000606180	0.3226199284841786	T	T	T

0.3326263877933168	0.5993835142639087	0.3225493435313855	T	T	T
0.4443223820474795	0.5995875163626786	0.3226104927019238	T	T	T
0.5559809713909297	0.599559952547855	0.3225794679811444	T	T	T
0.6675129660178264	0.6009408932248987	0.3227582004486327	T	T	T
0.7787673067504700	0.6012177732304469	0.3228500767740303	T	T	T
0.8896929070175078	0.6009918742464517	0.3229571505753909	T	T	T
0.0004398571369734	0.6005880564526467	0.3230070752626678	T	T	T
0.1113205705982186	0.6003913798491639	0.3229521910260245	T	T	T
0.1111111111111143	0.5000000000000000	0.2561864044279716	F	F	F
0.9999160443987836	0.8000691281598157	0.3230841302349041	T	T	T
0.2220031351637280	0.6000770576035924	0.3229136990141215	T	T	T
0.4438735786279545	0.7994320097885229	0.3225371844750877	T	T	T
0.5555447203715644	0.7997152960398324	0.3226750699517622	T	T	T
0.6672360257546527	0.8000542261001766	0.3227876505327138	T	T	T
0.7783706078018948	0.8002865186444421	0.3229498622235881	T	T	T
0.0007405438691996	0.4013611283257071	0.3226015238551168	T	T	T
0.8891154242721632	0.8002279916987258	0.3231760299526821	T	T	T
0.8887307848271750	0.1990438283002122	0.3226225427897127	T	T	T
0.2214775783513494	0.7993578663031832	0.3229515051191192	T	T	T
0.3325695464155094	0.7994000468082657	0.3227193281560450	T	T	T
0.1094382579577363	0.0972572714170990	0.3906130376680094	T	T	T
0.2201679412018386	0.0971863363840080	0.3903672730958906	T	T	T
0.3312960434912078	0.0973578710868917	0.3898006820615881	T	T	T
0.1108365300427467	0.7998584885276655	0.3230658416129798	T	T	T
0.4423886933612624	0.0970902226768403	0.3892422330909674	T	T	T
0.3333333333333357	0.2000000000000028	0.1894422798390494	F	F	F
0.6661775873361101	0.0981327838796643	0.3895944708760883	T	T	T
0.9989485497616002	0.0977340807080187	0.3903874263191711	T	T	T
0.2215006525622523	0.2990688393282309	0.3877054470140602	T	T	T
0.3325258022628673	0.2987999229419723	0.3876378126812866	T	T	T
0.4437041488813668	0.2992753722601821	0.3872791212439058	T	T	T
0.5552755829789561	0.3000250225378752	0.3865155833586652	T	T	T
0.6669236953460952	0.2999307874806917	0.3865826412555123	T	T	T
0.7784035811802599	0.3001789407985305	0.3871733710917030	T	T	T
0.8894044648046255	0.3003207167097300	0.3876338685928574	T	T	T
0.0003294697205784	0.3002937834542115	0.3878153058766221	T	T	T
0.1108114458048311	0.2996796426470746	0.3878188819514377	T	T	T
0.3336504886119414	0.5011022823852483	0.3897959009335689	T	T	T
0.4451215987936388	0.5010818539559018	0.3898615210975953	T	T	T
0.5565929225840778	0.5021048582890995	0.3898747467552096	T	T	T
0.6681813795405279	0.5028033940222071	0.3897319211369666	T	T	T
0.7793936958557828	0.5026943718450751	0.3897350343589251	T	T	T
0.8904677817455063	0.5023880010219456	0.3901631369247474	T	T	T
0.6676937953563609	0.9007169005260892	0.3889643662433375	T	T	T
0.7779733139694219	0.7004343390324608	0.3905337994743026	T	T	T
0.0014867595738141	0.5023370264996951	0.3904402223609112	T	T	T
0.1118647724400155	0.5016411351412604	0.3904483433677250	T	T	T
0.2225767552775337	0.5013396551444128	0.3902135792311408	T	T	T
0.4432819476496332	0.6987994082112311	0.3886830349993450	T	T	T
0.5553960580122416	0.6989221333179159	0.3889383343610055	T	T	T
0.8881011956818704	0.0979958159165679	0.3902997999587019	T	T	T
0.6671688113871929	0.6999969549325330	0.3898882551973651	T	T	T
0.8893144023697729	0.8999823889042381	0.3905464270264664	T	T	T
0.9999367529917859	0.7001725760342230	0.3904583811560881	T	T	T
0.1103517505887995	0.6995611868895656	0.3905621504756828	T	T	T
0.2210892357732704	0.6991725337966769	0.3901778120872842	T	T	T

0.3321276196312446	0.6991494800989564	0.3896807554574369	T	T	T
0.5558303533152186	0.9004321913785277	0.3888336820765442	T	T	T
0.8890933645750416	0.7004707086238279	0.3904336566369693	T	T	T
0.7787406286867659	0.9004235749702284	0.3900705005681093	T	T	T
0.0001149068393627	0.8999289991500096	0.3907449790871470	T	T	T
0.5558830811369244	0.6000472281545057	0.4575233107212974	T	T	T
0.3322531204103366	0.1985245236396583	0.4541712888124180	T	T	T
0.2214960940946262	0.1998913219937457	0.4542392782638392	T	T	T
0.1106670182282702	0.2003920490013428	0.4544168179230839	T	T	T
0.4452956606124305	0.0002349324940579	0.4563830365053386	T	T	T
0.3320722065487645	0.9995125365798897	0.4568128572042212	T	T	T
0.2210968327640358	0.9988187481970708	0.4582080761039434	T	T	T
0.4443975176065335	0.2000330009364117	0.4531124983891253	T	T	T
0.1108025052914379	0.9990436155103095	0.4588081925464298	T	T	T
0.8898999019787318	0.9999113947230630	0.4580092251787172	T	T	T
0.7782250987733311	0.0000085777756918	0.4576496036695767	T	T	T
0.6660357749431886	0.9983387949666743	0.4567714815935513	T	T	T
0.5556869500921549	0.9991545064137558	0.4572901746525755	T	T	T
0.3325473247632630	0.8992629768474879	0.3895449561844742	T	T	T
0.2212891474141168	0.8992647305242136	0.3900879911398145	T	T	T
0.0002230454653719	0.9994213594672454	0.4588412890767044	T	T	T
0.7772563467030591	0.0981728351178850	0.3898326944198175	T	T	T
0.5550164188039615	0.1994864811451426	0.4525530409490272	T	T	T
0.4445656558178184	0.6007119178318282	0.4562432975477150	T	T	T
0.5552919802944636	0.3991376957128199	0.4530819803637907	T	T	T
0.7778511431222174	0.1995421558290560	0.4537588608844044	T	T	T
0.4440881206705495	0.8994566729704837	0.3892399083956125	T	T	T
0.9999277356357515	0.2006319082149473	0.4544630911926656	T	T	T
0.2221598143064724	0.3994199678230487	0.4542876475536631	T	T	T
0.3330275359233642	0.3992359283096861	0.4536105053729985	T	T	T
0.6664674333974309	0.1999545044878585	0.4530367464375538	T	T	T
0.4439015783212752	0.3984525779067256	0.4536056049939262	T	T	T
0.1106446543244777	0.8995663493277539	0.3905104489311747	T	T	T
0.7771645944947601	0.3988254518325117	0.4531322800888069	T	T	T
0.8892411777639357	0.3993001813137190	0.4538442334679014	T	T	T
0.0001567056641712	0.3994654766138542	0.4545775194202250	T	T	T
0.1112422716681208	0.3995365581746169	0.4546708281163185	T	T	T
0.3322510769666284	0.5998922985637476	0.4571069137677043	T	T	T
0.6659904506141774	0.3983142372991156	0.4525358745218956	T	T	T
0.6661406637007296	0.6002561196155699	0.4578340276231522	T	T	T
0.8891762754891411	0.2008263046894434	0.4541809230858663	T	T	T
0.9264311404567236	0.4684878182076012	0.5375461845642969	T	T	T
0.1105908972037189	0.6001057388697534	0.4586772927795304	T	T	T
0.2213012212341572	0.6004186336894064	0.4579907140945830	T	T	T
0.4447176062187814	0.7994892598979559	0.4541151487092667	T	T	T
0.5552183966050378	0.7994314245966604	0.4539603971663230	T	T	T
0.6661121907371552	0.7999802340042473	0.4544010914086191	T	T	T
0.8886918070726203	0.7999560952522806	0.4565696948381271	T	T	T
0.9998156588009939	0.7997931902280603	0.4566837134542269	T	T	T
0.1106869446223746	0.7995761849091687	0.4566801936134406	T	T	T
0.2219185916395861	0.7995381179650553	0.4558244379397881	T	T	T
0.3335988938067020	0.8003178387921959	0.4552254728456506	T	T	T
0.1843676761371992	0.1310758038596230	0.5380469669260329	T	T	T
0.2953296214050573	0.1309144203146544	0.5386216480691735	T	T	T
0.4052944434356973	0.1300555846655443	0.5364624641948795	T	T	T
0.5173171567691237	0.1313801619437761	0.5370552110386514	T	T	T

0.6258234530801767	0.1284372099351186	0.5362312653038085	T	T	T
0.3717812472164507	0.4691804142488064	0.5368986913667896	T	T	T
0.1109724548491841	0.2998411766906368	0.5246230268795797	T	T	T
0.8891437804347558	0.6000660352221636	0.4578100558657076	T	T	T
0.4442484246666184	0.2996632358659745	0.5230485880671472	T	T	T
0.7381149652066297	0.1303316082199331	0.5375432411474893	T	T	T
0.8489507226142773	0.1300318830541419	0.5375792229445947	T	T	T
0.9611263087741899	0.1306790397291913	0.5381153540309783	T	T	T
0.0728000355280491	0.1308447116914811	0.5380739010532082	T	T	T
0.9997818121245251	0.6000899282950718	0.4586261897504317	T	T	T
0.2220642072808423	0.2994610097921143	0.5243527424304647	T	T	T
0.5552453256273194	0.2997454861267930	0.5220826091038994	T	T	T
0.5951795968658556	0.4708628650468149	0.5358546471891922	T	T	T
0.6662514558123430	0.2999471992040288	0.5233114507721915	T	T	T
0.7771257929607335	0.2996448902477133	0.5212484138925314	T	T	T
0.8878291529469827	0.2991766251083475	0.5252654841531252	T	T	T
0.9989578313861289	0.2989774238972195	0.5246535738816204	T	T	T
0.3336714469825247	0.2999480681336817	0.5226751228650772	T	T	T
0.4838907611307073	0.4700049601983708	0.5367203893976230	T	T	T
0.7775647540890185	0.8001988814302019	0.4565183101272163	T	T	T
0.7776495732322840	0.5998510965992390	0.4574856370997396	T	T	T
0.6668850050392237	0.7994424693569723	0.5424445634615446	T	T	T
0.5546104168170730	0.7987559104686229	0.5426542773877373	T	T	T
0.2963253401397322	0.6337563853647269	0.5360062065964805	T	T	T
0.1856718280810745	0.6344434055066710	0.5377376662646821	T	T	T
0.0748280084800195	0.6351439319159012	0.5376344157516969	T	T	T
0.7053157899198831	0.4699517258513604	0.5354201589490681	T	T	T
0.7779124528569383	0.8006180621511994	0.5456364221280864	T	T	T
0.8543652888523883	0.6378616495441640	0.5358110769372891	T	T	T
0.6311922925844338	0.6359852330133569	0.5378619777506207	T	T	T
0.5200836067793099	0.6362083870891774	0.5344370271085714	T	T	T
0.4085451174329666	0.6357723610590656	0.5340747667635720	T	T	T
0.2603822505545840	0.4680097784259040	0.5383441584920400	T	T	T
0.1485368314103869	0.4677568934735818	0.5386388539267966	T	T	T
0.0372512237626678	0.4679935738378706	0.5383453096802179	T	T	T
0.7435387410766209	0.6384299533128074	0.5349792813978395	T	T	T
0.8895517001347039	0.8012381762794291	0.5454484466426692	T	T	T
0.9640389765162730	0.6356706262162729	0.5374328104498705	T	T	T
0.3672364678139138	0.9614203443432630	0.5322319564286371	T	T	T
0.4785290255364066	0.9624687528352366	0.5359748683604491	T	T	T
0.0005481630063729	0.8004169171486264	0.5454994493325539	T	T	T
0.1109824781847028	0.7996181265638430	0.5454201639437837	T	T	T
0.7009531082573636	0.9627268758604020	0.5350283651690380	T	T	T
0.3320575915506664	0.7975262951426494	0.5438026476016926	T	T	T
0.4431837307710588	0.7993788321331576	0.5421965405052590	T	T	T
0.2211711736951231	0.7984160121287910	0.5444338733452405	T	T	T
0.8133831067114919	0.9640657782936205	0.5355072473055568	T	T	T
0.8158323646457268	0.4699177052195278	0.5363232558868258	T	T	T
0.9244459811169101	0.9643536144546565	0.5377524415150975	T	T	T
0.0359334803806373	0.9642645034435872	0.5377077498727354	T	T	T
0.1472251434959750	0.9643430982815914	0.5378443841344597	T	T	T
0.2573788709676897	0.9631578599040721	0.5367148833092266	T	T	T
0.5901402200210721	0.9624168045210393	0.5355452355392445	T	T	T
0.3007642086286444	0.9530342789004689	0.6522199946982765	T	T	T
0.6859193888637337	0.1638834144424891	0.6414547101783253	T	T	T
0.6655690182535469	0.4716745800581856	0.6410760061361025	T	T	T

0.3940497586996544	0.6463847467544890	0.6369599656404152	T	T	T
0.4960700634052612	0.5615106783153992	0.6447068974174118	T	T	T
0.3003116688359753	0.3319169967365517	0.6359233628278633	T	T	T
0.3593491465113048	0.4270581583216889	0.6395491232263532	T	T	T
0.4289384152133278	0.4631101192963866	0.6433349212145255	T	T	T
0.6844395310494797	0.8323416742996297	0.6470122857798487	T	T	T
0.7543348805221296	0.8701350688389574	0.6523871276569567	T	T	T
0.8133406329277505	0.9653738393417627	0.6503924795908327	T	T	T
0.3122852746931917	0.2753268347622999	0.6359349815104526	T	T	T
0.7297594991355740	0.9785483743372290	0.6380426130245771	T	T	T
0.3828443596008622	0.3156095514420371	0.6397823058733136	T	T	T
0.8005529776273254	0.0203175286796400	0.6432673588601742	T	T	T
0.3566986244962888	0.0487614009014012	0.6523242643616725	T	T	T
0.6187864935151691	0.7337285783865244	0.6465788845065813	T	T	T
0.4273437413775796	0.0912455247398263	0.6435242016469984	T	T	T
0.8134146688811407	0.3028184687745958	0.6430064798819146	T	T	T
0.6036323074293352	0.3702650564322889	0.6372076691946335	T	T	T
0.3235363694652010	0.6041079360185461	0.6444684471286697	T	T	T
0.3708086617664614	0.7531701882888978	0.6593317728676983	T	T	T
0.3175458688436128	0.9032515730721745	0.6423871776846471	T	T	T
0.7959884116867726	0.3518737577562359	0.6333674766135485	T	T	T
0.5048497743501368	0.8903303054104703	0.6484021291217535	T	T	T
0.7573355533710453	0.2072889508272786	0.6471209568560998	T	T	T
0.3114319150533399	0.6581546549556060	0.6561870001830636	T	T	T
0.4401273533479975	0.7912368378261858	0.6506567721604571	T	T	T
0.6228400268744892	0.0642137422934455	0.6433213592494860	T	T	T
0.3888790151758595	0.9502935184616452	0.6331509244561148	T	T	T
0.4885535437892997	0.1904362077818114	0.6403190130171452	T	T	T
0.7117226705824146	0.6190076419578755	0.6461886330495550	T	T	T
0.7830139747946631	0.6607825531343213	0.6452827694920262	T	T	T
0.7954100025922290	0.6049316534992015	0.6429301980800408	T	T	T
0.7361440099973289	0.5097797818903319	0.6403300766569460	T	T	T
0.7237088406338501	0.3040370985025762	0.6273889076436443	T	T	T
0.2787485621511991	0.5297454214298466	0.6400569269927976	T	T	T
0.3525437599725028	0.4735899665703476	0.6391463939460624	T	T	T
0.7608641318144312	0.8237113431328540	0.6570981033489901	T	T	T
0.2457742523566073	0.3023758809208315	0.6317585211332585	T	T	T
0.2566498345954883	0.6269440022187087	0.6617563407209147	T	T	T
0.7675215637756927	0.1652887780013841	0.6542979159280630	T	T	T
0.3649637649912281	0.7991878914820597	0.6677349946494717	T	T	T
0.8684625244937261	0.9963438000158863	0.6533311156847398	T	T	T
0.7432785652622219	0.4637979960623716	0.6372306493127552	T	T	T
0.8697758040681695	0.3383609293776622	0.6463024844694064	T	T	T
0.2677516191757233	0.2008534263083147	0.6319112313918865	T	T	T
0.8451070397035353	0.0950812218172217	0.6404135547372837	T	T	T
0.7168453720418755	0.0180833205042525	0.6323310731917812	T	T	T
0.3955398287589568	0.2751297312219141	0.6389382809101196	T	T	T
0.3473529872229372	0.0919960543925943	0.6583247662323463	T	T	T
0.2450109993722046	0.9178113751555332	0.6583237065267736	T	T	T
0.8275210259963356	0.7357784699675809	0.6456430935890664	T	T	T
0.2755253096268905	0.8281556649852347	0.6402669340109398	T	T	T
0.8503823740961628	0.6349598929033182	0.6415688051236037	T	T	T
0.6990211595937738	0.6596071960941746	0.6479762176751306	T	T	T
0.4067913288791951	0.6077710553393489	0.6282317694394368	T	T	T
0.7075575646465500	0.3388147648139216	0.6187276592079761	T	T	T
0.8379719716564129	0.4264776361663632	0.6289109223896907	T	T	T

0.4038159710775465	0.9141396688054205	0.6246448255532269	T	T	T
0.6688559506124551	0.2114776374751410	0.6311624718111022	T	T	T
0.6718999191405494	0.8859359068246839	0.6398060717035232	T	T	T
0.6223670814768725	0.6735057251722776	0.6501671297356642	T	T	T
0.5555296429850596	0.7135297696918079	0.6400316700354999	T	T	T
0.4921066377838054	0.6212778109547449	0.6420560540384236	T	T	T
0.4971982437675666	0.9466578948955999	0.6487968016301358	T	T	T
0.5569381620991656	0.0379947092569740	0.6400628786546283	T	T	T
0.6308570773688261	0.0082417130928704	0.6448228123868665	T	T	T
0.4523613183797305	0.7385994854995903	0.6402099589953303	T	T	T
0.4442671684092422	0.0433488921972269	0.6342413743911670	T	T	T
0.4398702825078927	0.4076101299572288	0.6436071782688545	T	T	T
0.5593705720535327	0.5817800867965920	0.6468722756172209	T	T	T
0.5565615686545793	0.2229007703201775	0.6344172252612165	T	T	T
0.6539354872499477	0.5267437176119431	0.6447698460304213	T	T	T
0.6148552132468535	0.3171950464924986	0.6396773216978761	T	T	T
0.5343863852590458	0.3318557283340549	0.6321866277587569	T	T	T
0.4758465089016690	0.2416496029496454	0.6394454659653611	T	T	T
0.5694031845754721	0.9146281192272959	0.6417626091595089	T	T	T
0.5563160834307881	0.1283104904167942	0.6172982352545633	T	T	T
0.5630808433322281	0.8141155167307604	0.6250951286842040	T	T	T
0.5478282645619423	0.4738580648093057	0.6545471830609479	T	T	T
0.5187078425469773	0.3773357099053907	0.6168182480984041	T	T	T
0.5426499697557503	0.4529391087236498	0.7055194015255136	T	T	T

Fig. 6f

Au C H N V O

1.000000000000000

26.0801187006857766 0.000000000000000 0.000000000000000

-14.4889548337143204 14.4889548337143204 0.000000000000000

0.000000000000000 0.000000000000000 31.000000000000000

Au C H N V O

279 36 24 18 3 2

Selective dynamics

Direct

0.000000000000000	0.000000000000000	0.1894422798390494	F	F	F
0.555555555555571	0.200000000000028	0.1894422798390494	F	F	F
0.444444444444429	0.200000000000028	0.1894422798390494	F	F	F
0.222222222222214	0.200000000000028	0.1894422798390494	F	F	F
0.111111111111143	0.200000000000028	0.1894422798390494	F	F	F
0.777777777777786	0.200000000000028	0.1894422798390494	F	F	F
0.888888888888857	0.000000000000000	0.1894422798390494	F	F	F
0.666666666666643	0.000000000000000	0.1894422798390494	F	F	F
0.555555555555571	0.000000000000000	0.1894422798390494	F	F	F
0.444444444444429	0.000000000000000	0.1894422798390494	F	F	F
0.333333333333357	0.000000000000000	0.1894422798390494	F	F	F
0.222222222222214	0.000000000000000	0.1894422798390494	F	F	F
0.111111111111143	0.000000000000000	0.1894422798390494	F	F	F
0.777777777777786	0.000000000000000	0.1894422798390494	F	F	F
0.888888888888857	0.500000000000000	0.2561864044279716	F	F	F
0.8888888888888928	0.200000000000028	0.1894422798390494	F	F	F
0.222222222222214	0.399999999999986	0.1894422798390494	F	F	F
0.8888888888888928	0.600000000000014	0.1894422798390494	F	F	F
0.000000000000000	0.399999999999986	0.1894422798390494	F	F	F
0.333333333333357	0.399999999999986	0.1894422798390494	F	F	F

0.444444444444429	0.399999999999986	0.1894422798390494	F	F	F
0.555555555555571	0.399999999999986	0.1894422798390494	F	F	F
0.666666666666643	0.399999999999986	0.1894422798390494	F	F	F
0.777777777777786	0.399999999999986	0.1894422798390494	F	F	F
0.6666666666666714	0.2000000000000028	0.1894422798390494	F	F	F
0.888888888888857	0.399999999999986	0.1894422798390494	F	F	F
0.000000000000000	0.2000000000000028	0.1894422798390494	F	F	F
0.333333333333357	0.6000000000000014	0.1894422798390494	F	F	F
0.444444444444429	0.6000000000000014	0.1894422798390494	F	F	F
0.555555555555571	0.6000000000000014	0.1894422798390494	F	F	F
0.5540479497791787	0.0985466454692618	0.3901208345529883	T	T	T
0.777777777777786	0.6000000000000014	0.1894422798390494	F	F	F
0.1111111111111072	0.399999999999986	0.1894422798390494	F	F	F
0.000000000000000	0.5000000000000000	0.2561864044279716	F	F	F
0.000000000000000	0.6000000000000014	0.1894422798390494	F	F	F
0.222222222222214	0.6000000000000014	0.1894422798390494	F	F	F
0.666666666666643	0.799999999999972	0.1894422798390494	F	F	F
0.777777777777786	0.799999999999972	0.1894422798390494	F	F	F
0.888888888888857	0.799999999999972	0.1894422798390494	F	F	F
0.000000000000000	0.799999999999972	0.1894422798390494	F	F	F
0.1111111111111072	0.799999999999972	0.1894422798390494	F	F	F
0.222222222222214	0.799999999999972	0.1894422798390494	F	F	F
0.3333333333333286	0.799999999999972	0.1894422798390494	F	F	F
0.111111111111143	0.1000000000000014	0.2561864044279716	F	F	F
0.222222222222214	0.1000000000000014	0.2561864044279716	F	F	F
0.333333333333357	0.1000000000000014	0.2561864044279716	F	F	F
0.444444444444429	0.1000000000000014	0.2561864044279716	F	F	F
0.555555555555571	0.1000000000000014	0.2561864044279716	F	F	F
0.666666666666643	0.1000000000000014	0.2561864044279716	F	F	F
0.777777777777786	0.1000000000000014	0.2561864044279716	F	F	F
0.8888888888888928	0.1000000000000014	0.2561864044279716	F	F	F
0.000000000000000	0.1000000000000014	0.2561864044279716	F	F	F
0.777777777777786	0.5000000000000000	0.2561864044279716	F	F	F
0.888888888888857	0.299999999999972	0.2561864044279716	F	F	F
0.222222222222214	0.299999999999972	0.2561864044279716	F	F	F
0.3333333333333286	0.299999999999972	0.2561864044279716	F	F	F
0.444444444444429	0.299999999999972	0.2561864044279716	F	F	F
0.555555555555571	0.299999999999972	0.2561864044279716	F	F	F
0.666666666666643	0.299999999999972	0.2561864044279716	F	F	F
0.111111111111143	0.6000000000000014	0.1894422798390494	F	F	F
0.777777777777786	0.299999999999972	0.2561864044279716	F	F	F
0.444444444444429	0.799999999999972	0.1894422798390494	F	F	F
0.1111111111111072	0.299999999999972	0.2561864044279716	F	F	F
0.333333333333357	0.5000000000000000	0.2561864044279716	F	F	F
0.444444444444429	0.5000000000000000	0.2561864044279716	F	F	F
0.555555555555571	0.5000000000000000	0.2561864044279716	F	F	F
0.666666666666643	0.5000000000000000	0.2561864044279716	F	F	F
0.000000000000000	0.299999999999972	0.2561864044279716	F	F	F
0.555555555555571	0.799999999999972	0.1894422798390494	F	F	F
0.666666666666643	0.6000000000000014	0.1894422798390494	F	F	F
0.9992836818038788	0.1984682346957265	0.3226756397766227	T	T	T
0.888888888888857	0.899999999999986	0.2561864044279716	F	F	F
0.777777777777786	0.899999999999986	0.2561864044279716	F	F	F
0.666666666666643	0.899999999999986	0.2561864044279716	F	F	F
0.555555555555571	0.899999999999986	0.2561864044279716	F	F	F
0.333333333333357	0.7000000000000028	0.2561864044279716	F	F	F

0.1111111111111072	0.8999999999999986	0.2561864044279716	F	F	F
0.222222222222214	0.7000000000000028	0.2561864044279716	F	F	F
0.6663667336351643	0.1990131979724120	0.3221293738064506	T	T	T
0.8888888888888928	0.7000000000000028	0.2561864044279716	F	F	F
0.7777777777777786	0.7000000000000028	0.2561864044279716	F	F	F
0.6666666666666714	0.7000000000000028	0.2561864044279716	F	F	F
0.5555555555555571	0.7000000000000028	0.2561864044279716	F	F	F
0.4444444444444429	0.7000000000000028	0.2561864044279716	F	F	F
0.1111111111111143	0.7000000000000028	0.2561864044279716	F	F	F
0.222222222222214	0.8999999999999986	0.2561864044279716	F	F	F
0.0000000000000000	0.7000000000000028	0.2561864044279716	F	F	F
0.4444444444444429	0.8999999999999986	0.2561864044279716	F	F	F
0.3333333333333357	0.8999999999999986	0.2561864044279716	F	F	F
0.1106805465780272	0.9994478104873750	0.3231963907624466	T	T	T
0.5547783893799987	-0.0000059611769976	0.3226184986844898	T	T	T
0.6666929311416182	0.0000329967656088	0.3223266366333138	T	T	T
0.7781893720185447	0.9998733741493561	0.3224536799627898	T	T	T
0.8888664336807041	0.9991580185447708	0.3228423817393653	T	T	T
0.0000000000000000	0.8999999999999986	0.2561864044279716	F	F	F
0.9995604141005715	0.9989526305863115	0.3229435660632691	T	T	T
0.3322246271136535	0.9993073570757142	0.3229128986180024	T	T	T
0.4433699952215481	0.9993000581634680	0.3227854003736663	T	T	T
0.1100713650081585	0.1980427659616745	0.3226013931377450	T	T	T
0.2211129080023122	0.1981170455888287	0.3225881608723341	T	T	T
0.3323350735047705	0.1983100299777994	0.3224845231175795	T	T	T
0.4434782338930937	0.1984846936319177	0.3223773593402262	T	T	T
0.2215815335118885	0.9997475256973880	0.3231444389196801	T	T	T
0.222222222222214	0.5000000000000000	0.2561864044279716	F	F	F
0.5545367696104999	0.1983428664003872	0.3224773705189682	T	T	T
0.7779264027892026	0.1995813127045737	0.3223753144490493	T	T	T
0.2224056680490200	0.4006357238393651	0.3225742959562187	T	T	T
0.3333556881206198	0.4003566342814981	0.3224750104471079	T	T	T
0.4446586729713298	0.4006484602243333	0.3224656440753300	T	T	T
0.5560389599004636	0.4015220041809307	0.3223325086501809	T	T	T
0.6673324053853011	0.4012752564922645	0.3222815997223869	T	T	T
0.7791812572491796	0.4019439235350279	0.3223327053686758	T	T	T
0.8901756109787661	0.4021151309994271	0.3225518144773893	T	T	T
0.1116652901877708	0.4011493848354876	0.3226048187458823	T	T	T
0.3327560558834851	0.5995155181901151	0.3225296561297157	T	T	T
0.4444957850923333	0.5996355422628832	0.3224537945235670	T	T	T
0.5560281053002141	0.5997420089794110	0.3226698783402574	T	T	T
0.6673769699938018	0.6008189256078454	0.3227403611780386	T	T	T
0.7785967917392138	0.6009805566034490	0.3227369880927051	T	T	T
0.8898262191443017	0.6011789487977925	0.3229668878388476	T	T	T
0.0006915631246526	0.6011760701983052	0.3229780798726494	T	T	T
0.1114899940322845	0.6009278508871906	0.3228802352765182	T	T	T
0.1111111111111143	0.5000000000000000	0.2561864044279716	F	F	F
0.9999408479301993	0.8002516489696416	0.3231769680457988	T	T	T
0.2221854154941410	0.6003114423659044	0.3228467661233754	T	T	T
0.4436845368229816	0.7995079107706469	0.3224896759455829	T	T	T
0.5555806019194468	0.7998114855953625	0.3226529533031349	T	T	T
0.6671682951987292	0.7996481021312370	0.3228006560396822	T	T	T
0.7782217064819552	0.7999289781218299	0.3229447569984549	T	T	T
0.0009045847003178	0.4017254031125275	0.3225974194813930	T	T	T
0.8888428397063763	0.7998573801851492	0.3232476562982356	T	T	T
0.8887089019742354	0.1991129291630494	0.3225724379752145	T	T	T

0.2218312237347572	0.8000349054455619	0.3230389463532287	T	T	T
0.3324841778836019	0.7996899032838912	0.3228162889599698	T	T	T
0.1091745284654944	0.0969525875137225	0.3903278163240398	T	T	T
0.2213786413602800	0.0982607804557525	0.3907337738649505	T	T	T
0.3317801045393390	0.0982269173831601	0.3904371499449990	T	T	T
0.1114738774697130	0.8008024714133782	0.3230893571363811	T	T	T
0.4422225338040038	0.0979011595627304	0.3900172078504992	T	T	T
0.3333333333333357	0.2000000000000028	0.1894422798390494	F	F	F
0.6657480789600941	0.0982504034802758	0.3892553387052897	T	T	T
0.9984946465276331	0.0973165140439144	0.3902339732528341	T	T	T
0.2213652012793393	0.2992563794599115	0.3875106764813477	T	T	T
0.3325574180093311	0.2985840861970047	0.3876667688566743	T	T	T
0.4443039822551026	0.2997266047669131	0.3873138536893728	T	T	T
0.5551650458010051	0.2999805859251982	0.3869729596942726	T	T	T
0.6669047527284646	0.2999409369941992	0.3866547991552253	T	T	T
0.7788857348469662	0.3008981877533197	0.3873139510015280	T	T	T
0.8897322840612729	0.3006832747551744	0.3875726650586735	T	T	T
0.0001891415590413	0.3001924685547073	0.3878398238231637	T	T	T
0.1106687883388784	0.2996379630704328	0.3877721956624750	T	T	T
0.3336964502003815	0.5014596805955182	0.3896381882109874	T	T	T
0.4450807761200127	0.5008093513832150	0.3895502463622708	T	T	T
0.5570539481851406	0.5018883501215851	0.3900408154372794	T	T	T
0.6680157774601220	0.5024768623016546	0.3894634210054181	T	T	T
0.7790310816752474	0.5020668007548108	0.3894453365747067	T	T	T
0.8908529190954223	0.5030090311780772	0.3900567535997990	T	T	T
0.6673064194606082	0.9003321898041114	0.3886028716092422	T	T	T
0.7774895483538390	0.6997457310708116	0.3908218965452709	T	T	T
0.0018555872082755	0.5030532800428285	0.3902954179462355	T	T	T
0.1120955649170070	0.5019542557653953	0.3902076332360384	T	T	T
0.2226827523231368	0.5015781099127326	0.3901811118119660	T	T	T
0.4436304560657284	0.6991511286965481	0.3885571983780998	T	T	T
0.5552616915104397	0.6985623291278116	0.3890369452078797	T	T	T
0.8879431972799874	0.0979888437908765	0.3900500371970553	T	T	T
0.6671389224050267	0.6993598815820593	0.3902486379670578	T	T	T
0.8890597429244503	0.8991969407188735	0.3904264123085114	T	T	T
0.0004960636076740	0.7011478625911767	0.3901809374377311	T	T	T
0.1111031140091363	0.7005929106985228	0.3904756434002675	T	T	T
0.2213725790709943	0.6996383290736086	0.3901623662740801	T	T	T
0.3321009715723166	0.6992026961359603	0.3896705648428831	T	T	T
0.5556417749007652	0.9005123579016666	0.3886024814200940	T	T	T
0.8887980782232497	0.7002836599920833	0.3903472603681903	T	T	T
0.7787023075837803	0.9002557174024347	0.3897025752477447	T	T	T
0.9999189147776109	0.8994712981778294	0.3906480611978268	T	T	T
0.5544184049484874	0.5986956651929782	0.4571146676158079	T	T	T
0.3338490533616600	0.2006512645684425	0.4550163792514974	T	T	T
0.2204150717805020	0.1996106800476453	0.4535209724892234	T	T	T
0.1101064158509049	0.2002073596313882	0.4543149684318069	T	T	T
0.4440685754486349	0.9998867359667768	0.4571103355890274	T	T	T
0.3323389731720626	0.0003820104630504	0.4576849448662997	T	T	T
0.2205514204103647	0.9985847808158294	0.4586775095613101	T	T	T
0.4459125478070252	0.2039669367113063	0.4539671986457011	T	T	T
0.1104443901269664	0.9992694839658850	0.4586015816942967	T	T	T
0.8896111109040267	0.0000117290454516	0.4576884083133778	T	T	T
0.7778192204474985	0.9997424581848854	0.4571323477373966	T	T	T
0.6662054083710497	0.9986705791317577	0.4558568430199275	T	T	T
0.5550606328290710	0.9998421695620598	0.4565943523107647	T	T	T

0.3325171891817364	0.8997772405600307	0.3900764649439735	T	T	T
0.2220204802899927	0.9004755287170164	0.3906226071127197	T	T	T
0.0001009771268352	0.9998285075336536	0.4585649448239106	T	T	T
0.7772728003238356	0.0983943044933748	0.3894537075785082	T	T	T
0.5546786125840736	0.1993559945953096	0.4540053856808124	T	T	T
0.4440773381353861	0.6009445666026860	0.4561132378814272	T	T	T
0.5559270459214878	0.3996322646714259	0.4550150259122337	T	T	T
0.7779995862435218	0.1996745557441659	0.4534596969755842	T	T	T
0.4438959148921445	0.9001939175878800	0.3892229188882603	T	T	T
0.9995057440282977	0.2000583220986790	0.4544438416559273	T	T	T
0.2222865571017527	0.3997748752061248	0.4541011716731666	T	T	T
0.3335274988856097	0.3995511030222258	0.4528550724192944	T	T	T
0.6675168623206725	0.2014053266080344	0.4523450816175120	T	T	T
0.4449841905142035	0.3974046903093616	0.4533653440075279	T	T	T
0.1112436464054919	0.9005134559673280	0.3904631536391838	T	T	T
0.7782051376008227	0.4006801099209362	0.4534823780434272	T	T	T
0.8898137488627995	0.4001563955584362	0.4538658892688965	T	T	T
0.0002712342169159	0.4000038426154239	0.4542745169661519	T	T	T
0.1111304950998218	0.3996889914551036	0.4544349949486612	T	T	T
0.3326575145286575	0.6002523017573164	0.4574373154459762	T	T	T
0.6652837285046502	0.3976992514966345	0.4522242361163691	T	T	T
0.6652751595634663	0.5982734690528363	0.4581396739867722	T	T	T
0.8886678477169537	0.2002002676777475	0.4542371538686660	T	T	T
0.9255938911949134	0.4678614565510468	0.5381269703617595	T	T	T
0.1107944599525535	0.6007360252598298	0.4584814761298066	T	T	T
0.2211075376537381	0.6004886044332185	0.4578222874279624	T	T	T
0.4448274479553498	0.7996850762635775	0.4533792565812715	T	T	T
0.5555891125348875	0.7998016988914807	0.4542709049668935	T	T	T
0.6663660537300905	0.8000423668849591	0.4539442019171927	T	T	T
0.8891105277787397	0.8001990146732464	0.4566031931399814	T	T	T
0.0002992996413541	0.7999159786359629	0.4566831182956899	T	T	T
0.1107777557889932	0.7993082404703953	0.4566525033134285	T	T	T
0.2222695298764406	0.7998776742882343	0.4562628995821739	T	T	T
0.3335700987360194	0.8001068234187265	0.4555764402096911	T	T	T
0.1812790489793154	0.1305353861376308	0.5375853720290834	T	T	T
0.2859372398152318	0.1229979349831382	0.5368154702486874	T	T	T
0.3994972220865812	0.1225058395366035	0.5343863848830919	T	T	T
0.5158409282295267	0.1249853787709537	0.5380356442546192	T	T	T
0.6264190437389303	0.1272250966140463	0.5348447117431638	T	T	T
0.3716316417330359	0.4698186591752103	0.5361558624723969	T	T	T
0.1112080310290404	0.3011324680554381	0.5246205314983904	T	T	T
0.8895696148064990	0.6006153336803410	0.4574098972428389	T	T	T
0.4292662504007365	0.2882115407295833	0.5305075412010717	T	T	T
0.7389440685366386	0.1315577446556735	0.5375931133936115	T	T	T
0.8502403551132439	0.1326921634753992	0.5386368323513073	T	T	T
0.9620453417563982	0.1331680850803844	0.5388280942348922	T	T	T
0.0728088744301817	0.1326295197200561	0.5385810681849028	T	T	T
0.9998637715788872	0.6005323656318333	0.4583837543862396	T	T	T
0.2218476320465599	0.3012626861413647	0.5243445308568854	T	T	T
0.5558418966855965	0.2910572791488933	0.5222606786354907	T	T	T
0.6031569825085297	0.4851482063121046	0.5380543426099450	T	T	T
0.6679908082745675	0.2986854073710891	0.5239513857490834	T	T	T
0.7780055421165173	0.3000514677116277	0.5212265274560747	T	T	T
0.8882540934559521	0.3000184277047445	0.5255771321335707	T	T	T
0.9990828123848586	0.2998280100983559	0.5235938969315058	T	T	T
0.3296862927869426	0.2988709451349285	0.5216084219320158	T	T	T

0.4845153860543285	0.4728866495561144	0.5346465061546374	T	T	T
0.7780803288400054	0.8011944526519070	0.4565314433145470	T	T	T
0.7774838703700090	0.5988655043704666	0.4571493467563958	T	T	T
0.6680724915232794	0.8039781732918174	0.5418649994622339	T	T	T
0.5551722810329287	0.7999242013540603	0.5434177471129522	T	T	T
0.2959097181480623	0.6338226013292234	0.5355693732935903	T	T	T
0.1848132952735891	0.6337134531590123	0.5379237106820686	T	T	T
0.0736771031513801	0.6341212903919783	0.5374242328241863	T	T	T
0.7079238708778016	0.4716364240059422	0.5339044623951913	T	T	T
0.7804621758307224	0.8059288347624963	0.5460020706038442	T	T	T
0.8540200034082531	0.6382197285443777	0.5353168477630480	T	T	T
0.6345070927523623	0.6439958370357426	0.5353362014827541	T	T	T
0.5208611871635801	0.6384174734868955	0.5339754953954167	T	T	T
0.4087666924061609	0.6355860480243338	0.5351533522284925	T	T	T
0.2603343182463774	0.4689697338295033	0.5382637807898255	T	T	T
0.1483349698428618	0.4682394141775167	0.5385383141056945	T	T	T
0.0368502655271496	0.4680823821825549	0.5383216903849991	T	T	T
0.7476312509618507	0.6456147349067803	0.5331549568965916	T	T	T
0.8909113651817615	0.8037639104128810	0.5455515521850125	T	T	T
0.9627595092696032	0.6344154609951546	0.5374743328663808	T	T	T
0.3654757427444437	0.9585441674558139	0.5335747560036755	T	T	T
0.4775400351987442	0.9592768632967287	0.5355476612359983	T	T	T
0.9980840223346941	0.7989868464977653	0.5457267731770503	T	T	T
0.1080564657982811	0.7969149200602473	0.5455758357051756	T	T	T
0.7022095198374255	0.9659824714529375	0.5349537836214833	T	T	T
0.3307935114364374	0.7965002912504799	0.5444389102407738	T	T	T
0.4424598189042429	0.7974631605134449	0.5411269686284527	T	T	T
0.2196029570865756	0.7967975007302563	0.5450948666480260	T	T	T
0.8145351451217204	0.9677641600760999	0.5355207544488265	T	T	T
0.8157921026777286	0.4693575174947651	0.5376663725259295	T	T	T
0.9255832487615301	0.9673259004708750	0.5377732741124012	T	T	T
0.0354794860693731	0.9653483460594325	0.5377718815226686	T	T	T
0.1423693800098520	0.9597754933060157	0.5378681671371172	T	T	T
0.2531971437881765	0.9588916395716438	0.5372498239677340	T	T	T
0.5901237224977930	0.9618898543689410	0.5335898218430233	T	T	T
0.3029622251881631	0.9752955774799604	0.6519499213738045	T	T	T
0.6772962325319075	0.1540127542919358	0.6398528762978831	T	T	T
0.6772356086608997	0.4832199607428294	0.6413600138388724	T	T	T
0.3898542759994241	0.6358074576106644	0.6415939835135123	T	T	T
0.4971055751842124	0.5474162106450535	0.6412098106156111	T	T	T
0.3053253988824146	0.3110742950058431	0.6326068479999098	T	T	T
0.3621904175332178	0.4067962664904187	0.6354702788521047	T	T	T
0.4330244604822238	0.4474007784891215	0.6401316746552995	T	T	T
0.6783631444879503	0.8210634389680808	0.6459878671206497	T	T	T
0.7492611179799162	0.8615378118100384	0.6505997323360085	T	T	T
0.8067481814045074	0.9571142329195037	0.6498864694959096	T	T	T
0.3209252144762427	0.2584636100319562	0.6341844066507512	T	T	T
0.7201247763231919	0.9659251327289891	0.6404062499640713	T	T	T
0.3925799581755648	0.3029478654726666	0.6391524405553344	T	T	T
0.7916410921052452	0.0100479849500858	0.6448284552068625	T	T	T
0.3607091980966242	0.0707226616778212	0.6524560791336564	T	T	T
0.6144475868727093	0.7218201822698841	0.6442799167046341	T	T	T
0.4309467243641515	0.1107243809559681	0.6448287393787275	T	T	T
0.8057909478584735	0.2899019394269586	0.6409746748262233	T	T	T
0.6125456839720614	0.3834675488893607	0.6409686282808348	T	T	T
0.3183486106414350	0.5920647803648093	0.6458194770411806	T	T	T

0.3611272029868330	0.7410021051211263	0.6493967240924975	T	T	T
0.3172122680069771	0.9221089078954514	0.6438859652042196	T	T	T
0.7906825660824344	0.3424470665741384	0.6346900129790100	T	T	T
0.4958901380360430	0.8803649012250372	0.6422222284704225	T	T	T
0.7481523929420894	0.1943968059767476	0.6437551635687246	T	T	T
0.3034442810506767	0.6453230220350022	0.6496084618202504	T	T	T
0.4318095488241950	0.7808744389788287	0.6449874283476547	T	T	T
0.6132239697019657	0.0544900368122776	0.6400020549992219	T	T	T
0.3880201922615656	0.9658297044451281	0.6362730360187784	T	T	T
0.4949786894655678	0.2095961063557121	0.6435875644335094	T	T	T
0.7198916988489640	0.6286667834372398	0.6462339950468037	T	T	T
0.7915545996981356	0.6721643031179763	0.6436898150872632	T	T	T
0.8059243359368691	0.6184335909401393	0.6398977263744670	T	T	T
0.7479258823019154	0.5227833197727255	0.6381834060203458	T	T	T
0.7189882762586668	0.2980009743790576	0.6305852780183138	T	T	T
0.2748913183462364	0.5169548664098002	0.6449047647464804	T	T	T
0.3530352692892042	0.4509186046418268	0.6335441888054674	T	T	T
0.7577846396969904	0.8168788045956096	0.6536028970374370	T	T	T
0.2498612669025511	0.2781710469339940	0.6279303683252961	T	T	T
0.2477826344058435	0.6127861412904815	0.6517945997798349	T	T	T
0.7566657292524558	0.1499709610546463	0.6482279801960351	T	T	T
0.3528103138285089	0.7859576910205327	0.6517138921481495	T	T	T
0.8624840859955811	0.9899450511349834	0.6521579677837478	T	T	T
0.7562608395038396	0.4780612262999698	0.6344465698415445	T	T	T
0.8615946129677279	0.3227746540339670	0.6426689000252286	T	T	T
0.2783488988494328	0.1836586757396345	0.6307008661594188	T	T	T
0.8349972605320977	0.0850853885879942	0.6429769932407594	T	T	T
0.7053112366940273	0.0037131069553816	0.6360615456051614	T	T	T
0.4081085409553364	0.2655672857718801	0.6407383218347154	T	T	T
0.3530547184979474	0.1157616185493448	0.6581643422595634	T	T	T
0.2476166613751763	0.9426038257283315	0.6568210334282911	T	T	T
0.8352046116020216	0.7472686107067497	0.6438942403003567	T	T	T
0.2736262816147165	0.8470617767402345	0.6421722906440527	T	T	T
0.8614579264237222	0.6506144215620420	0.6372527298047673	T	T	T
0.7051134488939640	0.6668374950476162	0.6486063619365832	T	T	T
0.4046315680414065	0.5978124660750233	0.6380392745899542	T	T	T
0.7040822365866213	0.3353022823967608	0.6247442627372632	T	T	T
0.8340171621910454	0.4172592661435763	0.6313794714816232	T	T	T
0.4018606236974622	0.9275867796171919	0.6296964066278935	T	T	T
0.6625872544471190	0.2052465049501476	0.6328498279093352	T	T	T
0.6636666976453008	0.8728181059597736	0.6408905100475895	T	T	T
0.6220128078899121	0.6651919960547237	0.6474385321807610	T	T	T
0.5493902720458634	0.6974030787000310	0.6378218477190105	T	T	T
0.4883910059736239	0.6030393126063636	0.6388519073527994	T	T	T
0.4876257479254019	0.9363927447552715	0.6410443699140923	T	T	T
0.5478800740283837	0.0295228272889990	0.6358447282105102	T	T	T
0.6214740138467545	0.9984815370490090	0.6413870145109191	T	T	T
0.4463116177685452	0.7287778439396231	0.6410426675107762	T	T	T
0.4448479417209881	0.0588678162877962	0.6366928401711572	T	T	T
0.4476647058075574	0.3954674646769098	0.6424562681032123	T	T	T
0.5621796542821227	0.5726035641121657	0.6438609963391851	T	T	T
0.5589475942376897	0.2337172535780138	0.6332245929670025	T	T	T
0.6636666648216740	0.5360059047192413	0.6456736415779116	T	T	T
0.6200420196375588	0.3274225726104498	0.6336171676463418	T	T	T
0.5487654793747571	0.3588389667210689	0.6489745963861848	T	T	T
0.4888331863643163	0.2668194119609047	0.6511794580295120	T	T	T

0.5610206213730438	0.9047368227147642	0.6387440583440067	T	T	T
0.5521651386087615	0.1307360655167111	0.6190629773525316	T	T	T
0.5551087444541187	0.8004308768666102	0.6264938360368798	T	T	T
0.5553423199780807	0.4663732306316891	0.6587894099730528	T	T	T
0.5540427208626777	0.4689913854575832	0.7107539372557224	T	T	T
0.5273319750237995	0.3481231174132895	0.5623968777097150	T	T	T

Fig. 6g

Au C H N V O

1.000000000000000

26.0801187006857766 0.000000000000000 0.000000000000000

-14.4889548337143204 14.4889548337143204 0.000000000000000

0.000000000000000 0.000000000000000 31.000000000000000

Au C H N V O

279 36 24 18 3 2

Selective dynamics

Direct

0.000000000000000	0.000000000000000	0.1894422798390494	F	F	F
0.5555555555555571	0.2000000000000028	0.1894422798390494	F	F	F
0.444444444444429	0.2000000000000028	0.1894422798390494	F	F	F
0.222222222222214	0.2000000000000028	0.1894422798390494	F	F	F
0.1111111111111143	0.2000000000000028	0.1894422798390494	F	F	F
0.777777777777786	0.2000000000000028	0.1894422798390494	F	F	F
0.888888888888857	0.000000000000000	0.1894422798390494	F	F	F
0.666666666666643	0.000000000000000	0.1894422798390494	F	F	F
0.555555555555571	0.000000000000000	0.1894422798390494	F	F	F
0.444444444444429	0.000000000000000	0.1894422798390494	F	F	F
0.333333333333357	0.000000000000000	0.1894422798390494	F	F	F
0.222222222222214	0.000000000000000	0.1894422798390494	F	F	F
0.1111111111111143	0.000000000000000	0.1894422798390494	F	F	F
0.777777777777786	0.000000000000000	0.1894422798390494	F	F	F
0.888888888888857	0.500000000000000	0.2561864044279716	F	F	F
0.8888888888888928	0.2000000000000028	0.1894422798390494	F	F	F
0.222222222222214	0.399999999999986	0.1894422798390494	F	F	F
0.8888888888888928	0.6000000000000014	0.1894422798390494	F	F	F
0.000000000000000	0.399999999999986	0.1894422798390494	F	F	F
0.333333333333357	0.399999999999986	0.1894422798390494	F	F	F
0.444444444444429	0.399999999999986	0.1894422798390494	F	F	F
0.555555555555571	0.399999999999986	0.1894422798390494	F	F	F
0.666666666666643	0.399999999999986	0.1894422798390494	F	F	F
0.777777777777786	0.399999999999986	0.1894422798390494	F	F	F
0.6666666666666714	0.2000000000000028	0.1894422798390494	F	F	F
0.888888888888857	0.399999999999986	0.1894422798390494	F	F	F
0.000000000000000	0.2000000000000028	0.1894422798390494	F	F	F
0.333333333333357	0.6000000000000014	0.1894422798390494	F	F	F
0.444444444444429	0.6000000000000014	0.1894422798390494	F	F	F
0.555555555555571	0.6000000000000014	0.1894422798390494	F	F	F
0.5543181871291156	0.0977485795738838	0.3892772963697990	T	T	T
0.777777777777786	0.6000000000000014	0.1894422798390494	F	F	F
0.1111111111111072	0.399999999999986	0.1894422798390494	F	F	F
0.000000000000000	0.500000000000000	0.2561864044279716	F	F	F
0.000000000000000	0.6000000000000014	0.1894422798390494	F	F	F
0.222222222222214	0.6000000000000014	0.1894422798390494	F	F	F
0.666666666666643	0.799999999999972	0.1894422798390494	F	F	F
0.777777777777786	0.799999999999972	0.1894422798390494	F	F	F

0.888888888888857	0.799999999999972	0.1894422798390494	F	F	F
0.000000000000000	0.799999999999972	0.1894422798390494	F	F	F
0.1111111111111072	0.799999999999972	0.1894422798390494	F	F	F
0.222222222222214	0.799999999999972	0.1894422798390494	F	F	F
0.3333333333333286	0.799999999999972	0.1894422798390494	F	F	F
0.1111111111111143	0.1000000000000014	0.2561864044279716	F	F	F
0.222222222222214	0.1000000000000014	0.2561864044279716	F	F	F
0.3333333333333357	0.1000000000000014	0.2561864044279716	F	F	F
0.444444444444429	0.1000000000000014	0.2561864044279716	F	F	F
0.555555555555571	0.1000000000000014	0.2561864044279716	F	F	F
0.666666666666643	0.1000000000000014	0.2561864044279716	F	F	F
0.777777777777786	0.1000000000000014	0.2561864044279716	F	F	F
0.8888888888888928	0.1000000000000014	0.2561864044279716	F	F	F
0.000000000000000	0.1000000000000014	0.2561864044279716	F	F	F
0.777777777777786	0.5000000000000000	0.2561864044279716	F	F	F
0.888888888888857	0.299999999999972	0.2561864044279716	F	F	F
0.222222222222214	0.299999999999972	0.2561864044279716	F	F	F
0.3333333333333286	0.299999999999972	0.2561864044279716	F	F	F
0.444444444444429	0.299999999999972	0.2561864044279716	F	F	F
0.555555555555571	0.299999999999972	0.2561864044279716	F	F	F
0.666666666666643	0.299999999999972	0.2561864044279716	F	F	F
0.1111111111111143	0.6000000000000014	0.1894422798390494	F	F	F
0.777777777777786	0.299999999999972	0.2561864044279716	F	F	F
0.444444444444429	0.799999999999972	0.1894422798390494	F	F	F
0.1111111111111072	0.299999999999972	0.2561864044279716	F	F	F
0.3333333333333357	0.5000000000000000	0.2561864044279716	F	F	F
0.444444444444429	0.5000000000000000	0.2561864044279716	F	F	F
0.555555555555571	0.5000000000000000	0.2561864044279716	F	F	F
0.666666666666643	0.5000000000000000	0.2561864044279716	F	F	F
0.000000000000000	0.299999999999972	0.2561864044279716	F	F	F
0.555555555555571	0.799999999999972	0.1894422798390494	F	F	F
0.666666666666643	0.6000000000000014	0.1894422798390494	F	F	F
0.9997686017956398	0.1985651562031531	0.3228306457009012	T	T	T
0.888888888888857	0.899999999999986	0.2561864044279716	F	F	F
0.777777777777786	0.899999999999986	0.2561864044279716	F	F	F
0.666666666666643	0.899999999999986	0.2561864044279716	F	F	F
0.555555555555571	0.899999999999986	0.2561864044279716	F	F	F
0.3333333333333357	0.7000000000000028	0.2561864044279716	F	F	F
0.1111111111111072	0.899999999999986	0.2561864044279716	F	F	F
0.222222222222214	0.7000000000000028	0.2561864044279716	F	F	F
0.6663837334275162	0.1987146155963847	0.3222524883182746	T	T	T
0.8888888888888928	0.7000000000000028	0.2561864044279716	F	F	F
0.777777777777786	0.7000000000000028	0.2561864044279716	F	F	F
0.6666666666666714	0.7000000000000028	0.2561864044279716	F	F	F
0.555555555555571	0.7000000000000028	0.2561864044279716	F	F	F
0.444444444444429	0.7000000000000028	0.2561864044279716	F	F	F
0.1111111111111143	0.7000000000000028	0.2561864044279716	F	F	F
0.222222222222214	0.899999999999986	0.2561864044279716	F	F	F
0.000000000000000	0.7000000000000028	0.2561864044279716	F	F	F
0.444444444444429	0.899999999999986	0.2561864044279716	F	F	F
0.3333333333333357	0.899999999999986	0.2561864044279716	F	F	F
0.1105632937952028	0.9997130374681474	0.3231208131903071	T	T	T
0.5549877237857446	0.9995900298673897	0.3223453016456305	T	T	T
0.6666290303132461	0.9997403960597789	0.3223853121398632	T	T	T
0.7786178374901773	0.0004773598176600	0.3226259864012115	T	T	T
0.8896093928712080	0.0002969362132263	0.3230980201152225	T	T	T

0.0000000000000000	0.8999999999999986	0.2561864044279716	F	F	F
0.0000075000551879	0.9998801906258543	0.3231273256499756	T	T	T
0.3321138210716034	0.9995184325256198	0.3227461290267088	T	T	T
0.4434867533262735	0.9994319860781894	0.3226092096776107	T	T	T
0.1102961190897388	0.1981518582425252	0.3228491934158584	T	T	T
0.2206788226106055	0.1977696694306933	0.3228061246761170	T	T	T
0.3318759027311855	0.1982339204154679	0.3226167589403386	T	T	T
0.4435554296564413	0.1988431112623627	0.3223492976526906	T	T	T
0.2213773634770573	0.9999177924202874	0.3230574178182194	T	T	T
0.2222222222222214	0.5000000000000000	0.2561864044279716	F	F	F
0.5548476034925222	0.1985829048923152	0.3223131879500905	T	T	T
0.7779969963417129	0.1990779524592885	0.3223459016366073	T	T	T
0.2218957827101601	0.3992548820796291	0.3231224987312287	T	T	T
0.3325318415797608	0.3994519495984457	0.3228726671596711	T	T	T
0.4446477101934675	0.4009727382645087	0.3224385821348691	T	T	T
0.5560915135590262	0.4017496521158733	0.3223012868406275	T	T	T
0.6673799309878247	0.4015572072595519	0.3222456208987208	T	T	T
0.7791177396243210	0.4019281105741456	0.3222005621841428	T	T	T
0.8900693520875446	0.4017335583978745	0.3224179906379164	T	T	T
0.1119315747376761	0.4009823081638114	0.3226226790424820	T	T	T
0.3323450571748339	0.5985135808546768	0.3226066200216320	T	T	T
0.4438635436256835	0.5991686296523042	0.3226812979691107	T	T	T
0.5557879257799113	0.6000832903787068	0.3226565384876884	T	T	T
0.6679037172042337	0.6013288614313077	0.3225831011816003	T	T	T
0.7787269686661382	0.6010024226666628	0.3227472923143000	T	T	T
0.8897086450537042	0.6011066084972895	0.3227861203215533	T	T	T
0.0005222658045891	0.6008509955401766	0.3228195786592301	T	T	T
0.1116825469325549	0.6010502924401694	0.3228462411054920	T	T	T
0.1111111111111143	0.5000000000000000	0.2561864044279716	F	F	F
0.0004091496618182	0.8005952509146301	0.3229775162582314	T	T	T
0.2225034750033085	0.6004001536254466	0.3228806080018610	T	T	T
0.4435751108473057	0.7988563475403168	0.3225180378736196	T	T	T
0.5552089292204105	0.7994082966462699	0.3227196673841788	T	T	T
0.6670187846689785	0.8003196018515673	0.3226794849682375	T	T	T
0.7782889907282849	0.8006984693732074	0.3227824510623271	T	T	T
0.0007291341666840	0.4012461153382589	0.3225330681657312	T	T	T
0.8892405196142869	0.8005091666326593	0.3229249550043377	T	T	T
0.8891951393502519	0.1991354609257249	0.3226149402921096	T	T	T
0.2221800678592877	0.8001154298231586	0.3229142105643359	T	T	T
0.3328277743530941	0.7996653297032348	0.3226648412313992	T	T	T
0.1091151486062516	0.0965593634759979	0.3918492046853395	T	T	T
0.2193649265400709	0.0975712588569267	0.3911421090499141	T	T	T
0.3316288816203372	0.0984531002431116	0.3900810689627283	T	T	T
0.1115431269656766	0.8005868332125665	0.3229810627720392	T	T	T
0.4426569931147566	0.0983579369689655	0.3894538603839240	T	T	T
0.3333333333333357	0.2000000000000028	0.1894422798390494	F	F	F
0.6663292746646465	0.0982518633527542	0.3893715504079361	T	T	T
0.0000145365349549	0.0973640438668097	0.3916345540904747	T	T	T
0.2199039167225369	0.2956970427847273	0.3893356585070250	T	T	T
0.3321591765840483	0.2981899303677541	0.3876087442450795	T	T	T
0.4447763924293718	0.3005107997347055	0.3872812096465237	T	T	T
0.5555872792673440	0.3008366905699474	0.3870693531718729	T	T	T
0.6667876283044085	0.3002148295723057	0.3864289847202953	T	T	T
0.7784766308993816	0.3005255407406981	0.3869181888706250	T	T	T
0.8895590098859087	0.3004396285795246	0.3875528593862082	T	T	T
0.0007007405377420	0.3001495333795396	0.3879017084905038	T	T	T

0.1104226453643510	0.2977226580895891	0.3886508882817361	T	T	T
0.3326322456566429	0.4992894774843621	0.3902804372348754	T	T	T
0.4448879916368804	0.5012181382530453	0.3895316327295902	T	T	T
0.5579948364453562	0.5032669874709647	0.3892127848554007	T	T	T
0.6686588648726773	0.5025998810780402	0.3896324784753272	T	T	T
0.7795182356263797	0.5024502676358829	0.3895896141925822	T	T	T
0.8906112135490446	0.5026772761170165	0.3898800240084833	T	T	T
0.6675470600914547	0.9008945473463751	0.3887615881143647	T	T	T
0.7779957264716540	0.7003299957306608	0.3897726121249425	T	T	T
0.0018282977475988	0.5031932219844184	0.3899340009201438	T	T	T
0.1122659983356139	0.5025443141555317	0.3896514410819185	T	T	T
0.2226719378681727	0.5007244985886565	0.3902600331683520	T	T	T
0.4425789416108141	0.6978412942961211	0.3888879095373838	T	T	T
0.5547338767735265	0.6989694993147197	0.3891155580389025	T	T	T
0.8890308969708776	0.0983397627336315	0.3905430160936680	T	T	T
0.6672046288017278	0.7009110029572794	0.3893413381715767	T	T	T
0.8892731065308047	0.9003125863039048	0.3900889285857491	T	T	T
0.0004471129415951	0.7009669469556280	0.3901020051118805	T	T	T
0.1111320488363470	0.7009330361406505	0.3902617110287643	T	T	T
0.2217841291166398	0.7003219099360817	0.3899842948790392	T	T	T
0.3321368660218717	0.6989327129244106	0.3897122481060942	T	T	T
0.5554800627950128	0.9000337103958485	0.3886371446406081	T	T	T
0.8890421826867291	0.7002261910821138	0.3899444565972265	T	T	T
0.7788234604623925	0.9010094011768554	0.3897877716180179	T	T	T
0.9999284931717017	0.9002009427422627	0.3905360056507960	T	T	T
0.5568897210767054	0.6013631673998729	0.4569270129862538	T	T	T
0.3330383779698121	0.2006224385072103	0.4535966401932970	T	T	T
0.2183561568606276	0.1947063932219333	0.4575996784777937	T	T	T
0.1086756492640904	0.1945737435262872	0.4583090271508558	T	T	T
0.4454014679505675	0.0006526447661362	0.4562846587037623	T	T	T
0.3335442473369493	0.0015814833590420	0.4572585916882237	T	T	T
0.2219027633308314	0.0006958121449741	0.4579643730100306	T	T	T
0.4454634360424827	0.2036124068927363	0.4532087572622779	T	T	T
0.1081330745913013	0.9960655177911358	0.4606224542528530	T	T	T
0.8901501065255173	0.9993797341458306	0.4579105848842996	T	T	T
0.7790397635987127	0.0006846166873389	0.4574221088904680	T	T	T
0.6666580836374943	0.9985197299352115	0.4559037876789032	T	T	T
0.5557023140763060	0.9998968376335888	0.4564786931515071	T	T	T
0.3331562440661029	0.9003857391215212	0.3896796844194693	T	T	T
0.2221201346977936	0.9007684936020487	0.3902549977618107	T	T	T
0.9995720570970003	0.9961431919913313	0.4609219199891476	T	T	T
0.7781075041238703	0.0988118206669122	0.3896755245383232	T	T	T
0.5546407471223379	0.1994414185921019	0.4531992656132975	T	T	T
0.4442951180657858	0.6006554375921802	0.4563479586528857	T	T	T
0.5579873830527641	0.4028788766841635	0.4547604130789007	T	T	T
0.7785142023110001	0.2002850614898143	0.4533542791148233	T	T	T
0.4439421141113153	0.8995550824254793	0.3889424280428847	T	T	T
0.0007532591171352	0.2004692561899470	0.4544999359522245	T	T	T
0.2202474624799443	0.3972424914515526	0.4541678301358921	T	T	T
0.3331064928723179	0.3971561193462214	0.4530733539855218	T	T	T
0.6670373888582410	0.2014034091596550	0.4521521144927692	T	T	T
0.4472382754280016	0.4008494342651468	0.4525963578256418	T	T	T
0.1109245257928970	0.9005182330084334	0.3906413504521963	T	T	T
0.7778941701104644	0.4000077613654144	0.4533293171208063	T	T	T
0.8893305118340841	0.4002516996633975	0.4535789285258339	T	T	T
0.9998387355452342	0.4005294282541816	0.4538346039432688	T	T	T

0.1107889168419894	0.4018618260083721	0.4536301112587391	T	T	T
0.3319974456441079	0.5987983103519843	0.4575545781604923	T	T	T
0.6664072772002660	0.3980777398972606	0.4526590262140244	T	T	T
0.6670325588066258	0.6012277896569528	0.4569404981638268	T	T	T
0.8901850581904406	0.2010955854178805	0.4544061997621808	T	T	T
0.9269039996623984	0.4691099742908825	0.5375155962335886	T	T	T
0.1114890566480926	0.6016739151896734	0.4579230636602390	T	T	T
0.2221947865191565	0.6020834519370484	0.4575483858077071	T	T	T
0.4442734342951210	0.7994481423834396	0.4536202499526301	T	T	T
0.5547801772194648	0.7997749281772617	0.4546803943831344	T	T	T
0.6660755212580383	0.8013066542472620	0.4540971899326567	T	T	T
0.8877224274959328	0.7992239126715203	0.4555493408846247	T	T	T
0.9990995025016212	0.7991511279118079	0.4560799426015364	T	T	T
0.1112391516136749	0.8005735082665982	0.4562461939239663	T	T	T
0.2228374229980307	0.8014474488878433	0.4557558969769377	T	T	T
0.3339106696176152	0.8012282145415954	0.4555266710757439	T	T	T
0.2052693796554683	0.1438491741490449	0.5442279401052966	T	T	T
0.3042704115009132	0.1345217889041817	0.5377759000248262	T	T	T
0.4096318398507743	0.1305869495036535	0.5358176469764856	T	T	T
0.5202389991176213	0.1317035590191251	0.5378982677038203	T	T	T
0.6273528949895586	0.1287882356203452	0.5346269399263773	T	T	T
0.3740594539381308	0.4706119403452604	0.5357725581574070	T	T	T
0.1112541342757634	0.3077571525589740	0.5224187811281865	T	T	T
0.8897131802492397	0.6003890903762568	0.4575833123369654	T	T	T
0.4497183369545703	0.3027689577360544	0.5274465810929653	T	T	T
0.7379784703384694	0.1304838446523027	0.5370697633523622	T	T	T
0.8473096821625162	0.1306916028096493	0.5382586198666708	T	T	T
0.9580479926626846	0.1347811309638822	0.5387989214182701	T	T	T
0.0698467839197238	0.1473662939668457	0.5463253135370685	T	T	T
0.0002829811804480	0.6007250347847212	0.4580466106510212	T	T	T
0.2256157686215836	0.3045096652800244	0.5218487231318322	T	T	T
0.5576748353103272	0.3009785458536746	0.5222846771087005	T	T	T
0.5952881382493979	0.4694512430080536	0.5401691026270776	T	T	T
0.6676541648398088	0.3006174667415804	0.5241441302362608	T	T	T
0.7772656236775263	0.2999754999330689	0.5211771067494420	T	T	T
0.8871074893207799	0.2997614508904390	0.5248539674573375	T	T	T
0.9983606890385833	0.3026926013571870	0.5253563425501275	T	T	T
0.3420922737530624	0.3063493299118581	0.5209427399264412	T	T	T
0.4880881215153677	0.4731041720685556	0.5357530517274873	T	T	T
0.7770010946473764	0.8003155014304312	0.4559119060990947	T	T	T
0.7777105736527854	0.5994855734084366	0.4572503415490148	T	T	T
0.6679206776361976	0.8001990980648156	0.5419794598084314	T	T	T
0.5553443860779096	0.7989245500873234	0.5438592638951137	T	T	T
0.2972502341448611	0.6352429385668634	0.5354968979448880	T	T	T
0.1871578456654632	0.6377910717339311	0.5372732119475171	T	T	T
0.0758164010079817	0.6369237768271161	0.5371122126418096	T	T	T
0.7061877440282676	0.4700217228423114	0.5355318699122216	T	T	T
0.7793361918170043	0.8019513622065427	0.5448933627859945	T	T	T
0.8538282820270778	0.6364566470848887	0.5353992574164114	T	T	T
0.6334608685639199	0.6376493571515386	0.5370137433705503	T	T	T
0.5216994110489976	0.6375399249190312	0.5335728075481802	T	T	T
0.4094815455337572	0.6360867444230819	0.5351707025165221	T	T	T
0.2619183820195740	0.4703986221870677	0.5376078429959179	T	T	T
0.1491105941634033	0.4721903831880643	0.5378224275420189	T	T	T
0.0375233083028731	0.4703382273436240	0.5378335405190386	T	T	T
0.7422401809581315	0.6367436005770636	0.5345229601570132	T	T	T

0.8869418106947516	0.7981459963063174	0.5436084162836422	T	T	T
0.9642574084687741	0.6351201761063947	0.5375397643871910	T	T	T
0.3692771802288343	0.9620940053491606	0.5331944661364716	T	T	T
0.4795317188021886	0.9626347341473129	0.5357707253380004	T	T	T
0.0002866489004596	0.7980606555606741	0.5443180831619681	T	T	T
0.1120258919492185	0.8005055143893220	0.5451654094832208	T	T	T
0.7010834885276741	0.9630487301993990	0.5349791332621827	T	T	T
0.3332746640407026	0.7987724698638485	0.5445008537359919	T	T	T
0.4438270950973315	0.7992989413639933	0.5414545796024285	T	T	T
0.2225352913138343	0.8004188683318283	0.5446512954086604	T	T	T
0.8134987153634707	0.9652662697244647	0.5356917129428594	T	T	T
0.8165428898123305	0.4695202127926251	0.5371893451476747	T	T	T
0.9248438367276169	0.9672109015351225	0.5374257135678351	T	T	T
0.0300794894480863	0.9553772163574681	0.5435184140295208	T	T	T
0.1490412332496815	0.9647355692525015	0.5370302675017150	T	T	T
0.2594121734124583	0.9642264226808438	0.5365057092225844	T	T	T
0.5902755461295659	0.9617169553937954	0.5334279331937289	T	T	T
0.3017292082332602	0.9765630392277468	0.6492256090856681	T	T	T
0.6772452308852109	0.1539215181332778	0.6392078981652649	T	T	T
0.6768509411581985	0.4840027221337508	0.6405976454419215	T	T	T
0.3892337638679037	0.6358731235077258	0.6411143440217255	T	T	T
0.4952010859594819	0.5484638170862202	0.6401627957196426	T	T	T
0.3021492465831158	0.3131255739463577	0.6346206064727168	T	T	T
0.3598339521996547	0.4088643329563760	0.6360398484508154	T	T	T
0.4306049395560687	0.4485769751496657	0.6392567402945027	T	T	T
0.6768573969084641	0.8214741612464612	0.6460288308377186	T	T	T
0.7476975475373022	0.8620158486646712	0.6510650341702541	T	T	T
0.8051766946624894	0.9575387440152255	0.6501052201532070	T	T	T
0.3169269198254532	0.2596254224328948	0.6361553511665526	T	T	T
0.7185796740251000	0.9662610593953863	0.6397421534418480	T	T	T
0.3886309248872066	0.3033338667437413	0.6388214235652672	T	T	T
0.7900285438976912	0.0103348967518663	0.6444353154630860	T	T	T
0.3593320002838650	0.0720225543727673	0.6477281826687190	T	T	T
0.6130019355793613	0.7225671502290150	0.6440856077567546	T	T	T
0.4296458725504829	0.1116002004037911	0.6411377626447595	T	T	T
0.8058959843473822	0.2893320178135750	0.6404548149405758	T	T	T
0.6120434972948674	0.3844554068111121	0.6378720838040193	T	T	T
0.3178265370019389	0.5922579033584895	0.6456577558325207	T	T	T
0.3607883502826550	0.7411514595552156	0.6502862105117222	T	T	T
0.3161743223369112	0.9229821033201520	0.6438895415218979	T	T	T
0.7911540674989881	0.3422557278243746	0.6341589196276290	T	T	T
0.4954503802156595	0.8802426722101485	0.6428060709676964	T	T	T
0.7479557475886032	0.1938335950182085	0.6431496210903747	T	T	T
0.3030123347703423	0.6455345272407226	0.6501461437117794	T	T	T
0.4314173630060645	0.7810002218217265	0.6455405333785131	T	T	T
0.6129079632387069	0.0543090006127492	0.6396298794374730	T	T	T
0.3871198464340626	0.9663639082064805	0.6370640704662421	T	T	T
0.4936977977888410	0.2105889445180996	0.6384467579780929	T	T	T
0.7195135318800242	0.6294640422884382	0.6446815548953592	T	T	T
0.7912185746706903	0.6727428123560655	0.6443841577675060	T	T	T
0.8056047795627735	0.6188153569769027	0.6423400592951140	T	T	T
0.7476228288832204	0.5232819607675078	0.6400390725680696	T	T	T
0.7195351878684458	0.2982121257476358	0.6300188058450182	T	T	T
0.2743525916691344	0.5171695991336485	0.6443940792176763	T	T	T
0.3512486972130389	0.4535827926882640	0.6344219653114191	T	T	T
0.7562032790516759	0.8173887880568271	0.6544499835780533	T	T	T

0.2465537183057550	0.2805356027291603	0.6313104705562880	T	T	T
0.2473778472181991	0.6130356372421897	0.6524513584608677	T	T	T
0.7562042500937202	0.1491478090006958	0.6476625933368113	T	T	T
0.3526118953017517	0.7861985007414224	0.6530048173569979	T	T	T
0.8609178015533323	0.9904626319425562	0.6525690888132478	T	T	T
0.7558592681976539	0.4783023537333831	0.6374729846350378	T	T	T
0.8615847196649640	0.3218624660793558	0.6423331474981591	T	T	T
0.2735256024893262	0.1846006071513914	0.6343518832239273	T	T	T
0.8333706976043257	0.0853475779228004	0.6423000642500412	T	T	T
0.7038046373816440	0.0040056341282360	0.6350848866327850	T	T	T
0.4036755534846644	0.2653476483265890	0.6393850389943072	T	T	T
0.3513714070828957	0.1172224603775666	0.6509287459039864	T	T	T
0.2463686214137437	0.9441847934220227	0.6534580837568725	T	T	T
0.8349361162951342	0.7478341656759255	0.6449752821373554	T	T	T
0.2726974646919514	0.8478407466394577	0.6437374161015621	T	T	T
0.8612128554877178	0.6508872848627199	0.6413847160713184	T	T	T
0.7048225536788574	0.6678145212772594	0.6460029510326607	T	T	T
0.4039568901190970	0.5979114675749110	0.6371130237191531	T	T	T
0.7050144731046248	0.3359672306421077	0.6242761900758462	T	T	T
0.8346788638207538	0.4170822668891647	0.6309556670333670	T	T	T
0.4011852062000920	0.9278609820334489	0.6323757101211147	T	T	T
0.6628558940834163	0.2055257807080822	0.6322597513680748	T	T	T
0.6620567852886050	0.8731007639971002	0.6404946924243997	T	T	T
0.6199690781490291	0.6653229733278612	0.6465070907142882	T	T	T
0.5480617406162913	0.6988316361097680	0.6375423611043367	T	T	T
0.4869218800459353	0.6045292948097449	0.6381928146171183	T	T	T
0.4875393767390951	0.9366092968539249	0.6421161542185304	T	T	T
0.5475611974620169	0.0294359634936296	0.6365149005911168	T	T	T
0.6210952380809519	0.9982086156351559	0.6405606634204509	T	T	T
0.4458610904930030	0.7289086679127437	0.6408833681612316	T	T	T
0.4437749245067846	0.0593510961131457	0.6358800374323839	T	T	T
0.4445533673682267	0.3959108542081445	0.6405848369374384	T	T	T
0.5600462550326853	0.5730844565006952	0.6424720504043950	T	T	T
0.5585794552913131	0.2344069245698958	0.6322086207224635	T	T	T
0.6632018105092715	0.5368912660714923	0.6433033482560442	T	T	T
0.6198406379720537	0.3279858020270610	0.6347978738612411	T	T	T
0.5473548615265922	0.3603961004601099	0.6387915697501857	T	T	T
0.4868824363304752	0.2679247288012910	0.6413748441565656	T	T	T
0.5604963358924142	0.9043341255092343	0.6382989665221656	T	T	T
0.5518964152536334	0.1312098057860882	0.6199575418195367	T	T	T
0.5541058494279667	0.8007236523561714	0.6258644557147678	T	T	T
0.5534193411536882	0.4658114157419923	0.6534744913343137	T	T	T
0.5514151507615968	0.4619390856550854	0.7055084802009802	T	T	T
0.1080085622473749	0.0922560860883762	0.5705423811169348	T	T	T

Fig. 6h

```

-----
Au C H N V O
1.000000000000000
26.0801187006857766 0.0000000000000000 0.0000000000000000
-14.4889548337143204 14.4889548337143204 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Au C H N V O
279 36 24 18 3 2
Selective dynamics
Direct

```

0.0000000000000000	0.0000000000000000	0.1894422798390494	F	F	F
0.5555555555555571	0.2000000000000028	0.1894422798390494	F	F	F
0.444444444444429	0.2000000000000028	0.1894422798390494	F	F	F
0.222222222222214	0.2000000000000028	0.1894422798390494	F	F	F
0.1111111111111143	0.2000000000000028	0.1894422798390494	F	F	F
0.777777777777786	0.2000000000000028	0.1894422798390494	F	F	F
0.888888888888857	0.0000000000000000	0.1894422798390494	F	F	F
0.666666666666643	0.0000000000000000	0.1894422798390494	F	F	F
0.5555555555555571	0.0000000000000000	0.1894422798390494	F	F	F
0.444444444444429	0.0000000000000000	0.1894422798390494	F	F	F
0.333333333333357	0.0000000000000000	0.1894422798390494	F	F	F
0.222222222222214	0.0000000000000000	0.1894422798390494	F	F	F
0.1111111111111143	0.0000000000000000	0.1894422798390494	F	F	F
0.777777777777786	0.0000000000000000	0.1894422798390494	F	F	F
0.888888888888857	0.5000000000000000	0.2561864044279716	F	F	F
0.8888888888888928	0.2000000000000028	0.1894422798390494	F	F	F
0.222222222222214	0.3999999999999986	0.1894422798390494	F	F	F
0.8888888888888928	0.6000000000000014	0.1894422798390494	F	F	F
0.0000000000000000	0.3999999999999986	0.1894422798390494	F	F	F
0.333333333333357	0.3999999999999986	0.1894422798390494	F	F	F
0.444444444444429	0.3999999999999986	0.1894422798390494	F	F	F
0.5555555555555571	0.3999999999999986	0.1894422798390494	F	F	F
0.666666666666643	0.3999999999999986	0.1894422798390494	F	F	F
0.777777777777786	0.3999999999999986	0.1894422798390494	F	F	F
0.6666666666666714	0.2000000000000028	0.1894422798390494	F	F	F
0.888888888888857	0.3999999999999986	0.1894422798390494	F	F	F
0.0000000000000000	0.2000000000000028	0.1894422798390494	F	F	F
0.333333333333357	0.6000000000000014	0.1894422798390494	F	F	F
0.444444444444429	0.6000000000000014	0.1894422798390494	F	F	F
0.5555555555555571	0.6000000000000014	0.1894422798390494	F	F	F
0.5538723154316877	0.0967144104950947	0.3891728561304516	T	T	T
0.777777777777786	0.6000000000000014	0.1894422798390494	F	F	F
0.1111111111111072	0.3999999999999986	0.1894422798390494	F	F	F
0.0000000000000000	0.5000000000000000	0.2561864044279716	F	F	F
0.0000000000000000	0.6000000000000014	0.1894422798390494	F	F	F
0.222222222222214	0.6000000000000014	0.1894422798390494	F	F	F
0.666666666666643	0.7999999999999972	0.1894422798390494	F	F	F
0.777777777777786	0.7999999999999972	0.1894422798390494	F	F	F
0.888888888888857	0.7999999999999972	0.1894422798390494	F	F	F
0.0000000000000000	0.7999999999999972	0.1894422798390494	F	F	F
0.1111111111111072	0.7999999999999972	0.1894422798390494	F	F	F
0.222222222222214	0.7999999999999972	0.1894422798390494	F	F	F
0.3333333333333286	0.7999999999999972	0.1894422798390494	F	F	F
0.1111111111111143	0.1000000000000014	0.2561864044279716	F	F	F
0.222222222222214	0.1000000000000014	0.2561864044279716	F	F	F
0.333333333333357	0.1000000000000014	0.2561864044279716	F	F	F
0.444444444444429	0.1000000000000014	0.2561864044279716	F	F	F
0.5555555555555571	0.1000000000000014	0.2561864044279716	F	F	F
0.666666666666643	0.1000000000000014	0.2561864044279716	F	F	F
0.777777777777786	0.1000000000000014	0.2561864044279716	F	F	F
0.8888888888888928	0.1000000000000014	0.2561864044279716	F	F	F
0.0000000000000000	0.1000000000000014	0.2561864044279716	F	F	F
0.777777777777786	0.5000000000000000	0.2561864044279716	F	F	F
0.888888888888857	0.2999999999999972	0.2561864044279716	F	F	F
0.222222222222214	0.2999999999999972	0.2561864044279716	F	F	F
0.3333333333333286	0.2999999999999972	0.2561864044279716	F	F	F

0.444444444444429	0.299999999999972	0.2561864044279716	F	F	F
0.555555555555571	0.299999999999972	0.2561864044279716	F	F	F
0.666666666666643	0.299999999999972	0.2561864044279716	F	F	F
0.111111111111143	0.600000000000014	0.1894422798390494	F	F	F
0.777777777777786	0.299999999999972	0.2561864044279716	F	F	F
0.444444444444429	0.799999999999972	0.1894422798390494	F	F	F
0.1111111111111072	0.299999999999972	0.2561864044279716	F	F	F
0.333333333333357	0.500000000000000	0.2561864044279716	F	F	F
0.444444444444429	0.500000000000000	0.2561864044279716	F	F	F
0.555555555555571	0.500000000000000	0.2561864044279716	F	F	F
0.666666666666643	0.500000000000000	0.2561864044279716	F	F	F
0.000000000000000	0.299999999999972	0.2561864044279716	F	F	F
0.555555555555571	0.799999999999972	0.1894422798390494	F	F	F
0.666666666666643	0.600000000000014	0.1894422798390494	F	F	F
0.9991977601262195	0.1984892370753030	0.3226559583028561	T	T	T
0.888888888888857	0.899999999999986	0.2561864044279716	F	F	F
0.777777777777786	0.899999999999986	0.2561864044279716	F	F	F
0.666666666666643	0.899999999999986	0.2561864044279716	F	F	F
0.555555555555571	0.899999999999986	0.2561864044279716	F	F	F
0.333333333333357	0.700000000000028	0.2561864044279716	F	F	F
0.1111111111111072	0.899999999999986	0.2561864044279716	F	F	F
0.222222222222214	0.700000000000028	0.2561864044279716	F	F	F
0.6663139775282910	0.1992561194200506	0.3224796718168256	T	T	T
0.8888888888888928	0.700000000000028	0.2561864044279716	F	F	F
0.777777777777786	0.700000000000028	0.2561864044279716	F	F	F
0.6666666666666714	0.700000000000028	0.2561864044279716	F	F	F
0.555555555555571	0.700000000000028	0.2561864044279716	F	F	F
0.444444444444429	0.700000000000028	0.2561864044279716	F	F	F
0.111111111111143	0.700000000000028	0.2561864044279716	F	F	F
0.222222222222214	0.899999999999986	0.2561864044279716	F	F	F
0.000000000000000	0.700000000000028	0.2561864044279716	F	F	F
0.444444444444429	0.899999999999986	0.2561864044279716	F	F	F
0.333333333333357	0.899999999999986	0.2561864044279716	F	F	F
0.1099268360452277	0.9984157059450910	0.3229780010719302	T	T	T
0.5549807424414012	0.9995313928875001	0.3222960369984166	T	T	T
0.6668191034259202	0.9997860443729472	0.3223288048428499	T	T	T
0.7783674543725911	-0.0000670922022588	0.3225162058049207	T	T	T
0.8887901592059708	0.9993051027877979	0.3229666222077916	T	T	T
0.000000000000000	0.899999999999986	0.2561864044279716	F	F	F
0.9993612252678783	0.9989556465029538	0.3229489800787040	T	T	T
0.3319214384986714	0.9986406005081787	0.3227238393617748	T	T	T
0.4434143762915587	0.9992993853754373	0.3226378784275982	T	T	T
0.1099888574922799	0.1981442226694391	0.3225741471850908	T	T	T
0.2207270498668930	0.1975428368200971	0.3224824821664496	T	T	T
0.3321586176912751	0.1976408396734445	0.3224696117205725	T	T	T
0.4437600939729811	0.1986292683010390	0.3224775692265976	T	T	T
0.2208895563786272	0.9985074569502753	0.3229254391551800	T	T	T
0.222222222222214	0.500000000000000	0.2561864044279716	F	F	F
0.5550254090124309	0.1990109426839920	0.3227543744444538	T	T	T
0.7778118100116836	0.1992935071296643	0.3223726267773612	T	T	T
0.2220977606149191	0.4005180291492738	0.3224956477880933	T	T	T
0.3332151388211008	0.4003073639770158	0.3223598588286311	T	T	T
0.4446947369779893	0.4004811005205184	0.3224909944734633	T	T	T
0.5561553624501679	0.4016469456270563	0.3224297602387945	T	T	T
0.6675585499460831	0.4020266894039695	0.3223086285040548	T	T	T
0.7791001580011354	0.4022782855650961	0.3223203787319721	T	T	T

0.8901613202648331	0.4019607887981952	0.3224898330626575	T	T	T
0.1115290590295192	0.4010759378997678	0.3226073078159035	T	T	T
0.3323925983049822	0.5993448725592487	0.3224801192368045	T	T	T
0.4442368250788362	0.5995485146662125	0.3224205711549324	T	T	T
0.5560669831827004	0.5996483198404340	0.3225381089445786	T	T	T
0.6676525673989591	0.6004474220123177	0.3228387319321296	T	T	T
0.7787124054406258	0.6008650801645710	0.3229850379111027	T	T	T
0.8894662873764426	0.6006857621874975	0.3231280527524716	T	T	T
0.0003485486443769	0.6005780518975653	0.3231014554263339	T	T	T
0.1111526922570459	0.6004150842737208	0.3230181158218655	T	T	T
0.1111111111111143	0.5000000000000000	0.2561864044279716	F	F	F
0.9996604526072451	0.7994201315362001	0.3231374421498889	T	T	T
0.2217111251120866	0.5999998385505405	0.3229033914879795	T	T	T
0.4436747875297580	0.7993416417332155	0.3225108044567765	T	T	T
0.5554546629376477	0.7996784935303078	0.3225643272105092	T	T	T
0.6671317886666089	0.7998745366304587	0.3226838792054334	T	T	T
0.7783391892967050	0.7999565749162093	0.3229004940750093	T	T	T
0.0007685011499735	0.4014329116086490	0.3225881866762925	T	T	T
0.8891080057134231	0.7998474487508204	0.3231563710017044	T	T	T
0.8887817797824938	0.1991177695255008	0.3226055045671044	T	T	T
0.2212379332429376	0.7992439493110741	0.3230463898466053	T	T	T
0.3322407195745835	0.7993799749150007	0.3226860751085477	T	T	T
0.1087221667618313	0.0964561869016998	0.3902206620076996	T	T	T
0.2192317144553419	0.0956284414536139	0.3899828801105162	T	T	T
0.3305020245558445	0.0956624110307478	0.3898330748636362	T	T	T
0.1107987047608906	0.7996526570687809	0.3232123889600954	T	T	T
0.4420550657802780	0.0971373476720134	0.3893727795902206	T	T	T
0.3333333333333357	0.2000000000000028	0.1894422798390494	F	F	F
0.6660504341815997	0.0975699590415124	0.3890134516333760	T	T	T
0.9986488942362571	0.0974647207292952	0.3902898588967159	T	T	T
0.2210608914240192	0.2990803947426575	0.3873531381952957	T	T	T
0.3320474171997262	0.2981486430780231	0.3869707472103751	T	T	T
0.4441268478968584	0.2991506183374884	0.3874070286105373	T	T	T
0.5563267823282138	0.3019944218596338	0.3874553430949766	T	T	T
0.6678503156557788	0.3024580326129712	0.3868383621862025	T	T	T
0.7789738050662108	0.3012102896862686	0.3869220420573635	T	T	T
0.8895971310522204	0.3004310801305649	0.3875877630470198	T	T	T
0.0002116300624904	0.3001950108171501	0.3879571451467266	T	T	T
0.1105584620738092	0.2997370170018981	0.3878452583703968	T	T	T
0.3330781489322298	0.5009246134813894	0.3894677771110000	T	T	T
0.4450878435175747	0.5010932013596370	0.3893101140620144	T	T	T
0.5570881658595163	0.5015810544766967	0.3899112611984707	T	T	T
0.6685735196694585	0.5024930243026535	0.3905838820294144	T	T	T
0.7795241430567156	0.5030833103335784	0.3904907642316056	T	T	T
0.8903688516033921	0.5024953496218162	0.3904779264806736	T	T	T
0.6674856737310945	0.9002957407259337	0.3887433880377232	T	T	T
0.7782450120476904	0.7000716702187950	0.3905448217628381	T	T	T
0.0010621903169030	0.5019173861679799	0.3905905625703072	T	T	T
0.1114363979594800	0.5012771551110710	0.3904799631681213	T	T	T
0.2220828924043640	0.5010117066255951	0.3903661263524978	T	T	T
0.4430597843067020	0.6983833526231756	0.3884839865614624	T	T	T
0.5551244647875061	0.6987104507010709	0.3887506275327428	T	T	T
0.8882035219976528	0.0978702223630919	0.3903189991060120	T	T	T
0.6672034619901572	0.6995083532312487	0.3895438764342516	T	T	T
0.8892844625436703	0.8994912295690631	0.3904526077317922	T	T	T
0.9995030744185841	0.6995323130840283	0.3906887420235229	T	T	T

0.1101222146045655	0.6992075741009204	0.3907692970438084	T	T	T
0.2207068626068351	0.6990840076821273	0.3903681206172681	T	T	T
0.3313561368245571	0.6985381323194237	0.3894860052267862	T	T	T
0.5554855578598639	0.8998353368123749	0.3885755133161111	T	T	T
0.8889252732763639	0.7000517784233252	0.3907938391700388	T	T	T
0.7787081641392332	0.9000208149436869	0.3898867992385637	T	T	T
0.9997346327267600	0.8990555760488672	0.3907055101102458	T	T	T
0.5565188779713613	0.5993677028889721	0.4565468073042510	T	T	T
0.3311143927728966	0.1971843591341002	0.4529625600150222	T	T	T
0.2204198258566615	0.1990508864962365	0.4531864266523900	T	T	T
0.1103562684170214	0.2002788683359428	0.4541213977142046	T	T	T
0.4430125128034156	0.9995747785181666	0.4564531364060882	T	T	T
0.3313695964910566	0.9981376966681247	0.4583193730577731	T	T	T
0.2203548352477750	0.9970322627799783	0.4585365079318186	T	T	T
0.4430156571562782	0.1985436080218812	0.4529567871218564	T	T	T
0.1102198106884703	0.9979201036576321	0.4585070527772159	T	T	T
0.8897547957868929	0.9990685852092410	0.4579460732514484	T	T	T
0.7784900787593478	0.9992644810297187	0.4575734100891852	T	T	T
0.6664817159836806	0.9979615268256434	0.4560682043313447	T	T	T
0.5545847454702927	0.9980346956185679	0.4561334210984768	T	T	T
0.3317036554246323	0.8987105354775901	0.3899830171203785	T	T	T
0.2210494897720832	0.8984181915312028	0.3907136126987708	T	T	T
0.0001752850112935	0.9991304215137905	0.4586539982960442	T	T	T
0.7775200909613837	0.0978556286644499	0.3895460324428031	T	T	T
0.5560220857659456	0.2004780360409756	0.4514145641960343	T	T	T
0.4438549000250750	0.6002004661987379	0.4557994618293620	T	T	T
0.5563822971484162	0.4015796330325533	0.4547405486951973	T	T	T
0.7781247942937352	0.1993003404880632	0.4530737359173292	T	T	T
0.4430485944114474	0.8990937081933283	0.3890242084178699	T	T	T
0.9996862516896010	0.2002776609443043	0.4545117036880802	T	T	T
0.2218420160453068	0.3993517796175266	0.4545616101843466	T	T	T
0.3323984254631805	0.3988607875075973	0.4527223849378684	T	T	T
0.6672192335221038	0.2000899046744248	0.4513677943357155	T	T	T
0.4432699641799215	0.3980326804826322	0.4526504562619736	T	T	T
0.1101924813854751	0.8983993384014403	0.3906684186991758	T	T	T
0.7780781206140063	0.3995628673978719	0.4537428392811786	T	T	T
0.8892194527422882	0.3988413808065935	0.4542011482404389	T	T	T
0.9999262556955875	0.3988402340685841	0.4549746919679977	T	T	T
0.1108691524515543	0.3991052210518811	0.4550266605246093	T	T	T
0.3321618663666898	0.5995012934055176	0.4571730681293757	T	T	T
0.6685546815242418	0.4023214024299691	0.4551608445904504	T	T	T
0.6678202795659471	0.6008917257603629	0.4581449187110258	T	T	T
0.8889883065545157	0.2002354202795156	0.4542587298987761	T	T	T
0.9232762537203580	0.4620886802816363	0.5387747757983827	T	T	T
0.1097013502065278	0.5992033936918258	0.4587839013962065	T	T	T
0.2204820978715521	0.5997171883142408	0.4578521506403155	T	T	T
0.4437832097439195	0.7985399319180915	0.4530910644686101	T	T	T
0.5546643180027097	0.7987231411218382	0.4542942189842904	T	T	T
0.6655690801078951	0.7994241015673883	0.4538027208847562	T	T	T
0.8885824823429503	0.8000262354595409	0.4569875169745539	T	T	T
0.9992053694824077	0.7988437441604165	0.4570435287950221	T	T	T
0.1098544131185345	0.7980229277945918	0.4570208082830928	T	T	T
0.2212271563260741	0.7983231847384823	0.4569439725244102	T	T	T
0.3327267232760669	0.7991238184808904	0.4556574339160460	T	T	T
0.1801993746877069	0.1245376510232486	0.5360299014337820	T	T	T
0.2913329547599284	0.1245964829400118	0.5365148395991062	T	T	T

0.4024244703869592	0.1256763443127448	0.5370956895060791	T	T	T
0.5119831517083731	0.1229588961653302	0.5341091728446598	T	T	T
0.6225493439180202	0.1212077474013643	0.5328784908081128	T	T	T
0.3687735780398574	0.4637817764557340	0.5365133918395437	T	T	T
0.1082847878302430	0.2950515365691964	0.5249811328344732	T	T	T
0.8888188664615599	0.6003696991290765	0.4589282615943081	T	T	T
0.4406118831576623	0.2942045696908713	0.5217243879363614	T	T	T
0.7349298476298157	0.1230847571245064	0.5357321094318334	T	T	T
0.8460080387145519	0.1232759106627088	0.5368864981086127	T	T	T
0.9579507684412191	0.1241995984948214	0.5371117822811536	T	T	T
0.0694290055660558	0.1246866653342673	0.5368175195939914	T	T	T
0.9989282145012353	0.5991891421171279	0.4589111204358096	T	T	T
0.2193963878684287	0.2950699919109467	0.5242606936023876	T	T	T
0.5521410084076941	0.2939568687002514	0.5194457525863465	T	T	T
0.5891159085238160	0.4595433813963997	0.5412270992834814	T	T	T
0.6633591241897320	0.2927514407595622	0.5212733549067288	T	T	T
0.7749726067351318	0.2940829409065882	0.5211521626396191	T	T	T
0.8852085610387528	0.2934906477026818	0.5256306302330022	T	T	T
0.9963967065421240	0.2939041932910447	0.5253618098635593	T	T	T
0.3306012231789480	0.2954701233897543	0.5202369539347851	T	T	T
0.4819013373454268	0.4640592679992084	0.5363225445576583	T	T	T
0.7770289346313122	0.7994794448834989	0.4563269860928537	T	T	T
0.7790113135236433	0.6015131735534945	0.4587792721089664	T	T	T
0.6639495187955944	0.7916151772362504	0.5414560127772163	T	T	T
0.5514652042235423	0.7918841099369915	0.5433978793271179	T	T	T
0.2927658060014947	0.6283370579961338	0.5355282934224849	T	T	T
0.1817429661150692	0.6283731270295712	0.5380989365947098	T	T	T
0.0712865488319837	0.6290727646592887	0.5381695483288184	T	T	T
0.699335677326363	0.4584845951696599	0.5416857609819129	T	T	T
0.7746599751558839	0.7920545195833316	0.5452539326214242	T	T	T
0.8478788720718311	0.6268468701042725	0.5391633457534346	T	T	T
0.6281842760377203	0.6276897119441088	0.5377943872032404	T	T	T
0.5171474046609887	0.6297014324404667	0.5327219460248018	T	T	T
0.4050488690309020	0.6292121814743116	0.5353783047492466	T	T	T
0.2571569284361195	0.4627896283041492	0.5394729528132101	T	T	T
0.1453322916004481	0.4622760246581676	0.5396839281807215	T	T	T
0.0339033015261927	0.4619107463048512	0.5395539974272567	T	T	T
0.7378358972280588	0.6267455129451107	0.5374683054771358	T	T	T
0.8847615530995790	0.7919742940972452	0.5458367837525775	T	T	T
0.9597379068297247	0.6281633782993249	0.5382629523982962	T	T	T
0.3634452013597749	0.9562399691529895	0.5353376514160463	T	T	T
0.4734025213696954	0.9542709061014911	0.5331622184524532	T	T	T
0.9951088258018355	0.7919488523251801	0.5456324706092449	T	T	T
0.1067795331099095	0.7929832444010708	0.5456355978492888	T	T	T
0.6977761798492771	0.9553559855753573	0.5341934013030533	T	T	T
0.3276221026945492	0.7919372517455227	0.5445339498005584	T	T	T
0.4395918779753992	0.7923635300155584	0.5406238131383786	T	T	T
0.2176280321729482	0.7928292036616784	0.5460077338849579	T	T	T
0.8100271715879310	0.9564277347215170	0.5351545140991864	T	T	T
0.8116651593303771	0.4618382140159175	0.5382321902245143	T	T	T
0.9207203028994631	0.9567189352248903	0.5372250574939754	T	T	T
0.0314222012294921	0.9565896879758589	0.5370519712693651	T	T	T
0.1425170186441841	0.9570156605171882	0.5372588412085404	T	T	T
0.2535922195649219	0.9573036833319041	0.5375380529465379	T	T	T
0.5864032316852841	0.9547536420415234	0.5329858047474501	T	T	T
0.3257179840275720	0.0027984631571958	0.6834529940513870	T	T	T

0.6741218783030907	0.1596850346782378	0.6370523851406568	T	T	T
0.6605495892740220	0.4719041311418672	0.6562571177091615	T	T	T
0.3827393766319009	0.6410555005716070	0.6420865386713261	T	T	T
0.4839225022679598	0.5439900795317243	0.6388867811709082	T	T	T
0.2897424144776559	0.3102738231308197	0.6340451661004698	T	T	T
0.3478164346270929	0.4057403756691117	0.6371052577279080	T	T	T
0.4184891882088665	0.4446046138398132	0.6367099749820712	T	T	T
0.6690307188790006	0.8164118012229409	0.6446164321929397	T	T	T
0.7391307674930158	0.8543863007160813	0.6493032841251045	T	T	T
0.7979034366925130	0.9497715859127802	0.6489369814814577	T	T	T
0.3037478885183231	0.2560768077579635	0.6301558378690725	T	T	T
0.7138925772177854	0.9631021982571702	0.6396830724757615	T	T	T
0.3752914133581140	0.2989716442205884	0.6292412112815382	T	T	T
0.7847941614690759	0.0048751357669454	0.6441487460976207	T	T	T
0.3872287221523352	0.0979348759904181	0.6826297436841785	T	T	T
0.6037865189273094	0.7174014935136659	0.6426238020396329	T	T	T
0.4488828907726857	0.1311942378150899	0.6615113770365153	T	T	T
0.8024032091839325	0.2958555511726578	0.6404741359205731	T	T	T
0.5974364572607291	0.3711061540229238	0.6478101652135405	T	T	T
0.3118105793771553	0.5993029496827470	0.6464941243747291	T	T	T
0.3572205535867774	0.7498849027087287	0.6477602050580493	T	T	T
0.3285001933505611	0.9450277634961479	0.6626049702373311	T	T	T
0.7872025104960406	0.3482913675881267	0.6339185481249884	T	T	T
0.4920719507384233	0.8867888792572161	0.6394970255303635	T	T	T
0.7448644353711180	0.2002672697674933	0.6422250622188466	T	T	T
0.2985567093003499	0.6544565425725292	0.6492163664973634	T	T	T
0.4272875327823917	0.7877306624557584	0.6432431454001238	T	T	T
0.6102241398123484	0.0604215124474104	0.6369614184593263	T	T	T
0.3928227238753180	0.9827805087513792	0.6432396726263686	T	T	T
0.5096849745705156	0.2296877568670724	0.6499591811531723	T	T	T
0.7085461836900554	0.6189987211298501	0.6455341867222104	T	T	T
0.7786766312584812	0.6595968768573213	0.6533768077557960	T	T	T
0.7889137597228373	0.6035124076430909	0.6642976520594094	T	T	T
0.7287973896848269	0.5080431975551747	0.6656812983244178	T	T	T
0.7157431099158360	0.3038458778332769	0.6281315325366742	T	T	T
0.2675028634458910	0.5242567107448109	0.6464860584207265	T	T	T
0.3397368984540180	0.4509050971690911	0.6395749827794420	T	T	T
0.7460686060758740	0.8080729813816625	0.6520809081624487	T	T	T
0.2342280981728169	0.2785461619269408	0.6334549040922929	T	T	T
0.2433704476862827	0.6235246312018062	0.6513745021344463	T	T	T
0.7532126474852430	0.1556844704808273	0.6468262749153324	T	T	T
0.3501715557863516	0.7962010876420149	0.6491336175662663	T	T	T
0.8531011375773089	0.9807821409999115	0.6512664711916376	T	T	T
0.7342117377890527	0.4610261350043854	0.6724980030153113	T	T	T
0.8581974722378749	0.3290077827331440	0.6431690276313797	T	T	T
0.2599604853788359	0.1813863257286918	0.6265991068389077	T	T	T
0.8292367241184270	0.0798264026127445	0.6425437092297762	T	T	T
0.7007917279137681	0.0028485145213557	0.6354590025964506	T	T	T
0.3890415036318965	0.2599020609649655	0.6251343381021470	T	T	T
0.3874367553423580	0.1468418289057256	0.6967094623974670	T	T	T
0.2760031040573743	0.9746972121633966	0.6989624103000669	T	T	T
0.8242248281629916	0.7340968458041741	0.6501622075844020	T	T	T
0.2810261255993718	0.8707909597199814	0.6605025429239028	T	T	T
0.8431492123776682	0.6333124676688002	0.6704146360794691	T	T	T
0.6968745436191091	0.6593139985791389	0.6376233546266985	T	T	T
0.3961800999372911	0.6014709429804257	0.6391102728193926	T	T	T

0.7019820353429200	0.3422151321770184	0.6212622257290711	T	T	T
0.8304195028899510	0.4232946574552755	0.6315451586850135	T	T	T
0.3982523354642078	0.9403461607765319	0.6276367923840934	T	T	T
0.6593776609873859	0.2108762395866521	0.6293054193919841	T	T	T
0.6562565308341347	0.8702936336371633	0.6399563691062563	T	T	T
0.6097322924914189	0.6589321214382359	0.6433775340535912	T	T	T
0.5395692981701922	0.6956525607070004	0.6382518432084936	T	T	T
0.4775175024930079	0.6019653194425866	0.6388891066455917	T	T	T
0.4845296536578566	0.9436006241379156	0.6363965055399516	T	T	T
0.5453585215384211	0.0362182077278242	0.6308208105295877	T	T	T
0.6175097344251845	0.0034400035603266	0.6397629947200403	T	T	T
0.4401654196163278	0.7337280372590256	0.6403046949012137	T	T	T
0.4528429783383349	0.0747637895806001	0.6426997638763585	T	T	T
0.4315365212357953	0.3912657883197174	0.6325761679494791	T	T	T
0.5483524982751143	0.5668234152158683	0.6390308344873740	T	T	T
0.5642627417657335	0.2455198519373671	0.6216760370084558	T	T	T
0.6505739212027417	0.5270585092633395	0.6470415388381520	T	T	T
0.6185356120224458	0.3367248443636739	0.6192356728335662	T	T	T
0.5360165944531872	0.3517204911973181	0.6258490159109070	T	T	T
0.4827728444775072	0.2634796333240771	0.6242412706841773	T	T	T
0.5568041041524376	0.9101079452402392	0.6373638406334134	T	T	T
0.5510031746502794	0.1370197760297852	0.6123944285369882	T	T	T
0.5483160981302748	0.8015516204914802	0.6266105037163786	T	T	T
0.5399232029952991	0.4590956421101534	0.6431273117221642	T	T	T
0.5266880495306455	0.4350013565405948	0.6940605415376563	T	T	T
0.5548558754311443	0.2999866290194078	0.6818627038225883	F	F	T

Fig. 6i

Au C H N V O

1.000000000000000

26.0801187006857766 0.0000000000000000 0.0000000000000000

-14.4889548337143204 14.4889548337143204 0.0000000000000000

0.0000000000000000 0.0000000000000000 31.0000000000000000

Au C H N V O

279 36 24 18 3 2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.1894422798390494	F	F	F
0.5555555555555571	0.2000000000000028	0.1894422798390494	F	F	F
0.4444444444444429	0.2000000000000028	0.1894422798390494	F	F	F
0.222222222222214	0.2000000000000028	0.1894422798390494	F	F	F
0.1111111111111143	0.2000000000000028	0.1894422798390494	F	F	F
0.7777777777777786	0.2000000000000028	0.1894422798390494	F	F	F
0.8888888888888857	0.0000000000000000	0.1894422798390494	F	F	F
0.6666666666666643	0.0000000000000000	0.1894422798390494	F	F	F
0.5555555555555571	0.0000000000000000	0.1894422798390494	F	F	F
0.4444444444444429	0.0000000000000000	0.1894422798390494	F	F	F
0.3333333333333357	0.0000000000000000	0.1894422798390494	F	F	F
0.222222222222214	0.0000000000000000	0.1894422798390494	F	F	F
0.1111111111111143	0.0000000000000000	0.1894422798390494	F	F	F
0.7777777777777786	0.0000000000000000	0.1894422798390494	F	F	F
0.8888888888888857	0.5000000000000000	0.2561864044279716	F	F	F
0.88888888888888928	0.2000000000000028	0.1894422798390494	F	F	F
0.222222222222214	0.3999999999999986	0.1894422798390494	F	F	F
0.88888888888888928	0.6000000000000014	0.1894422798390494	F	F	F

0.0000000000000000	0.3999999999999986	0.1894422798390494	F	F	F
0.3333333333333357	0.3999999999999986	0.1894422798390494	F	F	F
0.4444444444444429	0.3999999999999986	0.1894422798390494	F	F	F
0.5555555555555571	0.3999999999999986	0.1894422798390494	F	F	F
0.6666666666666643	0.3999999999999986	0.1894422798390494	F	F	F
0.7777777777777786	0.3999999999999986	0.1894422798390494	F	F	F
0.66666666666666714	0.2000000000000028	0.1894422798390494	F	F	F
0.8888888888888857	0.3999999999999986	0.1894422798390494	F	F	F
0.0000000000000000	0.2000000000000028	0.1894422798390494	F	F	F
0.3333333333333357	0.6000000000000014	0.1894422798390494	F	F	F
0.4444444444444429	0.6000000000000014	0.1894422798390494	F	F	F
0.5555555555555571	0.6000000000000014	0.1894422798390494	F	F	F
0.5540582358775882	0.0972797368604289	0.3894684760659227	T	T	T
0.7777777777777786	0.6000000000000014	0.1894422798390494	F	F	F
0.11111111111111072	0.3999999999999986	0.1894422798390494	F	F	F
0.0000000000000000	0.5000000000000000	0.2561864044279716	F	F	F
0.0000000000000000	0.6000000000000014	0.1894422798390494	F	F	F
0.2222222222222214	0.6000000000000014	0.1894422798390494	F	F	F
0.6666666666666643	0.7999999999999972	0.1894422798390494	F	F	F
0.7777777777777786	0.7999999999999972	0.1894422798390494	F	F	F
0.8888888888888857	0.7999999999999972	0.1894422798390494	F	F	F
0.0000000000000000	0.7999999999999972	0.1894422798390494	F	F	F
0.11111111111111072	0.7999999999999972	0.1894422798390494	F	F	F
0.2222222222222214	0.7999999999999972	0.1894422798390494	F	F	F
0.3333333333333286	0.7999999999999972	0.1894422798390494	F	F	F
0.1111111111111143	0.1000000000000014	0.2561864044279716	F	F	F
0.2222222222222214	0.1000000000000014	0.2561864044279716	F	F	F
0.3333333333333357	0.1000000000000014	0.2561864044279716	F	F	F
0.4444444444444429	0.1000000000000014	0.2561864044279716	F	F	F
0.5555555555555571	0.1000000000000014	0.2561864044279716	F	F	F
0.6666666666666643	0.1000000000000014	0.2561864044279716	F	F	F
0.7777777777777786	0.1000000000000014	0.2561864044279716	F	F	F
0.88888888888888928	0.1000000000000014	0.2561864044279716	F	F	F
0.0000000000000000	0.1000000000000014	0.2561864044279716	F	F	F
0.7777777777777786	0.5000000000000000	0.2561864044279716	F	F	F
0.8888888888888857	0.2999999999999972	0.2561864044279716	F	F	F
0.2222222222222214	0.2999999999999972	0.2561864044279716	F	F	F
0.3333333333333286	0.2999999999999972	0.2561864044279716	F	F	F
0.4444444444444429	0.2999999999999972	0.2561864044279716	F	F	F
0.5555555555555571	0.2999999999999972	0.2561864044279716	F	F	F
0.6666666666666643	0.2999999999999972	0.2561864044279716	F	F	F
0.1111111111111143	0.6000000000000014	0.1894422798390494	F	F	F
0.7777777777777786	0.2999999999999972	0.2561864044279716	F	F	F
0.4444444444444429	0.7999999999999972	0.1894422798390494	F	F	F
0.11111111111111072	0.2999999999999972	0.2561864044279716	F	F	F
0.3333333333333357	0.5000000000000000	0.2561864044279716	F	F	F
0.4444444444444429	0.5000000000000000	0.2561864044279716	F	F	F
0.5555555555555571	0.5000000000000000	0.2561864044279716	F	F	F
0.6666666666666643	0.5000000000000000	0.2561864044279716	F	F	F
0.0000000000000000	0.2999999999999972	0.2561864044279716	F	F	F
0.5555555555555571	0.7999999999999972	0.1894422798390494	F	F	F
0.6666666666666643	0.6000000000000014	0.1894422798390494	F	F	F
0.9991737010560321	0.1988363601815565	0.3226644131768560	T	T	T
0.8888888888888857	0.8999999999999986	0.2561864044279716	F	F	F
0.7777777777777786	0.8999999999999986	0.2561864044279716	F	F	F
0.6666666666666643	0.8999999999999986	0.2561864044279716	F	F	F

0.5555555555555571	0.8999999999999986	0.2561864044279716	F	F	F
0.3333333333333357	0.7000000000000028	0.2561864044279716	F	F	F
0.1111111111111072	0.8999999999999986	0.2561864044279716	F	F	F
0.222222222222214	0.7000000000000028	0.2561864044279716	F	F	F
0.6663855197833871	0.1992183412048140	0.3225368235493014	T	T	T
0.8888888888888928	0.7000000000000028	0.2561864044279716	F	F	F
0.7777777777777786	0.7000000000000028	0.2561864044279716	F	F	F
0.6666666666666714	0.7000000000000028	0.2561864044279716	F	F	F
0.5555555555555571	0.7000000000000028	0.2561864044279716	F	F	F
0.4444444444444429	0.7000000000000028	0.2561864044279716	F	F	F
0.1111111111111143	0.7000000000000028	0.2561864044279716	F	F	F
0.222222222222214	0.8999999999999986	0.2561864044279716	F	F	F
0.0000000000000000	0.7000000000000028	0.2561864044279716	F	F	F
0.4444444444444429	0.8999999999999986	0.2561864044279716	F	F	F
0.3333333333333357	0.8999999999999986	0.2561864044279716	F	F	F
0.1105153629121111	0.9994971387798665	0.3229084098422839	T	T	T
0.5551489866233278	0.9997372629781803	0.3225997140639199	T	T	T
0.6664968583632942	0.0000913336599189	0.3226911436600142	T	T	T
0.7779202408653876	0.0004018956250618	0.3226062821106312	T	T	T
0.8886030520833849	-0.0001968701738161	0.3228727694943771	T	T	T
0.0000000000000000	0.8999999999999986	0.2561864044279716	F	F	F
-0.0004234542973007	-0.0002991425452276	0.3228723133378796	T	T	T
0.3324210837837112	0.9993583876503250	0.3227779665698510	T	T	T
0.4437217761875792	0.9993344305777470	0.3227528958735289	T	T	T
0.1102964840638748	0.1986570217865205	0.3225269475853008	T	T	T
0.2213622067905166	0.1983526435589039	0.3225625881283380	T	T	T
0.3327462892788657	0.1985621189762885	0.3225860989125344	T	T	T
0.4439577599584193	0.1991514426203431	0.3225373125785949	T	T	T
0.2214669359712845	0.9994545858942665	0.3229259316972224	T	T	T
0.2222222222222214	0.5000000000000000	0.2561864044279716	F	F	F
0.5550003321699344	0.1990791043270880	0.3227861778069356	T	T	T
0.7775060548731112	0.1992084417257034	0.3225756601297912	T	T	T
0.2224668812857246	0.4009858549660625	0.3224955521830424	T	T	T
0.3334701632710561	0.4007010874787520	0.3224250806072484	T	T	T
0.4446246417264048	0.4007720032463161	0.3225132749393427	T	T	T
0.5559196834689136	0.4016945611399658	0.3223760888880328	T	T	T
0.6673595731583009	0.4019026843038635	0.3223063388797095	T	T	T
0.7790980483038109	0.4020678263121006	0.3222871191037243	T	T	T
0.8899979556609466	0.4016567697553762	0.3225356936840727	T	T	T
0.1115719846523725	0.4012395174213723	0.3226130696731216	T	T	T
0.3327761277157092	0.5999316848550188	0.3225491061201581	T	T	T
0.4442886315463471	0.5998749004257105	0.3224590506744833	T	T	T
0.5556654323481657	0.5998693461835505	0.3225651442138582	T	T	T
0.6672328153860480	0.6008542141448269	0.3226438779613617	T	T	T
0.7784421381436083	0.6008402536313227	0.3228198807563777	T	T	T
0.8895385092181530	0.6009478207065260	0.3228599701743287	T	T	T
0.0005474819188895	0.6006399655299863	0.3230437770661340	T	T	T
0.1112834207753128	0.6004077589669513	0.3230105222474502	T	T	T
0.1111111111111143	0.5000000000000000	0.2561864044279716	F	F	F
0.0002711674049208	0.8003401247515706	0.3228928887002737	T	T	T
0.2219866908749670	0.6001577967289994	0.3228465859776274	T	T	T
0.4439978048035422	0.8000553552166441	0.3227651551820703	T	T	T
0.5555269446428648	0.8003513349099138	0.3228092371047566	T	T	T
0.6669179392683346	0.8001843484522783	0.3226054908581406	T	T	T
0.7782206918674213	0.8004914824299815	0.3227375953417764	T	T	T
0.0007142053623232	0.4013796636240682	0.3226027325425525	T	T	T

0.8891218652551185	0.8002823005268265	0.3228907171462910	T	T	T
0.8884504234200941	0.1992706938942146	0.3227125477495645	T	T	T
0.2219164733753200	0.7997807952028708	0.3230422670139724	T	T	T
0.3328021498230719	0.7997066311612100	0.3228626616069113	T	T	T
0.1093683421449481	0.0976364499816855	0.3902131699664603	T	T	T
0.2204690947634649	0.0976500264592582	0.3901928867706374	T	T	T
0.3317976335818665	0.0981619035417942	0.3899465330255625	T	T	T
0.1110796031037232	0.7998811024785730	0.3229637751781272	T	T	T
0.4428784956736926	0.0983513801377212	0.3895062418570467	T	T	T
0.3333333333333357	0.2000000000000028	0.1894422798390494	F	F	F
0.6657302709275881	0.0983389564210121	0.3899389059940920	T	T	T
0.9987380932632366	0.0982898882076351	0.3901231380066897	T	T	T
0.2215674397304561	0.2995900082432059	0.3874892923798499	T	T	T
0.3326267462387841	0.2992040806883379	0.3875351202277483	T	T	T
0.4446963896675106	0.3007788802500445	0.3879255737006232	T	T	T
0.5562777347660068	0.3027060132750504	0.3873664112868336	T	T	T
0.6683689819387177	0.3028864418448353	0.3868508147344464	T	T	T
0.7788253573782984	0.3013447477782296	0.3875415406031280	T	T	T
0.8894592765332445	0.3009051603109019	0.3879791093322221	T	T	T
0.0000591927281567	0.3004650296288331	0.3879964786788062	T	T	T
0.1107913665287201	0.3000838871632995	0.3877512502382768	T	T	T
0.3334678843796914	0.5013950196331375	0.3897055804473620	T	T	T
0.4449938868980642	0.5014823314770481	0.3897469079978934	T	T	T
0.5562719484048751	0.5018511645411815	0.3901907305488122	T	T	T
0.6677670420488089	0.5030623387087499	0.3899500146996071	T	T	T
0.7793981184385425	0.5031094033549254	0.3900372047666232	T	T	T
0.8905655480395654	0.5027124023075219	0.3899983094503979	T	T	T
0.6674157317380601	0.9008077806605087	0.3890029212462826	T	T	T
0.7780366848857997	0.7009008921927551	0.3898320500928996	T	T	T
0.0012335314553586	0.5022480130822229	0.3905101142662639	T	T	T
0.1115992700676944	0.5016233738804277	0.3905199908818139	T	T	T
0.2223321970577772	0.5013510969513384	0.3902058503952188	T	T	T
0.4432920606024984	0.6990305522965821	0.3887190456086443	T	T	T
0.5549836121617048	0.6991286848440366	0.3889307611625663	T	T	T
0.8877537148448241	0.0982869752060254	0.3902704824514862	T	T	T
0.6666607393192376	0.7001104183840664	0.3894258369166575	T	T	T
0.8893517808324346	0.9004625307326527	0.3900312673731345	T	T	T
0.0001161823748568	0.7003592399104668	0.3901643538234649	T	T	T
0.1107081917490191	0.6997351021734571	0.3904388836537122	T	T	T
0.2212250727269580	0.6993902243351846	0.3901867053782426	T	T	T
0.3319040209596754	0.6989700343668842	0.3897504884534218	T	T	T
0.5554839136773522	0.9007828246840165	0.3894364158447050	T	T	T
0.8893945580349062	0.7009205954551514	0.3898894127980440	T	T	T
0.7785233658336204	0.9005858219178382	0.3897894241306368	T	T	T
0.0001677066634201	0.9002671220675670	0.3902397118534195	T	T	T
0.5553675421618367	0.5999160152489547	0.4572582403938424	T	T	T
0.3331233596763470	0.1993471543901772	0.4541151676844384	T	T	T
0.2211022846557101	0.1996042288117133	0.4538372461167421	T	T	T
0.1105238988771818	0.2004502020215918	0.4540127009020430	T	T	T
0.4421198067609102	0.9979422919008156	0.4559446819318409	T	T	T
0.3314869304080286	0.0010043238102887	0.4569506946432732	T	T	T
0.2198416350340847	0.9991422678229649	0.4578346376119526	T	T	T
0.4459489520460602	0.2028688924610831	0.4535037247024444	T	T	T
0.1097685360286498	-0.0008781107089483	0.4583923972235646	T	T	T
0.8891790675290330	0.9995320937134318	0.4577429952421099	T	T	T
0.7779167058119815	0.9997583509594620	0.4577332331124550	T	T	T

0.6660090098327411	0.9982403274849605	0.4569806759821934	T	T	T
0.5550992636380252	0.9986554148415230	0.4574652150232432	T	T	T
0.3325492894852382	0.8994692142821256	0.3898848472347959	T	T	T
0.2214984641394905	0.8995813009842301	0.3901454218025292	T	T	T
-0.0002952067461975	-0.0001775184574063	0.4583121489868836	T	T	T
0.7770658984463595	0.0985576289454893	0.3900956437988028	T	T	T
0.5579013074889403	0.2039888504609054	0.4515242065970732	T	T	T
0.4438871320489857	0.6009542313528086	0.4563522839610413	T	T	T
0.5568074369142585	0.4034344849651859	0.4560636641010534	T	T	T
0.7774431686133669	0.2000157896173966	0.4538430964395244	T	T	T
0.4436041662326123	0.8993181476220941	0.3900002345207254	T	T	T
-0.0005209437239096	0.2004062334951220	0.4544002783265239	T	T	T
0.2219686200615609	0.3994313329060479	0.4543733717297700	T	T	T
0.3327028780627945	0.3992899650743579	0.4534185275084110	T	T	T
0.6674542322376795	0.2028325202025997	0.4521815752374891	T	T	T
0.4436292531798738	0.3985063736280548	0.4537686438978645	T	T	T
0.1107133954204498	0.8996490255184660	0.3902406268399370	T	T	T
0.7807176269797863	0.4035503299920082	0.4542191370688859	T	T	T
0.8896484807621117	0.3998493320554616	0.4545931223059416	T	T	T
0.0004578179179465	0.3998814676502121	0.4549989469286066	T	T	T
0.1109658781296871	0.3993201652394445	0.4549845638885323	T	T	T
0.3316059406509401	0.5995111324877853	0.4573368861406909	T	T	T
0.6675009594500586	0.4031833627944448	0.4539169193944514	T	T	T
0.6666758422254497	0.6018547073669402	0.4572666596971174	T	T	T
0.8887493247956406	0.2007614859874224	0.4543581319081261	T	T	T
0.9205659546385410	0.4598084992699751	0.5397045316152697	T	T	T
0.1098683394828067	0.6004698562777220	0.4586750892827249	T	T	T
0.2197428420749082	0.5989634130850571	0.4580354503858124	T	T	T
0.4441454839391138	0.7980656579491259	0.4545497300371243	T	T	T
0.5552112811397434	0.7994473901260903	0.4544491860701981	T	T	T
0.6658419617345592	0.7999096722584557	0.4540879088884392	T	T	T
0.8892465908159332	0.8007589554208995	0.4557620789437022	T	T	T
0.0004086559370371	0.8003477404609249	0.4564394822618767	T	T	T
0.1109475916540120	0.7994255262282164	0.4564151183716141	T	T	T
0.2224537627098929	0.8000415815541979	0.4561615537778331	T	T	T
0.3319457430633969	0.7971511746864464	0.4559608492970126	T	T	T
0.1779870867457002	0.1247033707133871	0.5371268002165954	T	T	T
0.2865145377943887	0.1235850767403389	0.5372151764360783	T	T	T
0.3938618856998585	0.1225784777424844	0.5356523295315060	T	T	T
0.4964730038366528	0.1157663838559048	0.5285919687779665	T	T	T
0.6284407197785141	0.1206688353584143	0.5319118427048578	T	T	T
0.3673240020628572	0.4638071410032084	0.5374221684114392	T	T	T
0.1079999411204104	0.2954414430588749	0.5244742365950305	T	T	T
0.8896470639535059	0.6022934689603797	0.4576848472985129	T	T	T
0.4390749223057782	0.2943978668915455	0.5256568452385725	T	T	T
0.7380616158485210	0.1233831458348594	0.5367464591764501	T	T	T
0.8470302796299243	0.1237405634144117	0.5371984836507707	T	T	T
0.9576349776084774	0.1245002901166956	0.5374196981958923	T	T	T
0.0678682685418188	0.1243770779177999	0.5367192786187985	T	T	T
0.9991341459009005	0.6006091133127071	0.4583989379382597	T	T	T
0.2184801367915226	0.2951933087609821	0.5245901589037831	T	T	T
0.5508389532675351	0.2948264844988178	0.5236928049454022	T	T	T
0.5865355515582416	0.4590569924396913	0.5436274436932673	T	T	T
0.6647280007496970	0.2974306726114909	0.5193985572418338	T	T	T
0.7740196405981840	0.2940840951966905	0.5233140849820975	T	T	T
0.8857184800277966	0.2945740601679585	0.5251593016724214	T	T	T

0.9964599862621260	0.2942976759535663	0.5250292630505643	T	T	T
0.3295194258850647	0.2957463471126934	0.5218236518983304	T	T	T
0.4796730309230087	0.4637878013543592	0.5375625909344042	T	T	T
0.7775293671190546	0.8001020852712173	0.4559813500935282	T	T	T
0.7784861659104654	0.6023863270513989	0.4572487566295375	T	T	T
0.6626690568833551	0.7911655576250828	0.5419992786395456	T	T	T
0.5510803707066945	0.7916473396427303	0.5435062907912458	T	T	T
0.2926115420588513	0.6289159312350381	0.5361175050156769	T	T	T
0.1809663746217484	0.6280739730737920	0.5380720463026168	T	T	T
0.0671442707742911	0.6253187182344372	0.5381519491313659	T	T	T
0.6981437666384495	0.4598215211305748	0.5396779495474003	T	T	T
0.7727779526762232	0.7915122415858539	0.5448808596661086	T	T	T
0.8461103288677930	0.6260633583549886	0.5366019071326283	T	T	T
0.6263523682578795	0.6271343096773857	0.5378120264538960	T	T	T
0.5154415076901107	0.6288294529463898	0.5344109436085136	T	T	T
0.4048671386424966	0.6303794030634892	0.5352993452869141	T	T	T
0.2566577964628448	0.4633853989608956	0.5391634024854340	T	T	T
0.1450856233778220	0.4626627827027580	0.5398094864743017	T	T	T
0.0334349885893113	0.4616189848363291	0.5400188163853595	T	T	T
0.7356347850730173	0.6264543903233305	0.5356464048543078	T	T	T
0.8827127843888251	0.7912459983796130	0.5442955890097394	T	T	T
0.9563079111900835	0.6253853437683560	0.5383315701946531	T	T	T
0.3550026419016921	0.9479522807007286	0.5326419969856517	T	T	T
0.4736431497992039	0.9558131859729723	0.5325303029157813	T	T	T
0.9922708417691504	0.7904171541310694	0.5451597704340876	T	T	T
0.1017936676452154	0.7895463265101627	0.5452056671279589	T	T	T
0.6975649695155067	0.9548387259059321	0.5349397850064214	T	T	T
0.3271435376048331	0.7917919182688027	0.5452059944461028	T	T	T
0.4388544849575288	0.7933305814023488	0.5427766199294835	T	T	T
0.2114775958354001	0.7879346035317861	0.5449042519324937	T	T	T
0.8094549295805196	0.9563700806792662	0.5351446832309465	T	T	T
0.8095908516343426	0.4599816296697779	0.5406981477407230	T	T	T
0.9192741180906195	0.9562543552968810	0.5368514580417640	T	T	T
0.0294141951414833	0.9558790844566405	0.5368630741119484	T	T	T
0.1392578481165846	0.9554421551151485	0.5371295139808370	T	T	T
0.2477565849239345	0.9529928902738817	0.5354751825620711	T	T	T
0.5858017699612412	0.9532508387490279	0.5356321409985885	T	T	T
0.3063957162905278	0.9791907509281894	0.6444106737453121	T	T	T
0.6835026925562381	0.1569588460549605	0.6476321889872293	T	T	T
0.6808517800456509	0.4894110824351935	0.6458788250220125	T	T	T
0.3916848958685221	0.6390774593003542	0.6401339547665459	T	T	T
0.4974724198232695	0.5502622670107259	0.6420812324104732	T	T	T
0.3048331507722455	0.3152424529094349	0.6339497477801230	T	T	T
0.3622449521508105	0.4107704223333642	0.6371877028538228	T	T	T
0.4329700276903841	0.4504397952678129	0.6407462903702942	T	T	T
0.6797700761940748	0.8233666845090016	0.6467102891791275	T	T	T
0.7503915139506151	0.8630419920090598	0.6516424181400221	T	T	T
0.8083852551748411	0.9584634103254619	0.6502364816777132	T	T	T
0.3198183053691573	0.2619139484364137	0.6340230844675503	T	T	T
0.7226977698689991	0.9685525253032436	0.6395601654711026	T	T	T
0.3913807750385298	0.3054959482373281	0.6378483972867168	T	T	T
0.7940053316257156	0.0119534924382999	0.6440547450606355	T	T	T
0.3633954873537730	0.0748269765139149	0.6461541789801567	T	T	T
0.6154687231714095	0.7243769951193456	0.6451869933644524	T	T	T
0.4347566024329384	0.1159030254532405	0.6467399757566158	T	T	T
0.8114825089518594	0.2910127869676989	0.6391425077479821	T	T	T

0.6167910943938594	0.3897103535446059	0.6460430228361841	T	T	T
0.3204273379608180	0.5959508646128319	0.6446960865742344	T	T	T
0.3646452720351675	0.7448553411426966	0.6542129329831241	T	T	T
0.3223973773166133	0.9268884398848150	0.6425286730406823	T	T	T
0.7976138685889788	0.3455195470646439	0.6412425407348058	T	T	T
0.4997181340776922	0.8833504539243151	0.6489248058403337	T	T	T
0.7537286754626736	0.1956508783059672	0.6425481570126932	T	T	T
0.3063689784796982	0.6495779948313326	0.6517571383825934	T	T	T
0.4351352442550362	0.7842620681567553	0.6490450602758814	T	T	T
0.6183730321021468	0.0573668313264327	0.6483503484432719	T	T	T
0.3944151755705952	0.9716413278704005	0.6430715506315713	T	T	T
0.4986211712601724	0.2152416355124616	0.6472922885358501	T	T	T
0.7217061954457339	0.6339464794463235	0.6452698471100886	T	T	T
0.7936976007181867	0.6784349898488408	0.6445320225299701	T	T	T
0.8092995364803429	0.6256880200825362	0.6447292743395987	T	T	T
0.7520639113742106	0.5300053387344688	0.6450674243619109	T	T	T
0.7265363139758055	0.3029282237277987	0.6464359811361481	T	T	T
0.2765080024888881	0.5211714503485144	0.6415222209256783	T	T	T
0.3536261290176756	0.4555087067660855	0.6365680305316469	T	T	T
0.7583161437273956	0.8178993563535749	0.6555068248150684	T	T	T
0.2494447827749336	0.2830514532702826	0.6300640966791395	T	T	T
0.2508791951905429	0.6175486475581458	0.6542756330241274	T	T	T
0.7615545347931820	0.1502330958130565	0.6400794817543238	T	T	T
0.3570517666271227	0.7901056005716043	0.6592489325343494	T	T	T
0.8639354791387085	0.9907293945677372	0.6527833650965985	T	T	T
0.7611204298422278	0.4857498901106946	0.6439934575029655	T	T	T
0.8662949374847577	0.3223195006927248	0.6335059951156984	T	T	T
0.2767662375566881	0.1872065722618722	0.6301781226990035	T	T	T
0.8377447901904622	0.0868710441812888	0.6415533533238866	T	T	T
0.7083262117178593	0.0066853646974260	0.6346877651030526	T	T	T
0.4065661164458377	0.2676672303677819	0.6378150551061603	T	T	T
0.3541370099162801	0.1189082094608925	0.6464898050441069	T	T	T
0.2504329108185881	0.9458432014127353	0.6431544179969334	T	T	T
0.8367194276005293	0.7535314507525293	0.6430552931263550	T	T	T
0.2796507522137613	0.8519891969720419	0.6395918335953106	T	T	T
0.8651640900188842	0.6587295705217487	0.6433635381329561	T	T	T
0.7061353469940772	0.6713203166276157	0.6450691113947288	T	T	T
0.4058027705177428	0.6007801715499447	0.6345932401911063	T	T	T
0.7117018853544947	0.3411495371397099	0.6470572678099302	T	T	T
0.8410120383186943	0.4202018576070420	0.6374628265996707	T	T	T
0.4100410069506826	0.9344346494507294	0.6414940132375345	T	T	T
0.6703180447620786	0.2104561823907152	0.6496735799391141	T	T	T
0.6656840865471729	0.8756087819688402	0.6409477529786373	T	T	T
0.6224610375009576	0.6671765693650771	0.6479713110236486	T	T	T
0.5506735856532228	0.7005723596074359	0.6389124432816193	T	T	T
0.4894107565941810	0.6065313223237083	0.6399214587704208	T	T	T
0.4930648663570506	0.9404791642139028	0.6540452508080684	T	T	T
0.5538110029979790	0.0335207408414482	0.6525906120893403	T	T	T
0.6255531175593142	0.0006862589731858	0.6432506975404312	T	T	T
0.4488717532356196	0.7319176441382871	0.6420245335884625	T	T	T
0.4501685852290916	0.0645201244457575	0.6459476595669955	T	T	T
0.4470646427106363	0.3978629512990264	0.6414753652847038	T	T	T
0.5623870571566183	0.5749421088091986	0.6442618601645491	T	T	T
0.5641193535164738	0.2403730575078839	0.6499503708904362	T	T	T
0.6660074524774904	0.5411695161030937	0.6463933069260760	T	T	T
0.6250960040086332	0.3338247855365461	0.6490188177531727	T	T	T

0.5513621741851181	0.3643852933060985	0.6435536732387169	T	T	T
0.4907495589257612	0.2716301559348764	0.6446877217204207	T	T	T
0.5641927977568922	0.9070407919329753	0.6412804820860386	T	T	T
0.5608399628363944	0.1391625339195748	0.6386111281020642	T	T	T
0.5571555160794556	0.8036727960747262	0.6263892257724590	T	T	T
0.5556661283355218	0.4683287991618468	0.6562130402152442	T	T	T
0.5514902731037153	0.4639864994226296	0.7082756156462346	T	T	T
0.5689052481427560	0.1462531473345051	0.5856942849224792	T	T	T

Fig. 6j

Au C H N V O

1.000000000000000

26.0801187006857766 0.0000000000000000 0.0000000000000000

-14.4889548337143204 14.4889548337143204 0.0000000000000000

0.0000000000000000 0.0000000000000000 31.0000000000000000

Au C H N V O

279 36 24 18 3 2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.1894422798390494	F	F	F
0.5555555555555571	0.2000000000000028	0.1894422798390494	F	F	F
0.444444444444429	0.2000000000000028	0.1894422798390494	F	F	F
0.222222222222214	0.2000000000000028	0.1894422798390494	F	F	F
0.1111111111111143	0.2000000000000028	0.1894422798390494	F	F	F
0.777777777777786	0.2000000000000028	0.1894422798390494	F	F	F
0.888888888888857	0.0000000000000000	0.1894422798390494	F	F	F
0.666666666666643	0.0000000000000000	0.1894422798390494	F	F	F
0.555555555555571	0.0000000000000000	0.1894422798390494	F	F	F
0.444444444444429	0.0000000000000000	0.1894422798390494	F	F	F
0.333333333333357	0.0000000000000000	0.1894422798390494	F	F	F
0.222222222222214	0.0000000000000000	0.1894422798390494	F	F	F
0.1111111111111143	0.0000000000000000	0.1894422798390494	F	F	F
0.777777777777786	0.0000000000000000	0.1894422798390494	F	F	F
0.888888888888857	0.5000000000000000	0.2561864044279716	F	F	F
0.8888888888888928	0.2000000000000028	0.1894422798390494	F	F	F
0.222222222222214	0.3999999999999986	0.1894422798390494	F	F	F
0.8888888888888928	0.6000000000000014	0.1894422798390494	F	F	F
0.0000000000000000	0.3999999999999986	0.1894422798390494	F	F	F
0.333333333333357	0.3999999999999986	0.1894422798390494	F	F	F
0.444444444444429	0.3999999999999986	0.1894422798390494	F	F	F
0.555555555555571	0.3999999999999986	0.1894422798390494	F	F	F
0.666666666666643	0.3999999999999986	0.1894422798390494	F	F	F
0.777777777777786	0.3999999999999986	0.1894422798390494	F	F	F
0.6666666666666714	0.2000000000000028	0.1894422798390494	F	F	F
0.888888888888857	0.3999999999999986	0.1894422798390494	F	F	F
0.0000000000000000	0.2000000000000028	0.1894422798390494	F	F	F
0.333333333333357	0.6000000000000014	0.1894422798390494	F	F	F
0.444444444444429	0.6000000000000014	0.1894422798390494	F	F	F
0.555555555555571	0.6000000000000014	0.1894422798390494	F	F	F
0.5543326137185948	0.0978128953099885	0.3899321431167748	T	T	T
0.777777777777786	0.6000000000000014	0.1894422798390494	F	F	F
0.1111111111111072	0.3999999999999986	0.1894422798390494	F	F	F
0.0000000000000000	0.5000000000000000	0.2561864044279716	F	F	F
0.0000000000000000	0.6000000000000014	0.1894422798390494	F	F	F
0.222222222222214	0.6000000000000014	0.1894422798390494	F	F	F

0.6666666666666643	0.799999999999972	0.1894422798390494	F	F	F
0.7777777777777786	0.799999999999972	0.1894422798390494	F	F	F
0.8888888888888857	0.799999999999972	0.1894422798390494	F	F	F
0.0000000000000000	0.799999999999972	0.1894422798390494	F	F	F
0.1111111111111072	0.799999999999972	0.1894422798390494	F	F	F
0.222222222222214	0.799999999999972	0.1894422798390494	F	F	F
0.333333333333286	0.799999999999972	0.1894422798390494	F	F	F
0.1111111111111143	0.1000000000000014	0.2561864044279716	F	F	F
0.222222222222214	0.1000000000000014	0.2561864044279716	F	F	F
0.333333333333357	0.1000000000000014	0.2561864044279716	F	F	F
0.444444444444429	0.1000000000000014	0.2561864044279716	F	F	F
0.555555555555571	0.1000000000000014	0.2561864044279716	F	F	F
0.666666666666643	0.1000000000000014	0.2561864044279716	F	F	F
0.777777777777786	0.1000000000000014	0.2561864044279716	F	F	F
0.8888888888888928	0.1000000000000014	0.2561864044279716	F	F	F
0.0000000000000000	0.1000000000000014	0.2561864044279716	F	F	F
0.777777777777786	0.5000000000000000	0.2561864044279716	F	F	F
0.8888888888888857	0.299999999999972	0.2561864044279716	F	F	F
0.222222222222214	0.299999999999972	0.2561864044279716	F	F	F
0.333333333333286	0.299999999999972	0.2561864044279716	F	F	F
0.444444444444429	0.299999999999972	0.2561864044279716	F	F	F
0.555555555555571	0.299999999999972	0.2561864044279716	F	F	F
0.666666666666643	0.299999999999972	0.2561864044279716	F	F	F
0.1111111111111143	0.6000000000000014	0.1894422798390494	F	F	F
0.777777777777786	0.299999999999972	0.2561864044279716	F	F	F
0.444444444444429	0.799999999999972	0.1894422798390494	F	F	F
0.1111111111111072	0.299999999999972	0.2561864044279716	F	F	F
0.333333333333357	0.5000000000000000	0.2561864044279716	F	F	F
0.444444444444429	0.5000000000000000	0.2561864044279716	F	F	F
0.555555555555571	0.5000000000000000	0.2561864044279716	F	F	F
0.666666666666643	0.5000000000000000	0.2561864044279716	F	F	F
0.0000000000000000	0.299999999999972	0.2561864044279716	F	F	F
0.555555555555571	0.799999999999972	0.1894422798390494	F	F	F
0.666666666666643	0.6000000000000014	0.1894422798390494	F	F	F
0.9994031817364978	0.1987151372530374	0.3226556141252629	T	T	T
0.8888888888888857	0.899999999999986	0.2561864044279716	F	F	F
0.777777777777786	0.899999999999986	0.2561864044279716	F	F	F
0.666666666666643	0.899999999999986	0.2561864044279716	F	F	F
0.555555555555571	0.899999999999986	0.2561864044279716	F	F	F
0.333333333333357	0.7000000000000028	0.2561864044279716	F	F	F
0.1111111111111072	0.899999999999986	0.2561864044279716	F	F	F
0.222222222222214	0.7000000000000028	0.2561864044279716	F	F	F
0.6662669986604828	0.1990622274508990	0.3224214342633736	T	T	T
0.8888888888888928	0.7000000000000028	0.2561864044279716	F	F	F
0.777777777777786	0.7000000000000028	0.2561864044279716	F	F	F
0.6666666666666714	0.7000000000000028	0.2561864044279716	F	F	F
0.555555555555571	0.7000000000000028	0.2561864044279716	F	F	F
0.444444444444429	0.7000000000000028	0.2561864044279716	F	F	F
0.1111111111111143	0.7000000000000028	0.2561864044279716	F	F	F
0.222222222222214	0.899999999999986	0.2561864044279716	F	F	F
0.0000000000000000	0.7000000000000028	0.2561864044279716	F	F	F
0.444444444444429	0.899999999999986	0.2561864044279716	F	F	F
0.333333333333357	0.899999999999986	0.2561864044279716	F	F	F
0.1104563221515808	0.9991759293936634	0.3229714280281021	T	T	T
0.5551573935729184	0.0000808683376688	0.3225002815992777	T	T	T
0.6667694903142181	0.0002171853645218	0.3225101833831887	T	T	T

0.7784139059421006	0.0004032518796006	0.3225571221093669	T	T	T
0.8889688347322915	0.9996728440008514	0.3229060495330753	T	T	T
0.0000000000000000	0.8999999999999986	0.2561864044279716	F	F	F
0.9996844666978822	0.9993618124718318	0.3229966915330817	T	T	T
0.3326129448035963	0.9993167875831325	0.3228619572334889	T	T	T
0.4437156176350731	0.9993673434095313	0.3227372314283747	T	T	T
0.1102662478979830	0.1983673710224070	0.3226179518651137	T	T	T
0.2211802568715803	0.1981420549023634	0.3225821611336247	T	T	T
0.3324891889200617	0.1983851872760160	0.3224882069794217	T	T	T
0.4438811723957481	0.1987966289583929	0.3224835389319323	T	T	T
0.2215622588762820	0.9993222926852801	0.3229240988884233	T	T	T
0.222222222222214	0.5000000000000000	0.2561864044279716	F	F	F
0.5548380864476562	0.1985846212212967	0.3225090590985025	T	T	T
0.7776686993130778	0.1993595099447474	0.3224603396997131	T	T	T
0.2223375506097710	0.4006512963177703	0.3225827427901670	T	T	T
0.3334648319446233	0.4006484112460743	0.3224696894655589	T	T	T
0.4448578619343952	0.4009478927126005	0.3224142446617045	T	T	T
0.5563001046453374	0.4014642193937753	0.3224920091270696	T	T	T
0.6672691802755802	0.4012482800259414	0.3224840540531319	T	T	T
0.7786507046528651	0.4016466800863077	0.3224869377185096	T	T	T
0.8899618686489295	0.4019031764500266	0.3225663415004327	T	T	T
0.1117078021857717	0.4012717301908654	0.3226561881655133	T	T	T
0.3327027672341867	0.5996033378373051	0.3225601508083109	T	T	T
0.4443517400545775	0.5997954825659751	0.3224940175994688	T	T	T
0.5559550223856287	0.5999203226552137	0.3225063427347478	T	T	T
0.6674152394579188	0.6006737104583382	0.3227490210824960	T	T	T
0.7785036898491250	0.6006891439106511	0.3228572489112043	T	T	T
0.8895717804379062	0.6006988987205534	0.3229224361173972	T	T	T
0.0006899433391481	0.6008645026176357	0.3229742560390678	T	T	T
0.1114222882626106	0.6006249935022951	0.3230032203263997	T	T	T
0.1111111111111143	0.5000000000000000	0.2561864044279716	F	F	F
0.0000804926351059	0.8000339366206072	0.3230370115759655	T	T	T
0.2221195613395722	0.6002988638860460	0.3229049654987919	T	T	T
0.4439290426473210	0.7998354092432204	0.3226229114543169	T	T	T
0.5555547819542028	0.8000095143488773	0.3226427248160972	T	T	T
0.6671874142139271	0.8001952214162183	0.3226301001210511	T	T	T
0.7783837978466863	0.8002389866107075	0.3228627059418148	T	T	T
0.0008575098367172	0.4016304410795687	0.3226259912759364	T	T	T
0.8891403177256030	0.8000321098485798	0.3230514342139496	T	T	T
0.8887784401517970	0.1993557027445028	0.3225927083945785	T	T	T
0.2219449551580706	0.7999367612143902	0.3230536176778602	T	T	T
0.3327134831656840	0.7997601101069299	0.3228638986411743	T	T	T
0.1095167755932355	0.0972945758227934	0.3905088927877189	T	T	T
0.2205377987140412	0.0974520424894420	0.3901590031922629	T	T	T
0.3320675335456579	0.0978781026346149	0.3898611695269108	T	T	T
0.1110769754086257	0.8000156791828611	0.3230440616036273	T	T	T
0.4433532982831552	0.0981043934883213	0.3899204991440744	T	T	T
0.3333333333333357	0.2000000000000028	0.1894422798390494	F	F	F
0.6658903206945428	0.0985476978302033	0.3897340785838287	T	T	T
0.9990685530346743	0.0979371827354186	0.3903664524752554	T	T	T
0.2215797050876326	0.2992549791127079	0.3876138402769820	T	T	T
0.3329260723593389	0.2993385459474168	0.3873974422568596	T	T	T
0.4448479476513301	0.3005730886986117	0.3873479301062316	T	T	T
0.5555925045320802	0.3000644420336255	0.3876190807438545	T	T	T
0.6663215224369733	0.2995532087497773	0.3873385300696108	T	T	T
0.7782501745552938	0.3007251478216764	0.3873773453396029	T	T	T

0.8895649710669887	0.3008183310566798	0.3876061926779741	T	T	T
0.0002954998288276	0.3002854864506358	0.3878631506133710	T	T	T
0.1108409283459879	0.2997094543847053	0.3878610897287195	T	T	T
0.3336019727961539	0.5012650484799441	0.3897312192825690	T	T	T
0.4452563453644416	0.5014743149001227	0.3897364826811747	T	T	T
0.5568231237742475	0.5022290153421206	0.3899450010284905	T	T	T
0.6678050731624307	0.5019382050385613	0.3899194103116392	T	T	T
0.7790834097191643	0.5021791597713303	0.3898774967468094	T	T	T
0.8906300370240808	0.5026410115679901	0.3901694554145552	T	T	T
0.6678821434364361	0.9011391349936212	0.3886157824549923	T	T	T
0.7780210504236675	0.7000751251331876	0.3901625549283370	T	T	T
0.0016119797342368	0.5027436410096375	0.3905123586860369	T	T	T
0.1120510100252332	0.5020716240161890	0.3903696580421234	T	T	T
0.2227391897912331	0.5016081355311518	0.3902853604353156	T	T	T
0.4432384412812362	0.6989011835327137	0.3886015390604168	T	T	T
0.5552776175759352	0.6990679653341088	0.3887861543180597	T	T	T
0.8883906531527085	0.0984063505747492	0.3902896277711628	T	T	T
0.6671916455623343	0.7002885091379016	0.3895100625932060	T	T	T
0.8895307869474330	0.9000496758147440	0.3902803333836051	T	T	T
0.0001808425283236	0.7003517569459464	0.3904123826929564	T	T	T
0.1108669327221601	0.7001741461056840	0.3905779428195201	T	T	T
0.2215695564368100	0.6999586081574511	0.3902901792590674	T	T	T
0.3320711521371522	0.6992559298503371	0.3897833948927216	T	T	T
0.5558208532657560	0.9009596603080230	0.3887939644622831	T	T	T
0.8891071537594812	0.7000665689199709	0.3902801732002225	T	T	T
0.7790284009664378	0.9007648642732357	0.3898016154456099	T	T	T
0.0002495048409429	0.8998362041528480	0.3905497031568450	T	T	T
0.5559452825835327	0.6003719435776728	0.4571930693588718	T	T	T
0.3333872373965879	0.1999581251724154	0.4537433412353684	T	T	T
0.2217836208988340	0.2001164474858219	0.4539038422104040	T	T	T
0.1108008553133764	0.2002786756340695	0.4544815548257858	T	T	T
0.4446122195375988	0.9994263943388032	0.4572784226256329	T	T	T
0.3336920973505254	0.0007616987509851	0.4574146102891782	T	T	T
0.2217640579746651	0.9998610244340157	0.4578634195989228	T	T	T
0.4454140056052127	0.2025036705926908	0.4532126126583354	T	T	T
0.1109425062501796	0.9992573973552202	0.4585987839069084	T	T	T
0.8899051707822032	0.9996698699354413	0.4579099862081433	T	T	T
0.7784934226107165	0.0000183189346549	0.4574791823607323	T	T	T
0.6666447354216710	0.9988284770043352	0.4563185158322456	T	T	T
0.5551755520186371	0.9996354463206661	0.4572120132894320	T	T	T
0.3330950541850251	0.8999516461282765	0.3901515465215403	T	T	T
0.2220174177670712	0.8999546623102079	0.3903051845318830	T	T	T
0.0001955822838704	0.9993177847430637	0.4586558640196565	T	T	T
0.7775505583649074	0.0987652666010669	0.3897437756783618	T	T	T
0.5544086344620207	0.1981173155100625	0.4548628066218807	T	T	T
0.4444427983910987	0.6011773216001597	0.4563162099331702	T	T	T
0.5567844791303325	0.4019742355729906	0.4548701987559879	T	T	T
0.7779885381746341	0.2004701340488311	0.4533833159645503	T	T	T
0.4439369538672072	0.8997895457878489	0.3895039020303682	T	T	T
0.9999174472550615	0.2004486554809989	0.4546056805629722	T	T	T
0.2221089882060376	0.3993929188775624	0.4543049341647808	T	T	T
0.3331772630746268	0.3995593007146295	0.4533756361160549	T	T	T
0.6668032793044215	0.2012265495540326	0.4534040034379126	T	T	T
0.4444347315785012	0.3989624903806905	0.4535069283842259	T	T	T
0.1109870553412999	0.8997359709708516	0.3904196055212434	T	T	T
0.7778274223306415	0.4001837160681394	0.4537424955056911	T	T	T

0.8893851372541396	0.3999678119492561	0.4539031764866853	T	T	T
0.0003418647805935	0.3997249332782187	0.4544841297694717	T	T	T
0.1112324606535972	0.3995721065353676	0.4545886433844047	T	T	T
0.3326865808852464	0.6000421236923965	0.4574633850239846	T	T	T
0.6657806024165660	0.3976050425717774	0.4532731692485253	T	T	T
0.6665699493891860	0.6006946404613968	0.4572724451745700	T	T	T
0.8890446013905610	0.2006817122238962	0.4542912488004403	T	T	T
0.9268993211042744	0.4690112392327456	0.5376081749868050	T	T	T
0.1108953187924753	0.6006565688356937	0.4586679053703916	T	T	T
0.2212271081822834	0.6003737973758796	0.4578949617567853	T	T	T
0.4447521096957167	0.7995897508202058	0.4538919396965629	T	T	T
0.5555220109172248	0.7999863227895360	0.4536576352030087	T	T	T
0.6663183260730056	0.8004452321649074	0.4539038887485216	T	T	T
0.8886512587801073	0.7996603928337772	0.4560969937864155	T	T	T
0.0000420501079906	0.7999464572492436	0.4565885125488752	T	T	T
0.1111084313960050	0.8001662412621423	0.4565994663489059	T	T	T
0.2224352175518113	0.8003148580853197	0.4561173194618643	T	T	T
0.3334950464123333	0.7999336255206367	0.4560498400777797	T	T	T
0.1841801970217264	0.1309866158447429	0.5375995563551184	T	T	T
0.2949524385606302	0.1303283319408104	0.5375656824135114	T	T	T
0.4059842815907694	0.1303125903561639	0.5358239915264166	T	T	T
0.5183554150562697	0.1322091766528246	0.5402378987383343	T	T	T
0.6264798551585258	0.1294988265753766	0.5362552319113865	T	T	T
0.3722991639237125	0.4696412416717380	0.5366161942119024	T	T	T
0.1115305887597222	0.3004063630020074	0.5245423704572738	T	T	T
0.8893809214167235	0.6003054699120401	0.4578801789335158	T	T	T
0.4442409476848756	0.2995457532986119	0.5253537042046671	T	T	T
0.7388224037919193	0.1303524866036119	0.5366327875906295	T	T	T
0.8496802775629225	0.1306252356149733	0.5380813168994582	T	T	T
0.9618788943837256	0.1314589008071861	0.5385052732906281	T	T	T
0.0731369411779309	0.1313337859879030	0.5383183636279708	T	T	T
0.0001952121390671	0.6008464316592552	0.4586180474444018	T	T	T
0.2225147716115050	0.3000618993488209	0.5243946650419128	T	T	T
0.5555280570274430	0.2999573393016802	0.5223675602630689	T	T	T
0.5926536135030838	0.4677028467024926	0.5402192674742132	T	T	T
0.6668049294289393	0.3003335260703967	0.5253318641505659	T	T	T
0.7771883013188313	0.2998012680605565	0.5216865309128750	T	T	T
0.8885871513552006	0.2999626545931421	0.5244290577052121	T	T	T
0.9995735396013958	0.2995918206556518	0.5245330566542299	T	T	T
0.3339406187307995	0.3002204451899401	0.5217430768671828	T	T	T
0.4845946015401819	0.4703964135360939	0.5364716478559030	T	T	T
0.7776449634327053	0.8001694882585182	0.4560588065219734	T	T	T
0.7774604436724381	0.5992669761319773	0.4574335447709636	T	T	T
0.6676160159440496	0.7999069115738907	0.5417804667140454	T	T	T
0.5555587870797873	0.7999904747664397	0.5422510348359256	T	T	T
0.2969832132797176	0.6352138018800413	0.5355294091397235	T	T	T
0.1864165212226583	0.6353363250813941	0.5376895796687685	T	T	T
0.0753807302486734	0.6357686198086014	0.5375568215342656	T	T	T
0.7050141093180445	0.4695256074268944	0.5359709642343905	T	T	T
0.7781743258015347	0.8004883778410454	0.5450997654762672	T	T	T
0.8538123505315532	0.6371536796430363	0.5356648107150671	T	T	T
0.6317049800797666	0.6359061116300776	0.5368751111751452	T	T	T
0.5206494796025031	0.6368255318801800	0.5338701049655704	T	T	T
0.4093761022021104	0.6365918712655870	0.5352352159780873	T	T	T
0.2614034405916740	0.4693573452084278	0.5381146040255947	T	T	T
0.1492026153605287	0.4685277996123309	0.5384825331095128	T	T	T

0.0379645711110631	0.4686874206960539	0.5383156722335704	T	T	T
0.7422559126755779	0.6367642379657138	0.5345376369870269	T	T	T
0.8891681845179672	0.8007521553699829	0.5447885529978230	T	T	T
0.9640992926926339	0.6358603409953238	0.5376461063906871	T	T	T
0.3688005159740677	0.9631367245335591	0.5345744631489810	T	T	T
0.4793639230126913	0.9640464410725860	0.5368586180778415	T	T	T
0.0001802856688480	0.8003040208543042	0.5453984104125785	T	T	T
0.1108302865311566	0.7996142356719190	0.5454097858000142	T	T	T
0.7017070026789491	0.9633413637651330	0.5351406458388913	T	T	T
0.3329406324089739	0.7994632798631776	0.5450823946105168	T	T	T
0.4435429040343400	0.8000619111158147	0.5417721611854411	T	T	T
0.2219214903458981	0.7992057604942631	0.5448187126883145	T	T	T
0.8141465847065594	0.9647748214111127	0.5355960859569137	T	T	T
0.8160511102081023	0.4696014442720490	0.5375931464953816	T	T	T
0.9246937995202590	0.9646448359624901	0.5376895718242534	T	T	T
0.0357165378538628	0.9642338757739014	0.5375460567735768	T	T	T
0.1469046005431062	0.9640714503798612	0.5376552302444328	T	T	T
0.2571581002733610	0.9627012946197404	0.5355348198572318	T	T	T
0.5904845266167236	0.9631655860344731	0.5339407203941047	T	T	T
0.3026141395610821	0.9784107014132951	0.6429501651340904	T	T	T
0.6791065538456007	0.1524113583012104	0.6396971036498980	T	T	T
0.6783749859568936	0.4863397921843448	0.6405055290305338	T	T	T
0.3898443606637901	0.6346439869719404	0.6409827780984337	T	T	T
0.4947306191483409	0.5465919368139427	0.6406361932315040	T	T	T
0.3016765500678157	0.3118421767494839	0.6346893212985524	T	T	T
0.3593289964040985	0.4074170290053838	0.6373134236646590	T	T	T
0.4300826990508955	0.4468850922149404	0.6396936496893468	T	T	T
0.6767618760452828	0.8195555218277489	0.6462516741493534	T	T	T
0.7475064243894949	0.8594933178401725	0.6507931696093823	T	T	T
0.8052942567339396	0.9549923616942375	0.6500386239918037	T	T	T
0.3164547400648403	0.2583014031857778	0.6342185312389551	T	T	T
0.7191101402343055	0.9646414602952934	0.6407986114212751	T	T	T
0.3881245425258747	0.3018291019919874	0.6367110407352149	T	T	T
0.7905299084558708	0.0082765938297463	0.6450279639827255	T	T	T
0.3603090486714704	0.0739032892913395	0.6404223605526979	T	T	T
0.6127406987686451	0.7205920001070110	0.6440488346344526	T	T	T
0.4312315711894937	0.1135324691805320	0.6404146299198604	T	T	T
0.8075413277061186	0.2873136694260492	0.6345952014144383	T	T	T
0.6140080454694403	0.3870144667164728	0.6375803993738680	T	T	T
0.3184018293978066	0.5909820908379608	0.6451184856580519	T	T	T
0.3613816221580620	0.7398002999687167	0.6506071725618064	T	T	T
0.3174524419271361	0.9248970694303568	0.6446016141896578	T	T	T
0.7928592502992725	0.3409550504468226	0.6339680054901605	T	T	T
0.4962140627682972	0.8787221316884580	0.6440346927777659	T	T	T
0.7498268127135922	0.1917546262270194	0.6373236309824131	T	T	T
0.3036157481521629	0.6442864348071948	0.6498999777279727	T	T	T
0.4321456947634315	0.7797581443912103	0.6462280386089801	T	T	T
0.6143736168711367	0.0527239262753960	0.6406901232949169	T	T	T
0.3892487423408583	0.9685440552000050	0.6444091855443720	T	T	T
0.4956306760587896	0.2128393449203551	0.6375615688296918	T	T	T
0.7203333078963560	0.6313458776888994	0.6439273220796118	T	T	T
0.7921389209481494	0.6750113151067827	0.6443030734142491	T	T	T
0.8069754176030686	0.6214743014287674	0.6432334829847532	T	T	T
0.7492868903255545	0.5259518038701215	0.6409527214875131	T	T	T
0.7212217485383250	0.2975500642339997	0.6364849567689331	T	T	T
0.2748534842732195	0.5159515708457775	0.6433212231560077	T	T	T

0.3507768806736670	0.4522192140664315	0.6371004513288698	T	T	T
0.7557082180601549	0.8144996848108794	0.6536971755218616	T	T	T
0.2461875152348155	0.2797292478467618	0.6318501150845002	T	T	T
0.2479586691314025	0.6118247658111321	0.6519159749075053	T	T	T
0.7583037580063694	0.1468671073062514	0.6372614873180812	T	T	T
0.3531197480415631	0.7847517516352297	0.6533310482245726	T	T	T
0.8609301113408090	0.9874401223193693	0.6521814539174143	T	T	T
0.7578117589210600	0.4812063719737997	0.6389841645882652	T	T	T
0.8630084615806918	0.3193173056370037	0.6318145890117459	T	T	T
0.2731573123522257	0.1834744619132617	0.6310428667499981	T	T	T
0.8340772781788365	0.0832931399176173	0.6431319967007755	T	T	T
0.7044577212099973	0.0026031821155958	0.6365312155929139	T	T	T
0.4032837674771111	0.2640114608720927	0.6361479289183783	T	T	T
0.3517193869140280	0.1185160686035522	0.6378668701099061	T	T	T
0.2468993315637625	0.9459982629875190	0.6424245274962062	T	T	T
0.8356377810885153	0.7501332548695011	0.6447421614358743	T	T	T
0.2739685516866021	0.8497918665309565	0.6453669731591648	T	T	T
0.8626734349961154	0.6538329930335562	0.6429735444215771	T	T	T
0.7052901169626465	0.6692846685911079	0.6447493863961427	T	T	T
0.4045367933613861	0.5966983249078974	0.6368296411875541	T	T	T
0.7061593815554911	0.3354780607733086	0.6358034042651808	T	T	T
0.8362103191466033	0.4157491325333426	0.6306679046923233	T	T	T
0.4043237902191727	0.9306404626515359	0.6455788327708714	T	T	T
0.6652367562047496	0.2051828181635345	0.6395690697885016	T	T	T
0.6623205201423611	0.8716069274155926	0.6413635183206056	T	T	T
0.6198323810771892	0.6634629000114861	0.6464031872270883	T	T	T
0.5480433330478054	0.6967619907304023	0.6373945147595009	T	T	T
0.4867625443157083	0.6028749138434610	0.6388482645832104	T	T	T
0.4892637061332985	0.9359794938117674	0.6464395341965437	T	T	T
0.5494561955521930	0.0281120083910201	0.6421864227087341	T	T	T
0.6222088749479097	0.9963069502894091	0.6388311189090872	T	T	T
0.4465961837113277	0.7276882213421461	0.6414561351078969	T	T	T
0.4453955839163484	0.0611560928044337	0.6428262856082593	T	T	T
0.4440623664864264	0.3942374372410317	0.6396302889888105	T	T	T
0.5597033085517114	0.5713302030746068	0.6420822008703709	T	T	T
0.5606803071649745	0.2375869366793132	0.6359645598312631	T	T	T
0.6641627913204976	0.5387078779326657	0.6425753922493385	T	T	T
0.6216219680041030	0.3301516477161536	0.6377949817727916	T	T	T
0.5489408003706127	0.3622441210197313	0.6359036410469416	T	T	T
0.4879981299873706	0.2696937729646016	0.6377504570960832	T	T	T
0.5608909557427386	0.9024658342483666	0.6373772883548656	T	T	T
0.5559288697831921	0.1344135717660790	0.6522878625685613	T	T	T
0.5544398299821842	0.7995979592526895	0.6246773126912988	T	T	T
0.5534893601365097	0.4652307824525552	0.6521149843866019	T	T	T
0.5500979598713975	0.4578616137557142	0.7040888938990938	T	T	T
0.5593481449349395	0.1417812365177208	0.7042632146801439	T	T	T