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Electronic Supporting Information

Modulating the Surface Defects of Titanium Oxides and Consequent Reactivity of Pt Catalysts

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S1. Experimental and Computational Section

1.1 The pre-treatment processes of TiO_2 supports

The preparation process of the different catalysts is presented in Figure S1. The TiO_2 support (rutile, 40 nm, 99.8% metals basis, Aladdin) of different surface states were prepared in specific atmosphere. Firstly, the commercial rutile TiO_2 was calcinated in Ar for 4 h and O_2 for 2 h at 600 °C to remove the contaminants, such as carbonate and moister. Then the prepared surface clean support was processed at elevated temperature (700 °C) in Ar for 1, 2 or 4 hours to generate reduced TiO_2 with different amount of surface vacancies[1] and the as-prepared TiO_2 support are denoted as *r*-TiO_2-1h, *r*-TiO_2-2h and *r*-TiO_2-4h, respectively. As for the hydroxylated TiO_2 or oxidized TiO_2 (denoted as *h*-TiO_2-xh or *o*-TiO_2-xh respectively, x indicates the preparation time of the corresponding *r*-TiO_2. If there is no specific indication in main text and SI, the pre-treatment time is 1 h for supports.) was prepared by letting Ar through water bubbler or O_2 to flow the *r*-TiO_2 at 130 °C or room temperature respectively for one hour. The prepared TiO_2 support were transferred into glove box without contacting with atmosphere, so the delicate surfaces can be preserved.

1.2 Preparation of catalysts

Pt/TiO_2 catalysts were synthesized by impregnation method. The loading of Pt is controlled at 0.1 wt%. The 200 μL platinum precursor solution (0.0514 g $Pt(acac)_2$ (98%, Pt > 48%, Energy Chemical Co. LTD) dissolved in 5 ml benzyl alcohol (99.8%, water free, Aladdin)) was added into the mixture of n-pentane (99.5%, 3ADry, with molecular sieves, water ≤ 50 ppm, 3A Chemicals) (30 ml) and TiO_2 (rutile, 40 nm, 99.8% metals basis, Aladdin) (1 g) in glove box. Then the mixture in the sealed flask was stirred for 36 h in ice-water bath for impregnation. After that, the solvent was removed by rotate-evaporation. The as-prepared catalysts were calcinated in air at 400 °C for 5 h.

1.3 Catalyst characterizations

The X-ray diffraction (XRD) patterns were acquired on an Empyrean diffractometer using Cu Kα (λ=1.6406Å) as the radiation source. The crystal size of different TiO_2 supports was calculated by X-ray broadening based on Scherrer equation: $d = 0.89\lambda / (B \cos\theta)$. Here, λ is the wavelength of the radiation source (0.15418 nm), B is the line broadening at half the maximum intensity, and θ is the diffraction angle. The visible Raman spectra were collected on a Renishaw inVia reflex system using the laser wavelength of 532nm. X-ray photoelectron spectroscopy (XPS) was conducted on a homemade system with a reaction cell and an analysis chamber equipped with Thermo Fisher ESCALAB 250Xi spectrometer. In XPS system, the support can be pre-treated in the reaction cell and then transferred to the analysis chamber without exposing to air. The charge effect of sample was mitigated with an electron flooding gun. The binding energies were calibrated using the C 1s peak at 284.5 eV as a reference.

High-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) images were collected on a Titan Cubed Themis G2 300 (FEI) aberration-corrected scanning transmission electron microscope (AC-STEM) at 200 kV, capable of sub-angstrom resolution. The *in situ* diffuse reflection infrared Fourier transform spectroscopy (DRIFTS) analysis was performed on Thermo Fisher Nicolet IS50 spectrometer.

The H_2-O_2 titration and CO chemisorption were tested on a Micromeritics AutoChem II 2920. It can be presumed that the adsorption stoichiometry factors of Pt/H_2 and Pt/CO are equal to 2/3 and 1/1 respectively. The platinum dispersion is calculated by the following equation:

$$\text{Dispersion (\%)} = 100 \times V_{H2} \times 2/3 \times M_{Pt} / (W_{Pt} \times 22414)$$

$$\text{Dispersion (\%)} = 100 \times V_{CO} \times M_{Pt} / (W_{Pt} \times 22414)$$

where V_{H2} and V_{CO} are the volume of adsorbed H_2 and CO (mL), M_{Pt} is the atomic weight of Pt (g mol^{-1}), and W_{Pt} is the nominal weight of Pt supported on the sample (g).

1.4 Reactivity Tests

CO oxidation (COOX) was performed in a fixed bed reactor at atmospheric pressure. Before the reaction, the as-prepared catalysts were reduced in 10% H_2/Ar at 200 °C for 30 min. The composition of the reaction gas was 1% CO, 20% O_2 and balance He and the gas hour space velocity (GHSV) is 18000 ml/(gcat.·h). The temperature ramp rate was 0.5 °C/min. As for the kinetic measurements, the CO conversion was limited below 15%. A gas chromatography (GC7900, Techcomp) equipped with TCD and TDX-01 column was applied to analyze the gas composition online. The CO conversion was calculated from the equation: Con (%) = 100 × ($[F_{CO}]_{inlet}$ - $[F_{CO}]_{outlet}$) / $[F_{CO}]_{inlet}$.

Turnover frequency (TOF) was calculated as moles of CO_2 formed per mole of exposed Pt per second:

$TOF_a = R_{CO2} / D_{Pt}$

$TOF_b = R_{CO2} / N_{Pt}$

where R_{CO2} is the specific activity of CO_2 formation (s^{-1}), D_{Pt} is the dispersion of Pt and N_{Pt} is the atomic ratio of Pt located at the interface of Pt nanoparticles and supports.

The reaction order of CO oxidation was tested at 100 °C by varying the relative pressure of CO and O_2. The CO conversion was kept less than 15% and mass and heat transfer limitation were eliminated.

1.5 Computational details

The first-principles density functional theory (DFT) calculations were performed the plane wave-based Vienna ab initio simulation package (VASP)[2]. The generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE)[3] functional was used to describe the exchange-correlation effects. To circumvent the well-known self-interaction error, which underestimates the band gap of semiconductors in DFT, we adopted GGA+U[4] approach with a U value of 4.0 eV[5] to better describe the electronic interaction of TiO_2. The TiO_2 support was modeled as a periodically repeating three-layer of 5×4 unit cell of rutile TiO_2(110) surface. A vacuum layer of ~15 Å thick was added in the slab cell along the direction perpendicular to the surface to minimize periodic interactions. The Brillouin zone was integrated using the Monkhorst–Pack sets of 2×2×1 k-points mesh for TiO_2 surface optimization with bottom layer fixed to its bulk structure. For Pt cluster and Pt/TiO_2 optimization, given the larger size of the adopted supercells, the sampling of the reciprocal space is reduced to the Γ-point only. To quantify the charge transfer between Pt clusters and different supports, Bader analysis developed by Henkelman *et al*. was applied in our calculation.[6]

To describe the low concentration of surface oxygen vacancies, hydroxyls and oxygen adatoms of titania in experiment, we construct the three kinds of TiO_2(110) supports as follows[7]: for *r*-TiO_2, one bridge oxygen was artificially removed to create a surface oxygen vacancy; for *h*-TiO_2, two bridge hydroxyls were introduced to the surface by adding two hydrogen atoms to bridge oxygens; for *o*-TiO_2, an oxygen adatom was placed onto one on-top site of Ti.

To simulate the 1-nm scale Pt clusters loaded on TiO_2, a pyramid-like Pt_{14} cluster[8] was constructed by cutting away the bottom of a Pt_{19} cluster, created by Wulff construction method[9]. The Pt_{19} and obtained Pt_{14} were both optimized by DFT calculation with all atoms relaxed. The most stable Pt/TiO_2 configuration (with lowest total energy calculated by DFT) was applied as respective catalytic surface for further adsorption and reaction calculation.

In our calculation, the first-hand ΔE of the desorption of CO_2 was done without considering the effect of entropy contribution in the desorption process. To better describe the reaction, we converted DFT calculated energy to free energy. The temperature for free energy calculation is 400 K, at which the conversion of CO reached 100% for all the three catalysts. At the same time, the pressure of CO_2 in outlet gas is same with that of CO in inlet gas, which equals to 0.01 bar. The calculation is based on $\Delta G = \Delta H - T\Delta S$, where ΔH is the energy change from DFT

calculation, and $S = S^0 - R\ln(P/P^0)$, where $P^0 = 1$ bar, S^0 is adapted from the database of NIST (https://webbook.nist.gov/cgi/cbook.cgi?ID=C124389&Units=SI&Mask=1#Thermo-Gas). And the entropy of adsorbate was calculated according the Campbell's method[10] with the following equation $S_{ads} = 0.7S_{gas} – 3.3R$, where S_{ads} is the entropy of adsorbate; S_{gas} is the entropy of the corresponding gas-phase species and R is the ideal gas constant. In this way, the temperature and pressure variables are considered in the reaction pathway, which is especially suitable to describe the CO_2 desorption process.

S2. Supplementary Figures and Tables

2.1 Supplementary figures

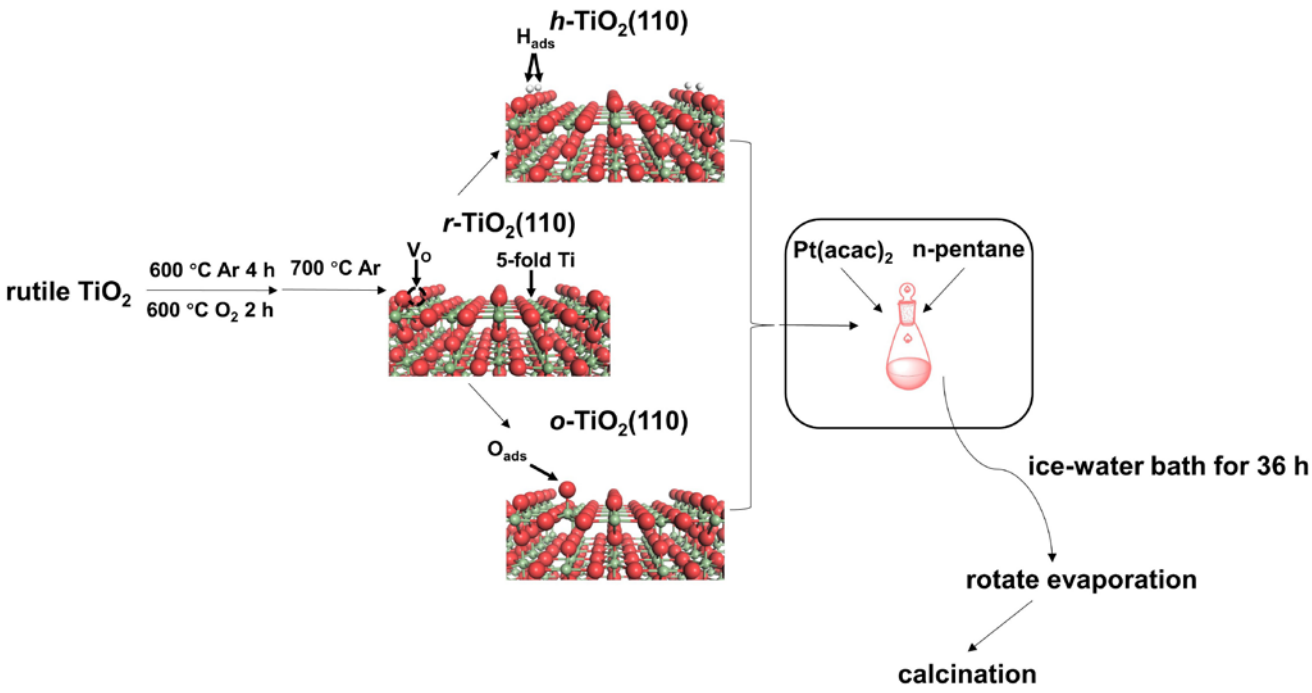

Figure S1. Scheme of preparation process for Pt/TiO_2 catalysts.

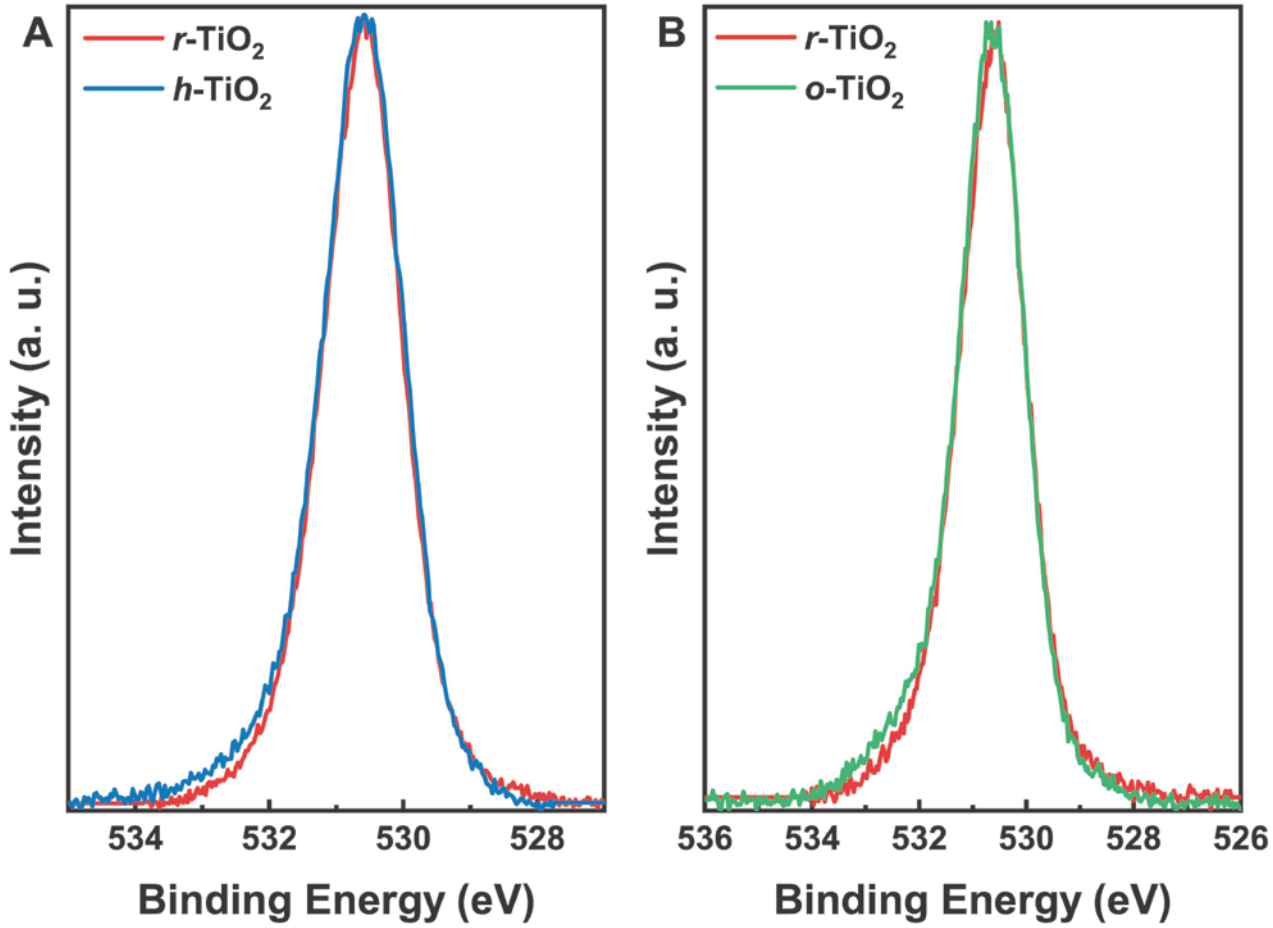

Figure S2. XPS O1s of TiO_2 supports. (A) overlapped normalization O1s spectra of reduced and hydroxylated TiO_2. (B) overlapped normalization O1s spectra of reduced and oxidized TiO_2.

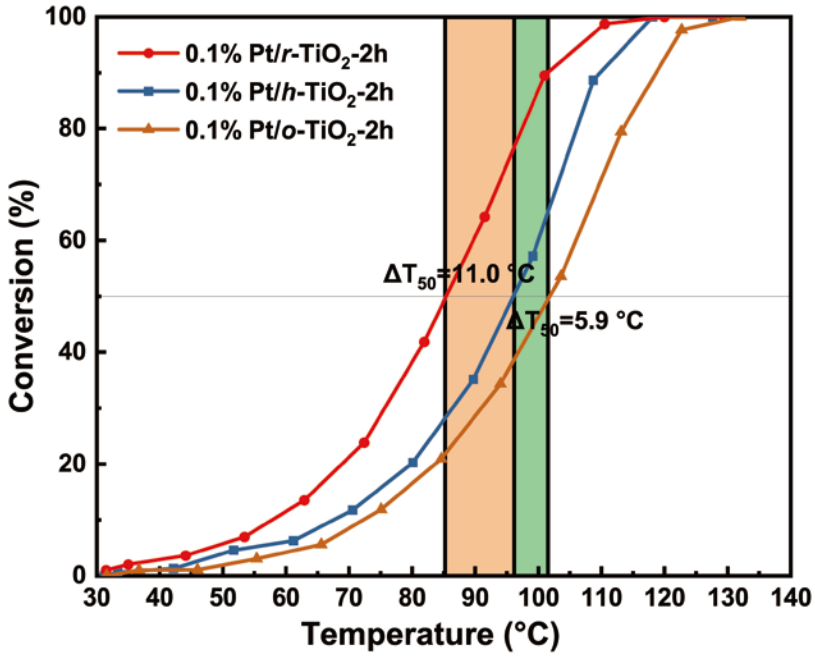

Figure S3. Light-off curves of CO conversion. TiO_2 supports were pre-treated for 2 h. The CO oxidation was conducted with a gas composition of 1% CO, 20% O_2 and He balanced, keeping GHSV at 18000 ml·gcat.$^{-1}$·h^{-1}.

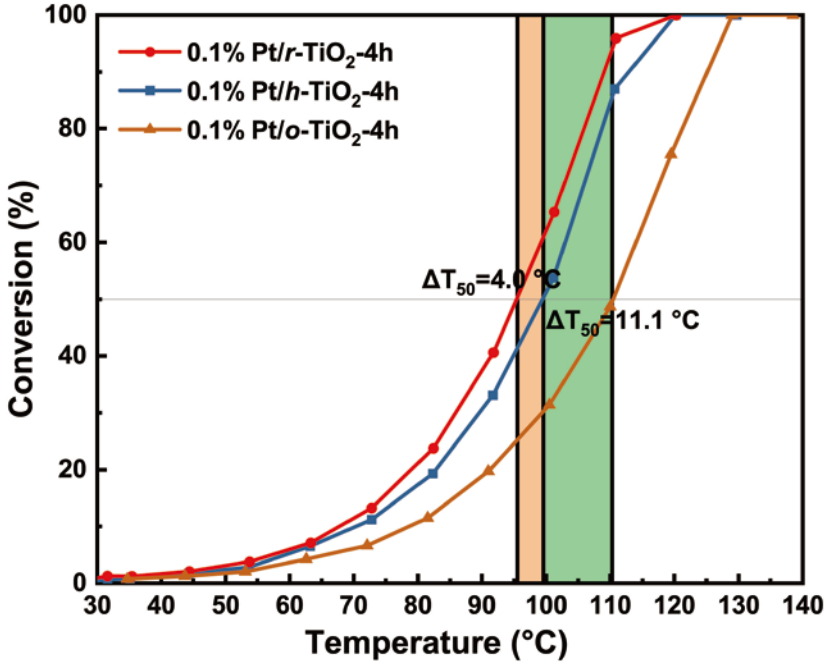

Figure S4. Light-off curves of CO conversion. TiO_2 supports were pre-treated for 4 h. The CO oxidation was conducted with a gas composition of 1% CO, 20% O_2 and He balanced, keeping GHSV at 18000 ml·gcat.$^{-1}$·h^{-1}.

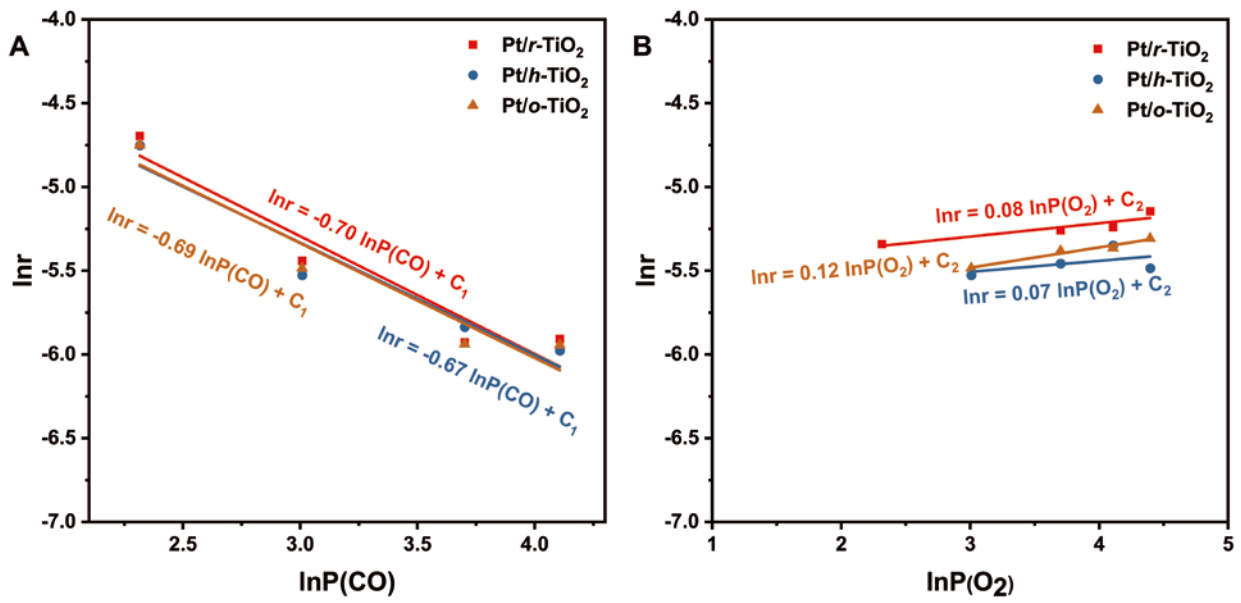

Figure S5. Reaction order of COOX on different Pt/TiO_2 catalysts at 100 °C. (A) reaction order of CO; (B) reaction order of O_2.

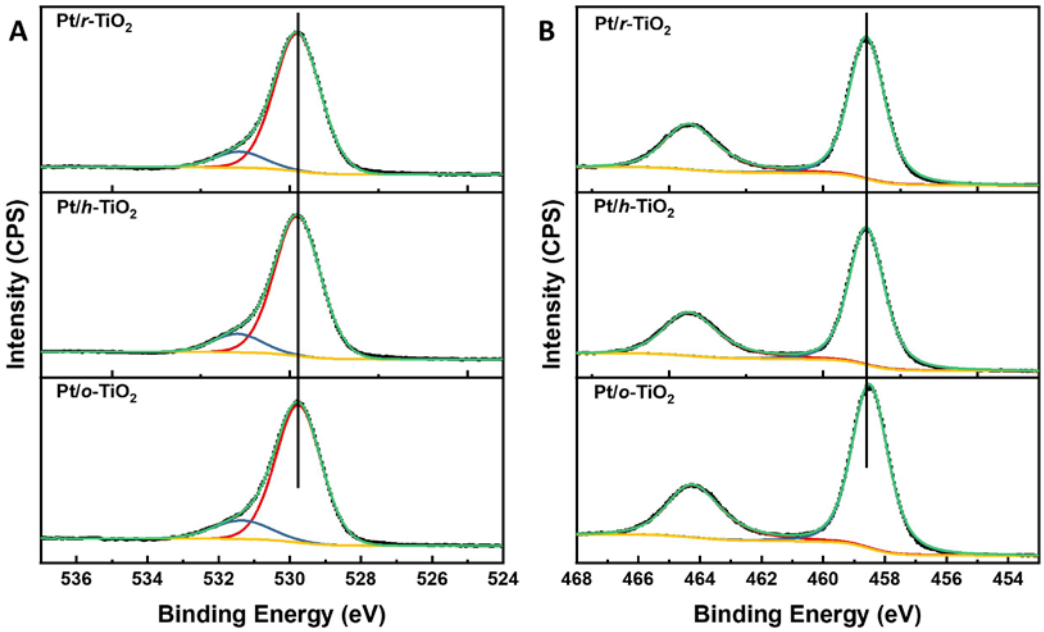

Figure S6. XPS O1s and Ti2p of different catalysts. (A) spectra of O1s; (B) spectra of Ti2p.

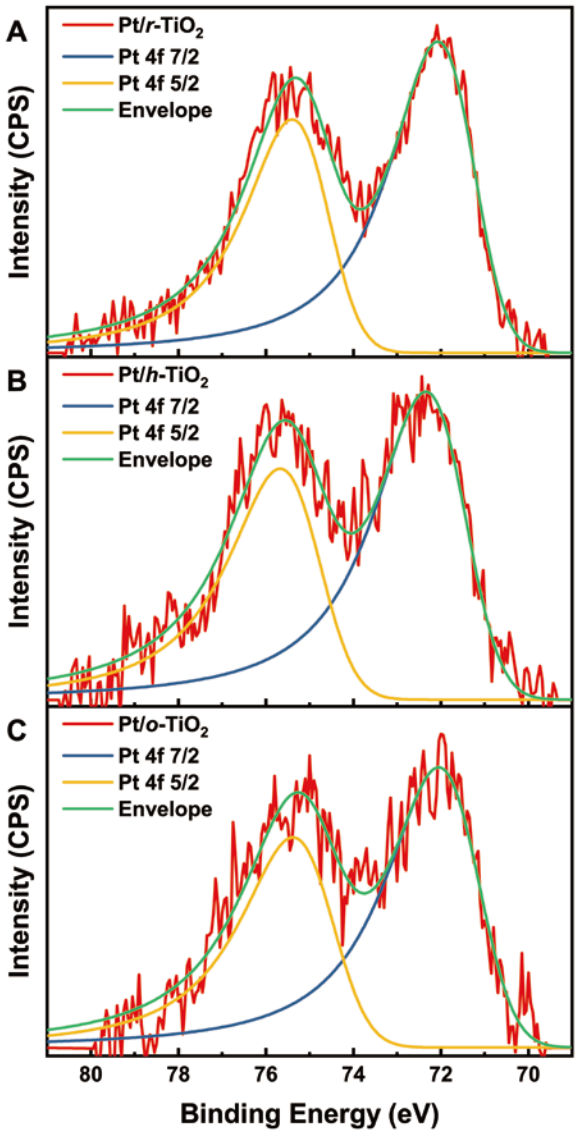

Figure S7. XPS Pt4f of different catalysts. (A) spectrum of catalyst Pt/*r*-TiO_2; (B) spectrum of catalyst Pt/*h*-TiO_2; (C) spectrum of catalyst Pt/*o*-TiO_2.

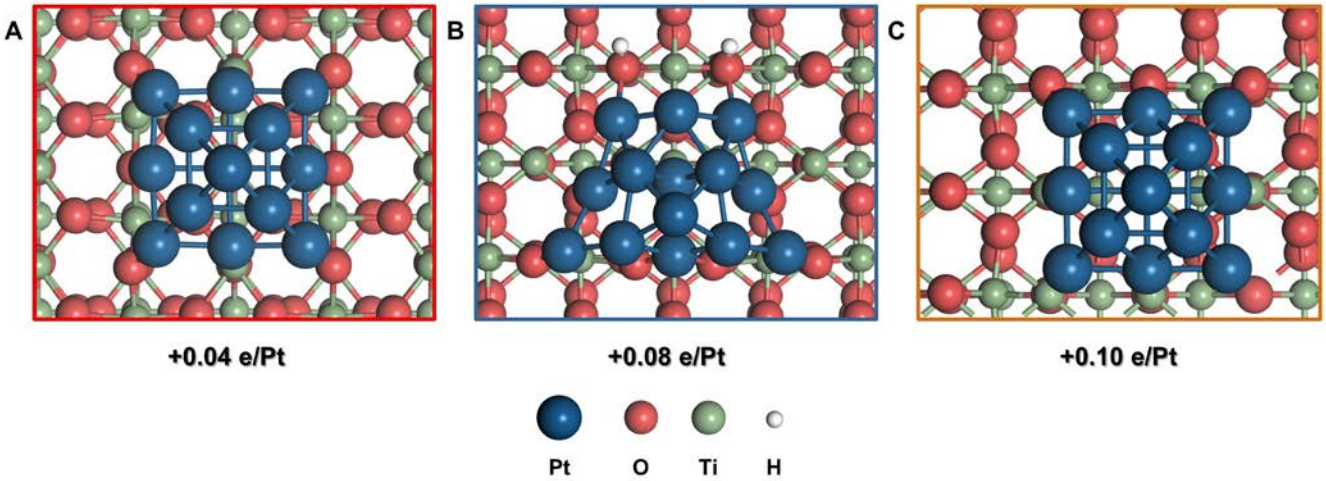

Figure S8. Average Bader charge analysis of Pt on different supports. (A) Pt/*r*-TiO_2; (B) Pt/*h*-TiO_2; (C) Pt/*o*-TiO_2.

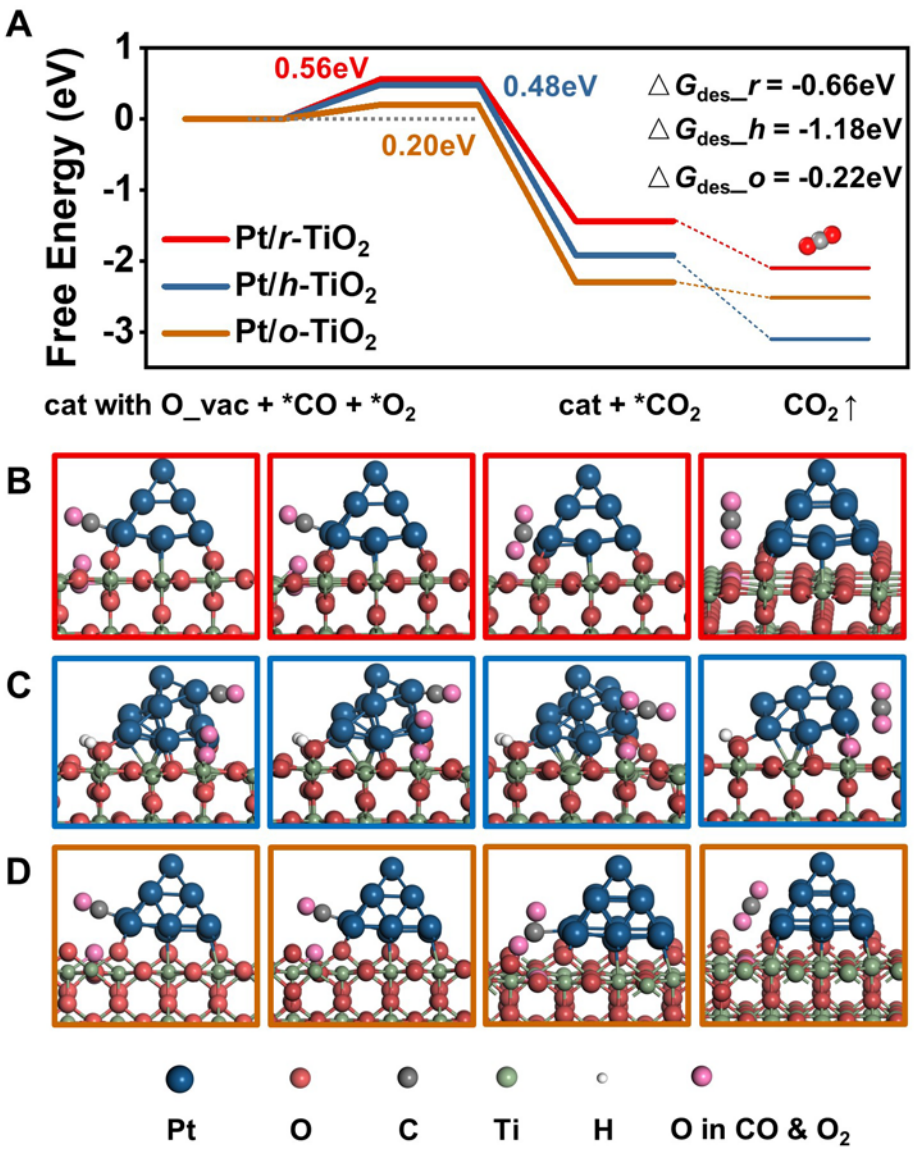

Figure S9. Calculated CO oxidation over Pt/TiO_2 catalysts with oxygen vacancies. (A) Free Energy barriers of CO oxidation. (B, C, D) Models from left to right represent the initial state (IS), transition state (TS), final state (FS) and CO_2 desorption of CO oxidation on Pt/*r*-TiO_2, Pt/*h*-TiO_2 and Pt/*o*-TiO_2, respectively.

2.2 Supplementary tables

Table S1. Crystal size of the different rutile TiO_2

Sample	Crystal size (nm)[a]
original TiO_2	28.1
r-TiO_2	31.4
h-TiO_2	34.4
o-TiO_2	33.5

[a]: The crystal size of different sample is derived from XRD by Scherrer equation

Table S2. Raman peak position and full width at half maximum (FWHM) of TiO_2 supports.

	original TiO_2		*r*-TiO_2		*h*-TiO_2		*o*-TiO_2	
	Peak position	FWHM	Peak position	FWHM	Peak position	FWHM	Peak position	FWHM
B_{1g}	184.5	3.0	184.7	5.2	185.7	3.1	184.6	4.3
Multi-photon process	265.8	64.8	267.6	63.9	268.1	59.1	266.7	64.6
E_g	459.2	35.1	459.3	35.5	459.3	36.9	459.0	36.9
A_{1g}	614.6	37.7	615.0	38.3	616.1	42.7	614.7	38.5

Table S3. Turn over frequency (TOF) of the different catalysts.

Sample	Dispersion[a]	$TOF_a \times 100(s^{-1})$[b]	$TOF_b \times 100(s^{-1})$[c]
Pt/*r*-TiO_2	118%	12.2	106.6
Pt/*h*-TiO_2	83%	6.2	75.9
Pt/*o*-TiO_2	62%	0.9	14.3

[a]: The dispersion is tested by H_2-O_2 titration and it is normalized while calculating TOF
[b]: The TOF_a is calculated based on the dispersion of metal nanoparticle
[c]: The TOF_b is calculated based on the length of perimeter between Pt nanoparticles and TiO_2

Table S4. XPS binding energy of $Pt4f_{7/2}$ peak and area ratio of Pt4f/Ti2p over the different catalysts.

	Pt/*r*-TiO_2	Pt/*h*-TiO_2	Pt/*o*-TiO_2
Binding energy	72.1 eV	72.3 eV	72.0 eV
Pt4f/Ti2p	0.013	0.009	0.007

Reference

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Coordinates

R_clean
Ti O Pt
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9.6705205423349163	6.7167973427417964	10.6410428258523524	T	T	T
11.2625541090915409	11.1751892135173385	2.8932940784072798	F	F	F
11.2870790814367226	7.9277868102395130	6.1163592644330178	T	T	T
11.2820679976491309	11.1009296976095033	9.4525510704417979	T	T	T
11.2625541090915409	8.6074080842651988	2.8932940784072798	F	F	F
11.2870911716552413	11.8546302706155089	6.1164826845268658	T	T	T
11.2816386122809522	8.6817036272201982	9.4504101115817747	T	T	T
12.8714904103903649	0.0000000000000001	1.6094667921785901	F	F	F
12.8825669558338785	3.2970235978810183	4.8069562297867447	T	T	T
12.9200219845386837	13.1150047349398555	8.1086474709353613	T	T	T
12.8714904103903649	0.0000000000000002	4.1771213646357834	F	F	F
12.9104558175915738	3.2973493723278886	7.3192627162265032	T	T	T
12.9043972744918474	13.0353629013528600	10.5710286160240798	T	T	T
14.4804267116891889	4.5809901142564922	2.8932940784072798	F	F	F
14.5221723014061688	1.3042378363381484	6.1151395095443650	T	T	T
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14.4804267116891889	2.0132089850043537	2.8932940784072798	F	F	F
14.5217646869004984	5.2902404715270368	6.1147341778730899	T	T	T
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12.9027429263849047	6.7482835664884417	10.5699104956645691	T	T	T
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14.2096536944073613	1.9128623101514488	14.2980102093533734	T	T	T
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12.8865930080152928	3.2992740508001415	16.0888143005336062	T	T	T
15.4308209353008774	5.7998597131320011	12.3102840259008648	T	T	T
15.4311043091156233	0.7996556646905321	12.3124104209145155	T	T	T

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*CO+O_bulk=*CO2
R_IS
Ti Pt  O  C
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16.1999999999999993    0.0000000000000000    0.0000000000000000
0.0000000000000008   13.1883981985216909    0.0000000000000000
0.0000000000000015    0.0000000000000015   25.7900218205815115
Ti   Pt   O    C
60    14   120     1
Selective dynamics
Direct
0.0000000000000000  0.2500000000000000  0.1121865699999987   F   F   F
  0.9979751599715807  0.9999566126054863  0.2364827716208705   T   T   T
  0.9973770012773223  0.2498887742551218  0.3565826297100866   T   T   T
  0.0993170559999967  0.0000000000000000  0.1121865699999987   F   F   F
  0.1030299102406444  0.2496844925292287  0.2372609935191415   T   T   T
  0.0892497928608610  0.9997648612901787  0.3675825133162814   T   T   T
  0.1986341109999969  0.2500000000000000  0.1121865699999987   F   F   F
  0.1963037823447786  0.9997408116732340  0.2374380022064250   T   T   T
  0.1976729696219894  0.2495266204771917  0.3675270354642631   T   T   T
  0.2979511670000008  0.0000000000000000  0.1121865699999987   F   F   F
  0.2984193941034535  0.2495431801552123  0.2386970080404822   T   T   T
  0.2938759122117029  0.0006882084170256  0.3629882354885609   T   T   T
  0.0000000000000000  0.7500000000000000  0.1121865699999987   F   F   F
  0.9977167814461877  0.4998626070458070  0.2363053419557999   T   T   T
  0.9962069246795285  0.7503094204399496  0.3571477923891788   T   T   T
  0.0993170559999967  0.5000000000000000  0.1121865699999987   F   F   F
  0.0974701109291258  0.7500399490123034  0.2352221337781300   T   T   T
  0.0856591963403035  0.5006220550775620  0.3681305709706273   T   T   T
  0.1986341109999969  0.7500000000000000  0.1121865699999987   F   F   F
  0.1958872294257033  0.4999859270874364  0.2358253833456535   T   T   T
  0.1972438188654802  0.7501700926566077  0.3579138805925393   T   T   T
  0.2979511670000008  0.5000000000000000  0.1121865699999987   F   F   F
  0.2974126460804860  0.7504361280656024  0.2348987275508393   T   T   T
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  0.3975613819237857  0.2531859393250731  0.3631261150716825   T   T   T
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  0.5983380237577774  0.9997607000488054  0.2375216743928002   T   T   T
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0.7994870912226436	0.7499861174577807	0.1855474643116273	T	T	T
0.7998737209922215	0.4999783510964020	0.3150585981225329	T	T	T
0.7945364449999985	0.5000000000000000	0.1619665699999970	F	F	F
0.8023978012894428	0.7498939225060286	0.2857608740151255	T	T	T
0.8003017318437906	0.5012385391684264	0.4130440224913685	T	T	T
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0.8971028311251833	0.5982982489851864	0.2364006810248341	T	T	T
0.8975375577273783	0.8432637801703259	0.3690358840621356	T	T	T
0.8938535010000024	0.6526500000000013	0.1121865699999987	F	F	F
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0.8975750911850654	0.6571864839495977	0.3689941513326278	T	T	T
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H_IS
Ti O Pt H O C
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16.1999999999999993 0.0000000000000000 0.0000000000000000
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Ti O Pt H O C
60 120 14 2 1 1
Selective dynamics
Direct
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0.0950883927365886	0.3450301501062870	0.3682143406047070	T	T	T
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0.0965028381967011	0.1582187188015491	0.3685429290554719	T	T	T
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0.1986341112714598	0.0000000000000000	0.1619665696173342	F	F	F
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0.1945654477128747	0.0033253346915822	0.4142359061477416	T	T	T
0.2979511669071826	0.3473499999999987	0.1121865696173359	F	F	F
0.2972473347995641	0.1007996204346366	0.2377500986133008	T	T	T
0.2931908468235045	0.3509149732669076	0.3667212829789076	T	T	T
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0.2979096291968313	0.4010730769688320	0.2395895857393586	T	T	T
0.2930298808960341	0.1569478564885052	0.3729979687368660	T	T	T
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0.9961909785138203	0.5031829461833192	0.3158767222373382	T	T	T
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0.9967628160188028	0.7504061986294613	0.2846355256728074	T	T	T
0.9955754257966709	0.5002532132269387	0.4138257141312348	T	T	T
0.0993170556357299	0.8473499999999987	0.1121865696173359	F	F	F
0.0969307125387556	0.6013682453631720	0.2368261089375722	T	T	T
0.0942211213603748	0.8460327270857868	0.3690848477971618	T	T	T
0.0993170556357299	0.6526500000000013	0.1121865696173359	F	F	F
0.0975275046241717	0.8997109389841822	0.2381765528702157	T	T	T
0.0926092125433544	0.6590952669327753	0.3701531306295395	T	T	T
0.1986341112714598	0.5000000000000000	0.0624065696173304	F	F	F
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0.1912760027162588	0.5049871454200353	0.3152497458988006	T	T	T
0.1986341112714598	0.5000000000000000	0.1619665696173342	F	F	F
0.1916888896186174	0.7493174279325694	0.2865769818358798	T	T	T
0.1902266224405417	0.5000721929748380	0.4131791395234971	T	T	T
0.2979511669071826	0.8473499999999987	0.1121865696173359	F	F	F
0.2971812051255694	0.5948866854557211	0.2383793828642923	T	T	T
0.2879190812037239	0.8452634370632377	0.3691850249655680	T	T	T
0.2979511669071826	0.6526500000000013	0.1121865696173359	F	F	F
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0.2871989414198033	0.6571705115368546	0.3724320467687687	T	T	T
0.3972682225429125	0.0000000000000000	0.0624065696173304	F	F	F
0.3984617644513022	0.2503616227761971	0.1872391818640617	T	T	T
0.3903664509276799	0.0010847788359591	0.3156481699966715	T	T	T
0.3972682225429125	0.0000000000000000	0.1619665696173342	F	F	F
0.3964160762525855	0.2502444535513583	0.2873680546760148	T	T	T
0.4034566699509418	0.9843862339840694	0.4122665095214073	T	T	T
0.4965852781786424	0.3473499999999987	0.1121865696173359	F	F	F
0.4969427730457247	0.0998401315297539	0.2403247914967443	T	T	T
0.4967208954397340	0.3557427110818756	0.3627593366697334	T	T	T
0.4965852781786424	0.1526500000000013	0.1121865696173359	F	F	F

0.4967900169001883	0.4005230000995724	0.2395586047491347	T	T	T
0.4958724925794024	0.1631729251857542	0.3691854281997278	T	T	T
0.5959023338143723	0.0000000000000000	0.0624065696173304	F	F	F
0.5949441930716926	0.2502490222953894	0.1872607949090418	T	T	T
0.6028776105406554	0.0032399386723044	0.3180911489875958	T	T	T
0.5959023338143723	0.0000000000000000	0.1619665696173342	F	F	F
0.5969595209894153	0.2497243951454718	0.2873714695757318	T	T	T
0.5714658380570206	0.9890940643326809	0.4165066105428765	T	T	T
0.6952193894500951	0.3473499999999987	0.1121865696173359	F	F	F
0.6965033197811407	0.1001784728619244	0.2379771917516753	T	T	T
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0.7007858456086269	0.1561634644109317	0.3745210031554493	T	T	T
0.3972682225429125	0.5000000000000000	0.0624065696173304	F	F	F
0.4010063990658146	0.7509067876748349	0.1852609458795313	T	T	T
0.4001296677583284	0.5100371143613329	0.3170062106857430	T	T	T
0.3972682225429125	0.5000000000000000	0.1619665696173342	F	F	F
0.4025179297377220	0.7472150808016232	0.2847814726075019	T	T	T
0.3868221051091214	0.5029814630553365	0.4186776924305489	T	T	T
0.4965852781786424	0.8473499999999987	0.1121865696173359	F	F	F
0.4977192910558418	0.5979835514224838	0.2370142716162224	T	T	T
0.5029775964147187	0.8406295011751832	0.3628014970338134	T	T	T
0.4965852781786424	0.6526500000000013	0.1121865696173359	F	F	F
0.4979358675744566	0.9031244683829081	0.2400951618529674	T	T	T
0.5051840255051776	0.6536144358861948	0.3774369011085704	T	T	T
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0.5925625964998648	0.7509742663409039	0.1853416482402228	T	T	T
0.5961689353168773	0.5062520696025331	0.3167031252534116	T	T	T
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0.5933488464225771	0.7452870087987230	0.2859688379502134	T	T	T
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0.6952193894500951	0.8473499999999987	0.1121865696173359	F	F	F
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0.6984537828841322	0.8442036934689929	0.3687368282371996	T	T	T
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0.6964743522451694	0.9049516151520276	0.2389469819230977	T	T	T
0.7013227710221456	0.6578694079842200	0.3698563286886234	T	T	T
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0.8972544918926167	0.3449667726310645	0.3679861622822245	T	T	T
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0.8969782497883463	0.1573472668654004	0.3691792069939936	T	T	T
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0.8016110309073565	0.5045816025115671	0.3147594903494633	T	T	T
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0.4861765844143777	0.0085369886623884	0.4743111132246822	T	T	T
0.4915804325075397	0.2071109579632176	0.4479334671367836	T	T	T
0.5834877550542702	0.2253806557170935	0.5358711459108647	T	T	T
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0.6604878010899932	0.1812621080600373	0.4516255161977427	T	T	T
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0.3869878925643089	0.5613302356909330	0.4418862143891834	T	T	T
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0.1515985676440337	-0.0713374007239865	0.5757983277084807	T	T	T
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O_IS
Ti O C Pt
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0.0000000000000015 0.0000000000000015 25.7900218205815115
60 122 1 14
Selective dynamics
Cartesian
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0.7016513716369899	0.3443365951043930	0.3682727832555515	T	T	T
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0.7010391680921044	0.1560652363641842	0.3685770239498163	T	T	T
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0.7987138760349880	1.0000582728422398	0.3148489141809097	T	T	T
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0.7998805452332381	0.5000230993993958	0.3149316561525547	T	T	T
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0.8975841039582925	0.8434771258545363	0.3690405606825278	T	T	T
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0.8975161555277802	0.6572645337387738	0.3687845060661639	T	T	T
0.2026444464472923	0.6778562302552924	0.4614146358163243	T	T	T
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H_TS
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Ti O Pt H O C
60 120 14 2 1 1
Selective dynamics
Direct

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0.0895908817331512	0.5029797623215763	0.3695782717348809	T	T	T
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0.9924082923405184	0.0024252265982768	0.4133645273225413	T	T	T
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0.9956402154009717	0.5004058399345349	0.4138992798512460	T	T	T
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0.0915634427101025	0.8440655409426461	0.3688181475278549	T	T	T
0.0993170556357293	0.6526500000000010	0.1121865696173359	F	F	F
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0.3974461335518458	0.2500084076710533	0.1931665059327708	T	T	T
0.4011395382136791	0.9999452210552598	0.3212306744223919	T	T	T
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0.3960177883294873	0.2496328865345468	0.2905812655012845	T	T	T
0.4386206090343522	0.9700116389203232	0.4296914150998604	T	T	T
0.4965852781786406	0.3473499999999987	0.1121865696173359	F	F	F
0.4965739623161254	0.0988825416497040	0.2401764555664748	T	T	T
0.4975167027422362	0.3552456231073594	0.3636717763447799	T	T	T
0.4965852781786406	0.1526500000000013	0.1121865696173359	F	F	F

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0.6013395445177498	0.0033317592557796	0.3164333392375762	T	T	T
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0.7010523296799127	0.3505176028000138	0.3646559736765229	T	T	T
0.6952193894500951	0.1526500000000013	0.1121865696173359	F	F	F
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0.7006864710765843	0.1581030475748156	0.3740293754577541	T	T	T
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0.3995089458702185	0.5092087115795452	0.3177940258332644	T	T	T
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0.3867079688801600	0.4995517226994659	0.4206788365538932	T	T	T
0.4965852781786297	0.8473499999999983	0.1121865696173359	F	F	F
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0.5049570362360001	0.6531073423152347	0.3773929417468420	T	T	T
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0.5957602031949413	0.5067630109123763	0.3165852426475667	T	T	T
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0.6076502723792315	0.5007835926364813	0.4186122412855804	T	T	T
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0.7918759461558761	0.2482152327312303	0.2868812957929160	T	T	T
0.7977476553603093	0.9964512531639139	0.4157966512200456	T	T	T
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0.8981946711044964	0.3450398938965076	0.3671799515895195	T	T	T
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0.8967880066313451	0.1583170492375810	0.3678358113185023	T	T	T
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0.8027846698957829	0.7488411973335640	0.2857410879596367	T	T	T
0.8011841680663473	0.5007893691428239	0.4122164372544008	T	T	T
0.8938535007215536	0.8473499999999983	0.1121865696173359	F	F	F
0.8976047346645565	0.6006818750343944	0.2359695045405200	T	T	T
0.8968957386516417	0.8449179433912547	0.3681012538846539	T	T	T
0.8938535007215536	0.6526500000000010	0.1121865696173359	F	F	F
0.8961475992107609	0.8998212653011728	0.2371206874589641	T	T	T
0.8984212138542300	0.6585532619692186	0.3696016066611426	T	T	T
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0.3780142025244960	0.3629366127816596	0.4663806312922507	T	T	T

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0.3253403910718662	0.9788881820346949	0.4643365964513801	T	T	T
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0.7592354588393877	0.0488027629616225	0.4843109168643899	T	T	T
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0.6062724288934348	0.5633334859040978	0.4388384692557096	T	T	T
0.1547162306656875	0.9850202824548169	0.5110276509255387	T	T	T
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O_TS
Ti  O  C Pt
1.00000000000000
16.1999999999999993    0.0000000000000000    0.0000000000000000
0.0000000000000008   13.1883981985216998    0.0000000000000000
0.0000000000000015    0.0000000000000015   25.7900218205815008
Ti   O    C    Pt
60   122     1    14
Selective dynamics
Direct
-0.0000000000000000  0.2499999999999999  0.1121865696173359   F   F   F
  0.9992664209661140  0.9998060568007261  0.2362597934620470   T   T   T
  0.9985034476692481  0.2497745093017261  0.3567621730810531   T   T   T
  0.0993170556357293 -0.0000000000000000  0.1121865696173359   F   F   F
  0.0993649382455975  0.2500020338832090  0.2335244175116010   T   T   T
  0.1064776478466732  0.9991774238846206  0.3677311870138444   T   T   T
  0.1986341112714587  0.2499999999999999  0.1121865696173359   F   F   F
  0.1982210037119130  0.0000248331919477  0.2372030460005906   T   T   T
  0.1991048810345918  0.2496670371053169  0.3578131612974598   T   T   T
  0.2979511669071808 -0.0000000000000000  0.1121865696173359   F   F   F
  0.3034272671765481  0.2499571780367179  0.2389236027684237   T   T   T
  0.2972264643635203  0.0018267961285900  0.3697662620374505   T   T   T
 -0.0000000000000000  0.7500000000000000  0.1121865696173359   F   F   F
  0.9992852883194229  0.5001395857352271  0.2362661098072703   T   T   T
  0.9978119303111549  0.7497272173225671  0.3570289252730899   T   T   T
  0.0993170556357293  0.4999999999999998  0.1121865696173359   F   F   F
  0.0982327357998801  0.7499048467654901  0.2354413836583078   T   T   T
  0.1064904968188279  0.5000143866559202  0.3677782567262833   T   T   T
  0.1986341112714587  0.7500000000000000  0.1121865696173359   F   F   F
  0.1981950385578060  0.4997592904735012  0.2372143024734525   T   T   T
  0.1990956540378672  0.7497300202743322  0.3583431717960168   T   T   T
  0.2979511669071808  0.4999999999999998  0.1121865696173359   F   F   F
  0.2975255027720176  0.7498783022447606  0.2344273646139453   T   T   T
  0.2971302931598334  0.4972682008349797  0.3698260754670039   T   T   T
  0.3972682225429125  0.2499999999999999  0.1121865696173359   F   F   F
  0.3975743159568270 -0.0000414008947183  0.2373814026867180   T   T   T
  0.4011705610695370  0.2494809129754170  0.3769771843245589   T   T   T
  0.4965852781786406 -0.0000000000000000  0.1121865696173359   F   F   F
  0.4943545064521642  0.2499504334552898  0.2389103402068734   T   T   T
  0.4891230992080615 -0.0002938998289163  0.3670044774369646   T   T   T
  0.5959023338143705  0.2499999999999999  0.1121865696173359   F   F   F
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  0.5972166405148890  0.2494898179995073  0.3594206972313164   T   T   T
  0.6952193894500951 -0.0000000000000000  0.1121865696173359   F   F   F
  0.6965161050799961  0.2499515978756713  0.2366067262449823   T   T   T
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  0.3959704058250991  0.7494742795374778  0.3582075378351695   T   T   T
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0.9022390695404886	0.4997551958489280	0.3619570259774423	T	T	T
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0.5038701086312587	0.3463774564023412	0.3657446922183873	T	T	T
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Selective dynamics
Direct
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0.7946028362764529	0.2498558815388268	0.1863506910328167	T	T	T
0.8002392592002093	0.0038046956783858	0.3149843224546726	T	T	T
0.7945364449999985	0.0000000000000000	0.1619665699999970	F	F	F
0.7971151838336450	0.2506051226331217	0.2839301098025571	T	T	T
0.8032749719988943	0.0075456459279572	0.4132998481107867	T	T	T
0.8938535010000024	0.3473499999999987	0.1121865699999987	F	F	F
0.8966288169596535	0.1008820485719993	0.2361329585458193	T	T	T
0.8968662586232913	0.3450621297590545	0.3670242913548928	T	T	T
0.8938535010000024	0.1526500000000013	0.1121865699999987	F	F	F
0.8962256638033766	0.3999307946046363	0.2362748244282225	T	T	T
0.8990440825718516	0.1597146600533834	0.3673547790638493	T	T	T
0.7945364449999985	0.5000000000000000	0.0624065700000003	F	F	F

0.7940338256500705	0.7500582795506573	0.1862673804246962	T	T	T
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0.7973305633100467	0.7496357198126650	0.2837844387726688	T	T	T
0.7996639699400929	0.5027755525407208	0.4123066928977182	T	T	T
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0.8997941435760766	0.6580025874299681	0.3682968819312458	T	T	T
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H_FS
Ti O Pt H O C
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Ti O Pt H O C
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Selective dynamics
Direct
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0.0945843187976670	0.3445682697435371	0.3692414024124281	T	T	T
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0.1904987128336005	0.5009666685488355	0.4131460593491147	T	T	T
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0.3972682225429125	0.0000000000000000	0.0624065696173304	F	F	F
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0.4011960467639039	-0.0005998720634348	0.3211463553169029	T	T	T
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0.3860981384025942	0.5002885731392538	0.4204077345041910	T	T	T
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0.4967659797073626	0.5979237724045426	0.2370139284109784	T	T	T
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Ti O C Pt
60 122 1 14
Selective dynamics
Direct
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CO2_desorption_1
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Ti Pt O C
60 14 120 1
Selective dynamics
Direct
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CO2+O2+O_vac=CO2
R_IS
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16.1999999999999993 0.0000000000000000 0.0000000000000000
0.0000000000000008 13.1883981985216909 0.0000000000000000
0.0000000000000015 0.0000000000000015 25.7900218205815115
Ti Pt O C
60 14 121 1
Selective dynamics
Direct
0.0000000000000000 0.2500000000000000 0.1121865699999987 F F F
0.9987282384317825 0.0010431259238123 0.2363245476619502 T T T
0.9976723729749325 0.2508502285677587 0.3561599960790170 T T T
0.0993170559999967 0.0000000000000000 0.1121865699999987 F F F
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0.1982422430523699 0.2497092611436598 0.3660194733943241 T T T
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0.8965602551472913	0.4004540594146330	0.2363342107622583	T	T	T
0.8989051058898113	0.1595760278350757	0.3674053745321597	T	T	T
0.7945364449999985	0.5000000000000000	0.0624065700000003	F	F	F

0.7946694715831881	0.7504691808081508	0.1861358422200206	T	T	T
0.7991917981946447	0.5013697518118830	0.3149215974245087	T	T	T
0.7945364449999985	0.5000000000000000	0.1619665699999970	F	F	F
0.7972971276797243	0.7502930930053018	0.2836810409514351	T	T	T
0.8006885395776852	0.4995304415152972	0.4130925522417789	T	T	T
0.8938535010000024	0.8473499999999987	0.1121865699999987	F	F	F
0.8964668349668201	0.5994367123275003	0.2361705231850313	T	T	T
0.8997271041094544	0.8456946247076534	0.3680175438865994	T	T	T
0.8938535010000024	0.6526500000000013	0.1121865699999987	F	F	F
0.8965537076762037	0.9020897740987684	0.2365170488512071	T	T	T
0.8993407546259971	0.6574290670890067	0.3685322022165927	T	T	T
0.4599197340604845	0.6380258407277591	0.4042558508913436	T	T	T
0.5105728468978644	0.6527808819750700	0.3569154386980067	T	T	T
0.3884736441107709	0.6806119548494836	0.5173294123330381	T	T	T
0.3910599679597884	0.5974773796646435	0.5025437076765068	T	T	T

H_IS
Ti O Pt H O C
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16.1999999999999993 0.0000000000000000 0.0000000000000000
0.0000000000000008 13.1883981985216909 0.0000000000000000
0.0000000000000015 0.0000000000000015 25.7900218205815115
Ti O Pt H O C
60 119 14 2 3 1
Selective dynamics
Direct
0.0000000000000000 0.2500000000000000 0.1121865696173359 F F F
0.9805673934100664 0.0055728725806497 0.2329014349238656 T T T
0.0005564047101769 0.2485275921912930 0.3503647425104421 T T T
0.0993170556357299 0.0000000000000000 0.1121865696173359 F F F
0.0968344958776742 0.2510341049864301 0.2296455702897748 T T T
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0.1986341112714598 0.2500000000000000 0.1121865696173359 F F F
0.1757356608225513 -0.0021958384708084 0.2341543794618222 T T T
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0.2979511669071826 0.0000000000000000 0.1121865696173359 F F F
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0.2848668192273937 0.9923451367767867 0.3527755263594626 T T T
0.0000000000000000 0.7500000000000000 0.1121865696173359 F F F
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0.7945364450858250	0.7500000000000000	0.1121865696173359	F	F	F
0.7781235789605074	0.5049423388838679	0.2341954593513936	T	T	T
0.8089821677432828	0.7470951784325595	0.3509851339365114	T	T	T
0.8938535007215549	0.5000000000000000	0.1121865696173359	F	F	F
0.8965189395123125	0.7536039383484577	0.2295582862988573	T	T	T
0.9006437041445222	0.4974985492231119	0.3658331766875595	T	T	T
0.0000000000000000	0.0000000000000000	0.0624065696173304	F	F	F
0.9979984513426204	0.2491696150216776	0.1828061122488409	T	T	T
0.9944472875038669	-0.0005685107955525	0.3108625979276821	T	T	T
0.0000000000000000	0.0000000000000000	0.1619665696173342	F	F	F
0.9978567044040588	0.2488601216090764	0.2804095339081398	T	T	T
0.9914278924299372	-0.0020440550559682	0.4088538566566718	T	T	T
0.0993170556357299	0.3473499999999987	0.1121865696173359	F	F	F
0.0942139732042035	0.0981391070852424	0.2348084168099172	T	T	T
0.0888929902175151	0.3422901702382656	0.3641544800018955	T	T	T
0.0993170556357299	0.1526500000000013	0.1121865696173359	F	F	F
0.1001289370975936	0.3939043124473784	0.2338892734948972	T	T	T
0.0892893464254808	0.1532196022263342	0.3639310908724256	T	T	T
0.1986341112714598	0.0000000000000000	0.0624065696173304	F	F	F
0.1995322490677423	0.2462889225484275	0.1845238341980730	T	T	T
0.1927796372498432	0.9920954651373775	0.3093890886935804	T	T	T
0.1986341112714598	0.0000000000000000	0.1619665696173342	F	F	F
0.1930777402020333	0.2429734496634645	0.2826974396251130	T	T	T
0.2979511669071826	0.3473499999999987	0.1121865696173359	F	F	F
0.3052043957580394	0.1001265513350373	0.2400201530958161	T	T	T
0.2779008545614050	0.3441622299831763	0.3635369551429450	T	T	T
0.2979511669071826	0.1526500000000013	0.1121865696173359	F	F	F
0.2957564201464722	0.3966393136086631	0.2375465947782285	T	T	T
0.2737846876228987	0.1428978496120320	0.3677866635348580	T	T	T
0.0000000000000000	0.5000000000000000	0.0624065696173304	F	F	F
0.9981234454752693	0.7463472392040392	0.1840180718342905	T	T	T
0.9936665423155215	0.5001277827941712	0.3111640350446652	T	T	T
0.0000000000000000	0.5000000000000000	0.1619665696173342	F	F	F
0.9968782840917141	0.7452938855548942	0.2807250615960709	T	T	T
0.9909218425846933	0.5000409753688284	0.4095079751547144	T	T	T
0.0993170556357299	0.8473499999999987	0.1121865696173359	F	F	F
0.0963818514459177	0.5995691709020240	0.2346008235362966	T	T	T
0.0885527606883446	0.8411130661358101	0.3624391435736132	T	T	T
0.0993170556357299	0.6526500000000013	0.1121865696173359	F	F	F
0.0963790043898018	0.8955604045711726	0.2340599115003947	T	T	T
0.0912710463495274	0.6545305856782849	0.3641806561180476	T	T	T
0.1986341112714598	0.5000000000000000	0.0624065696173304	F	F	F
0.1980324901296690	0.7500850900442130	0.1848961916772392	T	T	T
0.1840856935306266	0.4966054470365333	0.3118618482668311	T	T	T
0.1986341112714598	0.5000000000000000	0.1619665696173342	F	F	F
0.1927993552626898	0.7503504300271839	0.2829294384800683	T	T	T
0.1751435048103443	0.4954943623707538	0.4116546060550551	T	T	T
0.2979511669071826	0.8473499999999987	0.1121865696173359	F	F	F
0.2932387679442256	0.5986397070072544	0.2368078268020451	T	T	T
0.2871968593725975	0.8314342907253255	0.3665224397839067	T	T	T
0.2979511669071826	0.6526500000000013	0.1121865696173359	F	F	F
0.3032399718670550	0.8954538039951773	0.2381277121391434	T	T	T
0.2781043198904617	0.6432126001891935	0.3632881983327576	T	T	T
0.3972682225429125	0.0000000000000000	0.0624065696173304	F	F	F
0.3978638764846064	0.2499831035537080	0.1861571362858351	T	T	T
0.3962121725211221	0.9890000735378766	0.3227631293234352	T	T	T
0.3972682225429125	0.0000000000000000	0.1619665696173342	F	F	F
0.3979046558955945	0.2533883210519053	0.2897474176855790	T	T	T
0.4553145316074432	0.9712335574893320	0.4254927194401090	T	T	T
0.4965852781786424	0.3473499999999987	0.1121865696173359	F	F	F
0.4947718269163425	0.1003206879715967	0.2390573233160477	T	T	T
0.5000338291974089	0.3625912539478672	0.3627531599102013	T	T	T
0.4965852781786424	0.1526500000000013	0.1121865696173359	F	F	F
0.4993408941634067	0.3977021951376584	0.2361985306909716	T	T	T

0.5002005210227278	0.1639529969454661	0.3650151117499905	T	T	T
0.5959023338143723	0.0000000000000000	0.0624065696173304	F	F	F
0.5980515729157569	0.2499259244276830	0.1847788322405715	T	T	T
0.5993402478870933	0.9911318990650498	0.3102905314774312	T	T	T
0.5959023338143723	0.0000000000000000	0.1619665696173342	F	F	F
0.5953327980816255	0.2519997948482848	0.2852976124651179	T	T	T
0.6030602467182026	0.9940018749470632	0.4038017487260656	T	T	T
0.6952193894500951	0.3473499999999987	0.1121865696173359	F	F	F
0.6955588737695126	0.1038839490862609	0.2374744899768237	T	T	T
0.6930939184997068	0.3678562132319484	0.3588787363073208	T	T	T
0.6952193894500951	0.1526500000000013	0.1121865696173359	F	F	F
0.6924815555017931	0.4041983787110874	0.2385949632700763	T	T	T
0.7068921881553480	0.1591584303610249	0.3588519513334268	T	T	T
0.3972682225429125	0.5000000000000000	0.0624065696173304	F	F	F
0.3963793906192685	0.7496722203576031	0.1849865538840481	T	T	T
0.4047122035616178	0.5045272682753046	0.3074319087377425	T	T	T
0.3972682225429125	0.5000000000000000	0.1619665696173342	F	F	F
0.3959127473436809	0.7412782500932735	0.2858595121024266	T	T	T
0.3652882222117564	0.4874517399049956	0.4145506422362253	T	T	T
0.4965852781786424	0.8473499999999987	0.1121865696173359	F	F	F
0.5010115645897929	0.6057052379486212	0.2327629218627075	T	T	T
0.5193921869875998	0.8269443006451931	0.3629349959825798	T	T	T
0.4965852781786424	0.6526500000000013	0.1121865696173359	F	F	F
0.4934892024584107	0.9010670051431318	0.2384633807714703	T	T	T
0.4564653179839445	0.6410989168023949	0.3815300297925791	T	T	T
0.5959023338143723	0.5000000000000000	0.0624065696173304	F	F	F
0.5947803087693634	0.7540481285956528	0.1845240265512579	T	T	T
0.5853837055273673	0.5224261333665927	0.3119617595913988	T	T	T
0.5959023338143723	0.5000000000000000	0.1619665696173342	F	F	F
0.6057719379257605	0.7523286725909381	0.2809671741854218	T	T	T
0.6064160868312370	0.5184757530662693	0.4129654506684363	T	T	T
0.6952193894500951	0.8473499999999987	0.1121865696173359	F	F	F
0.6978191686963702	0.6051805167162168	0.2342811594212703	T	T	T
0.7164868029563122	0.8546790390435715	0.3613287962901248	T	T	T
0.6952193894500951	0.6526500000000013	0.1121865696173359	F	F	F
0.7015017803199094	0.8987245899071182	0.2351416423290960	T	T	T
0.7043964736253195	0.6666252776004514	0.3656843003767078	T	T	T
0.7945364450858250	0.0000000000000000	0.0624065696173304	F	F	F
0.7935392768888579	0.2520189623090104	0.1845306811706509	T	T	T
0.8041606106927603	0.0036662504680730	0.3113764243665918	T	T	T
0.7945364450858250	0.0000000000000000	0.1619665696173342	F	F	F
0.7982018313483107	0.2530471734931016	0.2834934314487538	T	T	T
0.8104990083315240	-0.0005923577704483	0.4105138669991224	T	T	T
0.8938535007215549	0.3473499999999987	0.1121865696173359	F	F	F
0.8951875533807306	0.1029421989233032	0.2336985890915649	T	T	T
0.8983094955918541	0.3462728576849411	0.3638700682852345	T	T	T
0.8938535007215549	0.1526500000000013	0.1121865696173359	F	F	F
0.8981962914932901	0.3965811664099381	0.2342684700163602	T	T	T
0.9007754077212732	0.1571372566135428	0.3632945430857143	T	T	T
0.7945364450858250	0.5000000000000000	0.0624065696173304	F	F	F
0.7965319062207801	0.7513287674481465	0.1847091363546987	T	T	T
0.8006317695651824	0.5090000800433602	0.3100112609091523	T	T	T
0.7945364450858250	0.5000000000000000	0.1619665696173342	F	F	F
0.8035538608311262	0.7487085920038659	0.2813985679892155	T	T	T
0.8025709902140004	0.5061880956417949	0.4076999801574627	T	T	T
0.8938535007215549	0.8473499999999987	0.1121865696173359	F	F	F
0.8955874713311198	0.6007209696913032	0.2328328288779293	T	T	T
0.8994929808866368	0.8430177276369020	0.3623541659482024	T	T	T
0.8938535007215549	0.6526500000000013	0.1121865696173359	F	F	F
0.9014449578032903	0.8969574496669649	0.2337194308599159	T	T	T
0.9003333019340484	0.6564052075854073	0.3645770700292894	T	T	T
0.3346683370905004	0.1747774467167510	0.4410041000481771	T	T	T
0.3656175500332278	0.3595744582736595	0.4618682470807228	T	T	T
0.4134745391947159	0.2112581101921965	0.5243235527997856	T	T	T

0.5113073674880614	0.3569532677660988	0.5006701988721440	T	T	T
0.3360864615550307	0.9822210316792510	0.4450712876190539	T	T	T
0.4753670570201727	0.0357593038136148	0.5620082835797415	T	T	T
0.5495699565909969	0.0061113747747609	0.4748479899059321	T	T	T
0.5260820704506388	0.1969900707174037	0.4428333525290175	T	T	T
0.6340774687146091	0.2441888538608977	0.5219496737459582	T	T	T
0.6460544497303792	0.0617663325773798	0.5484801402082230	T	T	T
0.7082673315365461	0.2032276812677505	0.4381779004542411	T	T	T
0.5301495863069472	0.2043721410876075	0.5961024843317579	T	T	T
0.6459808099348420	0.3818284698083317	0.4481390620112677	T	T	T
0.7406204638277949	0.0249725362293424	0.4739505669292998	T	T	T
0.3765731213624578	0.5502971355137565	0.4333578749196551	T	T	T
0.6079049084979885	0.5738381863880614	0.4380074297949096	T	T	T
0.2159206236216188	0.9744037758207789	0.4562940139651280	T	T	T
0.1856526868210253	0.9856271856804204	0.4039570695041462	T	T	T
0.3729473357542474	0.8460232232832190	0.5569787244626341	T	T	T
0.4126621429528993	0.9198436587013156	0.5565088573939934	T	T	T

O_IS
Ti O Pt O C
1.00000000000000
16.1999999999999993 0.0000000000000000 0.0000000000000000
0.0000000000000008 13.1883981985216909 0.0000000000000000
0.0000000000000015 0.0000000000000015 25.7900218205815115
Ti O Pt O C
60 119 14 3 1
Selective dynamics
Direct

0.0000000000000000	0.2500000000000000	0.1121865696173359	F	F	F
0.9986181905999527	0.0000570843446532	0.2363177547892416	T	T	T
0.9972209645153097	0.2499874060459332	0.3645609470012224	T	T	T
0.0993170556357299	0.0000000000000000	0.1121865696173359	F	F	F
0.0942462881379184	0.2502753664669732	0.2362499261950802	T	T	T
0.1049843105601800	0.9995163713856191	0.3674779119584096	T	T	T
0.1986341112714598	0.2500000000000000	0.1121865696173359	F	F	F
0.1971430652452309	0.0003089834351896	0.2372078097165751	T	T	T
0.1959121727267893	0.2517261476466363	0.3576454726594161	T	T	T
0.2979511669071826	0.0000000000000000	0.1121865696173359	F	F	F
0.2984253389010474	0.2501897846779650	0.2357846689988189	T	T	T
0.2953804669001376	0.0034854597247115	0.3698420237586692	T	T	T
0.0000000000000000	0.7500000000000000	0.1121865696173359	F	F	F
0.9986682367180505	0.5004795197668763	0.2363082480366392	T	T	T
0.9970512232022392	0.7514170358936224	0.3563965778186926	T	T	T
0.0993170556357299	0.5000000000000000	0.1121865696173359	F	F	F
0.0978854867739842	0.7502971725230075	0.2351337897529872	T	T	T
0.1051012169185133	0.5020681382017912	0.3673736716180533	T	T	T
0.1986341112714598	0.7500000000000000	0.1121865696173359	F	F	F
0.1972572178631525	0.5002449575774406	0.2371067853636050	T	T	T
0.1979040992780567	0.7500948047429354	0.3577922742977098	T	T	T
0.2979511669071826	0.5000000000000000	0.1121865696173359	F	F	F
0.2972880205587622	0.7502826448705801	0.2342385879719677	T	T	T
0.2957144565698506	0.4986868236716162	0.3694683043004228	T	T	T
0.3972682225429125	0.2500000000000000	0.1121865696173359	F	F	F
0.3969121732116201	0.9999450503731763	0.2374020845340155	T	T	T
0.3966787649956819	0.2472088469154157	0.3621947003578807	T	T	T
0.4965852781786424	0.0000000000000000	0.1121865696173359	F	F	F
0.4964134122766322	0.2495675961346744	0.2372737489694224	T	T	T
0.4884296871951749	0.0004328014361470	0.3669264494939721	T	T	T
0.5959023338143723	0.2500000000000000	0.1121865696173359	F	F	F
0.5957305588289334	0.9996007949344944	0.2372399690150536	T	T	T
0.5985907375862336	0.2437807177786557	0.3598401139892217	T	T	T
0.6952193894500951	0.0000000000000000	0.1121865696173359	F	F	F
0.6978814968413528	0.2501870112095123	0.2366654089819975	T	T	T
0.6926543799155601	0.9979981882440664	0.3632855852296524	T	T	T
0.3972682225429125	0.7500000000000000	0.1121865696173359	F	F	F
0.3971120536293898	0.5004736803262810	0.2375056458178013	T	T	T
0.3937089858114593	0.7542607937831675	0.3582257450739928	T	T	T
0.4965852781786424	0.5000000000000000	0.1121865696173359	F	F	F
0.4962533347128433	0.7504145624075715	0.2355382654312387	T	T	T
0.4884670490880683	0.5120314170887879	0.3683737486886777	T	T	T
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0.5953033942564334	0.5005347732341913	0.2372376957462037	T	T	T
0.5978273108702897	0.7534511618632844	0.3576460417145744	T	T	T
0.6952193894500951	0.5000000000000000	0.1121865696173359	F	F	F
0.6957566273231468	0.7501578646193849	0.2340908483011382	T	T	T
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0.7945364450858250	0.2500000000000000	0.1121865696173359	F	F	F
0.7965991482245605	0.0006504597272369	0.2371077675473677	T	T	T
0.7972270183805708	0.2524243810955057	0.3640968377608674	T	T	T
0.8938535007215549	0.0000000000000000	0.1121865696173359	F	F	F
0.8954323841341598	0.2503441206064090	0.2386732920497750	T	T	T
0.9006838748839063	0.9997414343009088	0.3614574021034254	T	T	T

0.7945364450858250	0.7500000000000000	0.1121865696173359	F	F	F
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0.7975623136606851	0.7489303453133158	0.3567910627092967	T	T	T
0.8938535007215549	0.5000000000000000	0.1121865696173359	F	F	F
0.8965470352522329	0.7501986759681508	0.2333506718535895	T	T	T
0.9006048525644568	0.5016905679620668	0.3612552381755297	T	T	T
0.0000000000000000	0.0000000000000000	0.0624065696173304	F	F	F
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0.9957463207368120	0.9978467519971305	0.3146343860882111	T	T	T
0.0000000000000000	0.0000000000000000	0.1619665696173342	F	F	F
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0.9978549830319130	0.9930784390373217	0.4124407987099420	T	T	T
0.0993170556357299	0.3473499999999987	0.1121865696173359	F	F	F
0.0970625258046684	0.1008440202740639	0.2378261383564406	T	T	T
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0.2900113344522929	0.3455621080893076	0.3691982935882746	T	T	T
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0.9978683034969460	0.5083992362766444	0.4121768468071303	T	T	T
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0.0969773999006379	0.8432749584458086	0.3667490943202370	T	T	T
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0.1977935133958884	0.5015523736498616	0.3152782127091756	T	T	T
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0.1963051182943399	0.5041633434109344	0.4123420317276743	T	T	T
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0.2972326578334927	0.5989601946577651	0.2375140270521527	T	T	T
0.2963414063539023	0.8448823084855003	0.3701302545378368	T	T	T
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0.2970184697391469	0.9016868794511060	0.2375132725654255	T	T	T
0.2968493849044876	0.6584431507236035	0.3699942416365301	T	T	T
0.3972682225429125	0.0000000000000000	0.0624065696173304	F	F	F
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0.3947560845697166	-0.0010956567527077	0.3153105877405010	T	T	T
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0.3962852089994847	0.0065535014637183	0.4118793363127496	T	T	T
0.4965852781786424	0.3473499999999987	0.1121865696173359	F	F	F
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0.4965852781786424	0.1526500000000013	0.1121865696173359	F	F	F
0.4971153514672551	0.4000503118078817	0.2388214868009993	T	T	T

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0.5996838356503303	0.9927123610545218	0.3152729418940623	T	T	T
0.5959023338143723	0.0000000000000000	0.1619665696173342	F	F	F
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0.5996880132818707	0.9970387661538395	0.4150511903858515	T	T	T
0.6952193894500951	0.3473499999999987	0.1121865696173359	F	F	F
0.6968244889173839	0.0988099669988071	0.2381689145875304	T	T	T
0.6949798642940158	0.3458580434907289	0.3647821587286508	T	T	T
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0.3962551576402374	0.5042915032452525	0.3156519472819616	T	T	T
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0.3968604621519710	0.4996382284417598	0.4121187779939098	T	T	T
0.4965852781786424	0.8473499999999987	0.1121865696173359	F	F	F
0.4965638275079482	0.5955067794225796	0.2381902408922142	T	T	T
0.4962363999108017	0.8449387807853401	0.3682915873950574	T	T	T
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0.4965121475018006	0.9051824876717953	0.2383634530507082	T	T	T
0.4957869870900902	0.6613971911399209	0.3691336762255210	T	T	T
0.5959023338143723	0.5000000000000000	0.0624065696173304	F	F	F
0.6000410686816092	0.7501270236961780	0.1855538014830806	T	T	T
0.5974998128850449	0.5072261627354185	0.3155699530512612	T	T	T
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0.5969440396821083	0.5055737619495234	0.4144099136766565	T	T	T
0.6952193894500951	0.8473499999999987	0.1121865696173359	F	F	F
0.6965600801115654	0.6001271622011419	0.2371786228591407	T	T	T
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0.8960903485305657	0.0991368235160765	0.2374697660444409	T	T	T
0.8956854611652879	0.3474531491344368	0.3629366225804933	T	T	T
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0.7962625288192456	0.5051007567747404	0.3149679511219889	T	T	T
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0.7975016824631477	0.5104782212295844	0.4102983731077667	T	T	T
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0.8964157433203539	0.9001560620986661	0.2363698476588317	T	T	T
0.8968241367971173	0.6579486780787789	0.3671284579630417	T	T	T
0.6282397082976254	0.2542021336999063	0.4926184990563930	T	T	T
0.6434432686215265	0.4455371894011355	0.4814235703517967	T	T	T
0.7248682284618008	0.3628376772822796	0.5587429743646468	T	T	T

0.7999625945632940	0.4440549378089506	0.4779504421849095	T	T	T
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0.7246499451301482	0.1453750032294381	0.5579972721632348	T	T	T
0.8002774231851995	0.0604821832711638	0.4777445156699372	T	T	T
0.7895496596162443	0.2522206261644082	0.4667674102275547	T	T	T
0.8881245814910170	0.3535924777366874	0.5531582982711594	T	T	T
0.8882849824792154	0.1486362173915282	0.5537675292399540	T	T	T
0.9565727354052198	0.2503245822531756	0.4670217415003312	T	T	T
0.8060818017782755	0.2528398756413185	0.6255645416110751	T	T	T
0.9585109513434147	0.4378530003073053	0.4762338036287835	T	T	T
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0.5012190466345171	0.3098718014904318	0.4096874102421308	T	T	T
0.5017582999575843	0.3525790483255218	0.3568608071513268	T	T	T
0.4545917880038890	0.2647950245504073	0.5361257940234062	T	T	T
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R_TS
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Ti Pt O C
60 14 121 1
Selective dynamics
Direct

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0.4966409816255580	0.2491329846680245	0.2387378912896304	T	T	T
0.5000369104289051	0.9962717729967723	0.3635743931204152	T	T	T
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0.5969208163790574	0.9991318549564244	0.2378563600968084	T	T	T
0.5966791941628760	0.2498396111718699	0.3674162283192820	T	T	T
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0.6031972661392158	0.7631713916838526	0.3618673272515678	T	T	T
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0.7969725525301923	0.0003467670482779	0.2374679600045383	T	T	T
0.7972757326206481	0.2518887565468783	0.3570536272071943	T	T	T
0.8938535010000024	0.0000000000000000	0.1121865699999987	F	F	F
0.8961951293257400	0.2498229993128641	0.2326654811528630	T	T	T
0.9001622127492962	0.0023503502616638	0.3689402171003611	T	T	T

0.7945364449999985	0.7500000000000000	0.1121865699999987	F	F	F
0.7971103374646504	0.5000526451840108	0.2371006854539382	T	T	T
0.8005441890334317	0.7508765051361009	0.3572896762557456	T	T	T
0.8938535010000024	0.5000000000000000	0.1121865699999987	F	F	F
0.8954912857898490	0.7504433291067445	0.2334456053008747	T	T	T
0.8971404091460625	0.5003131150463804	0.3687539878926714	T	T	T
0.2367947351359525	0.2521795574471666	0.4660397224580795	T	T	T
0.2376171875213422	0.4413088710837238	0.4757861096200057	T	T	T
0.3141532701648024	0.3522642558266165	0.5512003960665546	T	T	T
0.3946290500077435	0.4720095033131404	0.4793015135765419	T	T	T
0.2398368777349958	0.0622176313858655	0.4779827475092515	T	T	T
0.3149813283059443	0.1534737441156937	0.5530016682997281	T	T	T
0.3968137598180226	0.0681259325972381	0.4767167632913037	T	T	T
0.3964648509132835	0.2711307642489709	0.4592936913622495	T	T	T
0.4790280404829902	0.3533188301786377	0.5509502568809810	T	T	T
0.4794759651386785	0.1548427944074414	0.5521438038850253	T	T	T
0.5563909502453478	0.2548924919157602	0.4656758000033513	T	T	T
0.3974715742217877	0.2549091337238524	0.6243703331234018	T	T	T
0.5524124571323797	0.4446506936811413	0.4748292327815746	T	T	T
0.5539463691129374	0.0640005190295699	0.4764725835480733	T	T	T
0.0000000000000000	0.0000000000000000	0.0624065700000003	F	F	F
0.9980956844403217	0.2499054656120883	0.1852889525523482	T	T	T
0.9969478708005959	0.0016633077134200	0.3147165468293779	T	T	T
0.0000000000000000	0.0000000000000000	0.1619665699999970	F	F	F
0.9970295593903600	0.2503696739024497	0.2834767518902409	T	T	T
0.9979676334146196	0.0006103897104616	0.4121573831071062	T	T	T
0.0993170559999967	0.3473499999999987	0.1121865699999987	F	F	F
0.0979789363092540	0.1002176208889559	0.2376478461193088	T	T	T
0.0928900134130018	0.3441035506437661	0.3681640688348178	T	T	T
0.0993170559999967	0.1526500000000013	0.1121865699999987	F	F	F
0.0973438268747489	0.3996984791729629	0.2370233250719526	T	T	T
0.0946475370737621	0.1562880860880904	0.3677542059026365	T	T	T
0.1986341109999969	0.0000000000000000	0.0624065700000003	F	F	F
0.1990496458650684	0.2502954269293274	0.1864278308633678	T	T	T
0.1982689793094747	0.9962279132194037	0.3148002232554980	T	T	T
0.1986341109999969	0.0000000000000000	0.1619665699999970	F	F	F
0.1969758284831050	0.2498270278591885	0.2851290396465432	T	T	T
0.1957381685600237	0.9956187395340182	0.4125698648176589	T	T	T
0.2979511670000008	0.3473499999999987	0.1121865699999987	F	F	F
0.2978200688528960	0.0983378883662769	0.2382164431522706	T	T	T
0.2943931572663556	0.3481204420294140	0.3610321882726537	T	T	T
0.2979511670000008	0.1526500000000013	0.1121865699999987	F	F	F
0.2976136449863140	0.4018513471728462	0.2387648108226532	T	T	T
0.2974782873470826	0.1535697868710069	0.3623071146129400	T	T	T
0.0000000000000000	0.5000000000000000	0.0624065700000003	F	F	F
0.9933521538693713	0.7502342737831216	0.1844276247793775	T	T	T
0.9945677696091090	0.4997150131781836	0.3147434332532727	T	T	T
0.0000000000000000	0.5000000000000000	0.1619665699999970	F	F	F
0.9910423465579548	0.7503385622555498	0.2844322111220098	T	T	T
0.9942624799078099	0.5010901243017146	0.4129965772583878	T	T	T
0.0993170559999967	0.8473499999999987	0.1121865699999987	F	F	F
0.0971210806473413	0.5950942618918290	0.2373438916962626	T	T	T
0.0957271257429749	0.8439996347450590	0.3666222150987805	T	T	T
0.0993170559999967	0.6526500000000013	0.1121865699999987	F	F	F
0.0972668306034950	0.9048414806161550	0.2377279908376671	T	T	T
0.0944362787078394	0.6574003457062766	0.3664248791459089	T	T	T
0.1986341109999969	0.5000000000000000	0.0624065700000003	F	F	F
0.2026761975996029	0.7490727158487929	0.1852895465203890	T	T	T
0.1911930814705325	0.5004449989597545	0.3134862609111086	T	T	T
0.1986341109999969	0.5000000000000000	0.1619665699999970	F	F	F
0.2018628092494820	0.7507276967722771	0.2852230172527236	T	T	T
0.1907172521707656	0.5039216723369941	0.4108102713598773	T	T	T
0.2979511670000008	0.8473499999999987	0.1121865699999987	F	F	F
0.2974531884901456	0.5981783753523237	0.2386794543225393	T	T	T

0.2972730550130459	0.8384579650279521	0.3690357942584214	T	T	T
0.2979511670000008	0.6526500000000013	0.1121865699999987	F	F	F
0.2978669566234231	0.8997753555365242	0.2371587636074493	T	T	T
0.2891283710211692	0.6523610156552435	0.3670616393919401	T	T	T
0.3972682229999975	0.0000000000000000	0.0624065700000003	F	F	F
0.3974433374225707	0.2499929875171064	0.1862099742794587	T	T	T
0.3971761346596310	0.9937198548974918	0.3149220565619975	T	T	T
0.3972682229999975	0.0000000000000000	0.1619665699999970	F	F	F
0.3973251245706445	0.2504574491185944	0.2841051428892714	T	T	T
0.3957837280899117	0.9956466229375761	0.4101294696191850	T	T	T
0.4965852779999977	0.3473499999999987	0.1121865699999987	F	F	F
0.4971917700908668	0.0978906848631575	0.2385555278518632	T	T	T
0.4990847111967242	0.3488683660455528	0.3606900513286801	T	T	T
0.4965852779999977	0.1526500000000013	0.1121865699999987	F	F	F
0.4964876291225107	0.4021432582870962	0.2390316500996668	T	T	T
0.4972352489658940	0.1533880377522200	0.3626115220283546	T	T	T
0.5959023340000016	0.0000000000000000	0.0624065700000003	F	F	F
0.5955465393611699	0.2502807107375213	0.1865904672182209	T	T	T
0.5951141806123987	0.9908100951031682	0.3150638476776941	T	T	T
0.5959023340000016	0.0000000000000000	0.1619665699999970	F	F	F
0.5974519513988572	0.2500166324229880	0.2852770854036845	T	T	T
0.6001366977433227	0.9936331820894921	0.4126321574890415	T	T	T
0.6952193890000018	0.3473499999999987	0.1121865699999987	F	F	F
0.6959026171028058	0.0986558528729623	0.2384858127027795	T	T	T
0.7017635152527049	0.3451845597457845	0.3685118412239600	T	T	T
0.6952193890000018	0.1526500000000013	0.1121865699999987	F	F	F
0.6968120679794687	0.4010557661106144	0.2374912153805903	T	T	T
0.7001299715853611	0.1572639891542104	0.3683909516119687	T	T	T
0.3972682229999975	0.5000000000000000	0.0624065700000003	F	F	F
0.3983174683196582	0.7488347556323136	0.1866562201072555	T	T	T
0.3948923270670554	0.5016188340275156	0.3205330307793302	T	T	T
0.3972682229999975	0.5000000000000000	0.1619665699999970	F	F	F
0.3963826699392241	0.7479672057191238	0.2858291374131947	T	T	T
0.4965852779999977	0.8473499999999987	0.1121865699999987	F	F	F
0.4966555449799064	0.5982390676937863	0.2387788621276360	T	T	T
0.4914290046692976	0.8391184847301620	0.3720705052947373	T	T	T
0.4965852779999977	0.6526500000000013	0.1121865699999987	F	F	F
0.4960985862256166	0.8993085934719132	0.2371844033079946	T	T	T
0.5959023340000016	0.5000000000000000	0.0624065700000003	F	F	F
0.5959351611132770	0.7491581744913905	0.1860790542938900	T	T	T
0.6020402324990671	0.4998856661630481	0.3141043714062528	T	T	T
0.5959023340000016	0.5000000000000000	0.1619665699999970	F	F	F
0.5983370855617723	0.7529207900472542	0.2827201983293473	T	T	T
0.6030716667983628	0.5088884092529675	0.4110153361451375	T	T	T
0.6952193890000018	0.8473499999999987	0.1121865699999987	F	F	F
0.6970857521684115	0.5991659462530784	0.2373003837394470	T	T	T
0.7106943914335746	0.8488496373655433	0.3696221714319374	T	T	T
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0.6979115858829633	0.9011395102129636	0.2374728267515600	T	T	T
0.7048904751650329	0.6600346439203455	0.3683403440355904	T	T	T
0.7945364449999985	0.0000000000000000	0.0624065700000003	F	F	F
0.7947086387859622	0.2496344877036855	0.1864160657164779	T	T	T
0.7995959555359122	0.0030089559958187	0.3148548615038025	T	T	T
0.7945364449999985	0.0000000000000000	0.1619665699999970	F	F	F
0.7968591791440910	0.2503742138041097	0.2841637991289764	T	T	T
0.8016789574248530	0.0055868171849552	0.4128187325224026	T	T	T
0.8938535010000024	0.3473499999999987	0.1121865699999987	F	F	F
0.8968761699733032	0.1007917636531150	0.2362945410829351	T	T	T
0.8970646628620148	0.3439445714145336	0.3671781601121203	T	T	T
0.8938535010000024	0.1526500000000013	0.1121865699999987	F	F	F
0.8964889332116641	0.3997804871781495	0.2362787223601653	T	T	T
0.8984456119080056	0.1586204394669662	0.3675857546684848	T	T	T
0.7945364449999985	0.5000000000000000	0.0624065700000003	F	F	F
0.7947474941229233	0.7501546179537926	0.1862087370578396	T	T	T

0.7992467440602089	0.5013515333976719	0.3145399755179445	T	T	T
0.7945364449999985	0.5000000000000000	0.1619665699999970	F	F	F
0.7973352556541324	0.7502657086840253	0.2837604674137827	T	T	T
0.8000145555527265	0.5010301513710763	0.4125224271620763	T	T	T
0.8938535010000024	0.8473499999999987	0.1121865699999987	F	F	F
0.8964707013246968	0.5992032519904822	0.2360562675324248	T	T	T
0.8993121320473224	0.8451657938821729	0.3680989222256167	T	T	T
0.8938535010000024	0.6526500000000013	0.1121865699999987	F	F	F
0.8964818530718277	0.9013637534167148	0.2364889000300505	T	T	T
0.8987959688358685	0.6577016921004342	0.3682015595717280	T	T	T
0.4457621047627993	0.6184000876640577	0.4050650766858990	T	T	T
0.5076781251989229	0.6554732899053808	0.3521800919896401	T	T	T
0.3881450175814711	0.6854576285226298	0.5222091782484448	T	T	T
0.3913713207931006	0.6053682258873094	0.5036745407541011	T	T	T

H_TS
Ti O Pt H O C
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16.1999999999999993 0.0000000000000000 0.0000000000000000
0.0000000000000008 13.1883981985216998 0.0000000000000000
0.0000000000000015 0.0000000000000015 25.7900218205815008
Ti O Pt H O C
60 119 14 2 3 1
Selective dynamics
Direct

0.0000000000000000	0.2500000000000000	0.1121865696173359	F	F	F
0.9957392853392187	0.0006537616833558	0.2359786368598216	T	T	T
0.9968643401546641	0.2512416353876641	0.3568415511288112	T	T	T
0.0993170556357299	0.0000000000000000	0.1121865696173359	F	F	F
0.0997935929757786	0.2507093309581489	0.2343454188009916	T	T	T
0.0846010966252375	1.0003159444182563	0.3700822906308240	T	T	T
0.1986341112714598	0.2500000000000000	0.1121865696173359	F	F	F
0.1963044658653972	0.0005500969642271	0.2356434965699022	T	T	T
0.1899209903395025	0.2513113871796738	0.3608577188653897	T	T	T
0.2979511669071826	0.0000000000000000	0.1121865696173359	F	F	F
0.3026231344587807	0.2500302124644065	0.2378472861195801	T	T	T
0.2817867397750338	0.9978388646486798	0.3583382867816792	T	T	T
0.0000000000000000	0.7500000000000000	0.1121865696173359	F	F	F
0.9964788971942330	0.4998254486139164	0.2363354825791734	T	T	T
0.9956652564929310	0.7519413497578145	0.3568975357539604	T	T	T
0.0993170556357299	0.5000000000000000	0.1121865696173359	F	F	F
0.0984082973230403	0.7498553962121606	0.2346304945943948	T	T	T
0.0902118777509581	0.5030784793349461	0.3695640904255165	T	T	T
0.1986341112714598	0.7500000000000000	0.1121865696173359	F	F	F
0.1977317610768007	0.5003347056131979	0.2363365676171248	T	T	T
0.1915177736940736	0.7526675282937714	0.3588641589388322	T	T	T
0.2979511669071826	0.5000000000000000	0.1121865696173359	F	F	F
0.2976544187596893	0.7505876120136046	0.2360932523353312	T	T	T
0.2767605653369625	0.5096413335410220	0.3673510800480179	T	T	T
0.3972682225429125	0.2500000000000000	0.1121865696173359	F	F	F
0.3973428775186991	0.0003426616950688	0.2371231416546939	T	T	T
0.4004942081093768	0.2527459429921833	0.3666757814986500	T	T	T
0.4965852781786424	0.0000000000000000	0.1121865696173359	F	F	F
0.4966812136250148	0.2507253309728217	0.2392582859534376	T	T	T
0.5070294480526230	0.9902490670761290	0.3626211621378299	T	T	T
0.5959023338143723	0.2500000000000000	0.1121865696173359	F	F	F
0.5979975911687003	0.0001671372377018	0.2364182950385681	T	T	T
0.6001438977959423	0.2590367605420847	0.3641943893484921	T	T	T
0.6952193894500951	0.0000000000000000	0.1121865696173359	F	F	F
0.6936294585900213	0.2499173891524701	0.2365969669405920	T	T	T
0.7028742944041640	0.9954825850738611	0.3678444603654648	T	T	T
0.3972682225429125	0.7500000000000000	0.1121865696173359	F	F	F
0.3961510953572212	0.5005940263140897	0.2367377538531569	T	T	T
0.3973265667765685	0.7509863850515313	0.3590559366566394	T	T	T
0.4965852781786424	0.5000000000000000	0.1121865696173359	F	F	F
0.4953072474267378	0.7489663042157984	0.2348231135924735	T	T	T
0.4967622060980363	0.5040349791239658	0.3576031537290617	T	T	T
0.5959023338143723	0.7500000000000000	0.1121865696173359	F	F	F
0.5979363886264232	0.5002216446889288	0.2365770493192651	T	T	T
0.5998292389817391	0.7450293372610232	0.3561721590201766	T	T	T
0.6952193894500951	0.5000000000000000	0.1121865696173359	F	F	F
0.6965615480601459	0.7494567087509941	0.2345744578165858	T	T	T
0.7180488096830158	0.5026498501785115	0.3645448857856215	T	T	T
0.7945364450858250	0.2500000000000000	0.1121865696173359	F	F	F
0.7961812705379169	0.0005038979987954	0.2374372272136646	T	T	T
0.8020458093369582	0.2549824844053133	0.3585065762084508	T	T	T
0.8938535007215549	0.0000000000000000	0.1121865696173359	F	F	F
0.8956775796190600	0.2499054058468025	0.2341162333115687	T	T	T
0.8996144616903018	0.0021709915975085	0.3679208892790567	T	T	T

0.7945364450858250	0.7500000000000000	0.1121865696173359	F	F	F
0.7973675307311392	0.4996276968633424	0.2362045503100910	T	T	T
0.8004377989706530	0.7512458252534346	0.3568676115301517	T	T	T
0.8938535007215549	0.5000000000000000	0.1121865696173359	F	F	F
0.8966814442809148	0.7500269129361753	0.2331581677444294	T	T	T
0.9043203177251720	0.5026345714064513	0.3691192361855225	T	T	T
0.0000000000000000	0.0000000000000000	0.0624065696173304	F	F	F
0.0026192206215364	0.2500898753785621	0.1849229683769624	T	T	T
0.9937802573018490	0.0005927460951898	0.3161196671923580	T	T	T
0.0000000000000000	0.0000000000000000	0.1619665696173342	F	F	F
0.0023872674106693	0.2503573760632385	0.2854096682698333	T	T	T
0.9922479521378886	0.0010267031017203	0.4142575100322781	T	T	T
0.0993170556357299	0.3473499999999987	0.1121865696173359	F	F	F
0.0972919538180171	0.0998166707177675	0.2374385912924487	T	T	T
0.0950594206489826	0.3449637450364096	0.3700408036922328	T	T	T
0.0993170556357299	0.1526500000000013	0.1121865696173359	F	F	F
0.0983003230207851	0.4006363898820849	0.2377976559824501	T	T	T
0.0935237484224540	0.1577233923070644	0.3699336695977706	T	T	T
0.1986341112714598	0.0000000000000000	0.0624065696173304	F	F	F
0.1998317652948420	0.2497108667418959	0.1884768379341923	T	T	T
0.1889377675447895	0.0039932928514453	0.3147576308067361	T	T	T
0.1986341112714598	0.0000000000000000	0.1619665696173342	F	F	F
0.1971273685778452	0.2500120585866497	0.2888966062800603	T	T	T
0.2979511669071826	0.3473499999999987	0.1121865696173359	F	F	F
0.2974837155134792	0.0989449459811114	0.2411606068082112	T	T	T
0.2894646183687805	0.3486291706577875	0.3747463310599055	T	T	T
0.2979511669071826	0.1526500000000013	0.1121865696173359	F	F	F
0.2972993363590815	0.4010894364612556	0.2406749980035106	T	T	T
0.2892753788186380	0.1530376789204010	0.3755245350025742	T	T	T
0.0000000000000000	0.5000000000000000	0.0624065696173304	F	F	F
0.9982862387143173	0.7509364815043256	0.1856772599012053	T	T	T
0.9981760974122857	0.5029754484123039	0.3155240100054766	T	T	T
0.0000000000000000	0.5000000000000000	0.1619665696173342	F	F	F
0.9967554611150770	0.7506152759334789	0.2842318577791477	T	T	T
0.9971446088408997	0.5022123066080943	0.4140736556002590	T	T	T
0.0993170556357299	0.8473499999999987	0.1121865696173359	F	F	F
0.0975824035237014	0.6003692937661296	0.2369870535162838	T	T	T
0.0920432435492174	0.8458823471822741	0.3690487864383173	T	T	T
0.0993170556357299	0.6526500000000013	0.1121865696173359	F	F	F
0.0970689495533921	0.9011600109865928	0.2376754541287281	T	T	T
0.0927871736936172	0.6598168834210477	0.3693842903962821	T	T	T
0.1986341112714598	0.5000000000000000	0.0624065696173304	F	F	F
0.1939133947824519	0.7510679955180902	0.1857356678678004	T	T	T
0.1918918410983902	0.5029322652308267	0.3154218541627424	T	T	T
0.1986341112714598	0.5000000000000000	0.1619665696173342	F	F	F
0.1910418362729163	0.7504650396358633	0.2869424612937543	T	T	T
0.1898239159457701	0.5056118826293825	0.4136333939979696	T	T	T
0.2979511669071826	0.8473499999999987	0.1121865696173359	F	F	F
0.2966919098124439	0.5950929128564894	0.2386388757761637	T	T	T
0.2872691641146939	0.8486382299056278	0.3677630314406272	T	T	T
0.2979511669071826	0.6526500000000013	0.1121865696173359	F	F	F
0.2970268786297469	0.9063589360691878	0.2407457951320139	T	T	T
0.2874066397532661	0.6599289414410866	0.3720552312509573	T	T	T
0.3972682225429125	0.0000000000000000	0.0624065696173304	F	F	F
0.3977606013094209	0.2498439467250796	0.1934452009243705	T	T	T
0.3952972560090671	0.9988108918131023	0.3254984309240241	T	T	T
0.3972682225429125	0.0000000000000000	0.1619665696173342	F	F	F
0.3958122135358446	0.2488408569791298	0.2914936058506287	T	T	T
0.4479782876849421	0.9530063259632974	0.4344488378735216	T	T	T
0.4965852781786424	0.3473499999999987	0.1121865696173359	F	F	F
0.4953612466487283	0.0977203182763159	0.2409247713940238	T	T	T
0.4916857129631299	0.3537728265952320	0.3667760873618554	T	T	T
0.4965852781786424	0.1526500000000013	0.1121865696173359	F	F	F
0.4960739870167111	0.4014923143284695	0.2404496037410885	T	T	T

0.4922533481558782	0.1519793454203742	0.3752689386001670	T	T	T
0.5959023338143723	0.0000000000000000	0.0624065696173304	F	F	F
0.5947987342714688	0.2499868596680474	0.1881144858455428	T	T	T
0.6013621264403876	0.0049974449623666	0.3159896477804163	T	T	T
0.5959023338143723	0.0000000000000000	0.1619665696173342	F	F	F
0.5968601507973288	0.2483790002299970	0.2867031642396551	T	T	T
0.6028554194708153	0.9895605759630191	0.4110789016143329	T	T	T
0.6952193894500951	0.3473499999999987	0.1121865696173359	F	F	F
0.6967271354761055	0.0988963786160643	0.2379574420200511	T	T	T
0.7082269804306720	0.3527329796679345	0.3638485353859616	T	T	T
0.6952193894500951	0.1526500000000013	0.1121865696173359	F	F	F
0.6966442954854994	0.4011503068421435	0.2395290671716039	T	T	T
0.7102587129116738	0.1566493679615432	0.3763655037784368	T	T	T
0.3972682225429125	0.5000000000000000	0.0624065696173304	F	F	F
0.4003019549079581	0.7511402718585448	0.1854596697487812	T	T	T
0.3978357915029875	0.5091005012332529	0.3183507933581918	T	T	T
0.3972682225429125	0.5000000000000000	0.1619665696173342	F	F	F
0.4025507384749807	0.7480042731802390	0.2851857851300104	T	T	T
0.3801869917224627	0.5008052847226137	0.4218262234703218	T	T	T
0.4965852781786424	0.8473499999999987	0.1121865696173359	F	F	F
0.4965267935001725	0.5977758248013340	0.2371154658708473	T	T	T
0.5081740089243982	0.8401035046449680	0.3622341511504527	T	T	T
0.4965852781786424	0.6526500000000013	0.1121865696173359	F	F	F
0.4966359884899214	0.9026507201193625	0.2400410721578912	T	T	T
0.5048772888509120	0.6519252299451862	0.3770044402688899	T	T	T
0.5959023338143723	0.5000000000000000	0.0624065696173304	F	F	F
0.5923025375985816	0.7509390348773061	0.1853520473603772	T	T	T
0.5939244811882444	0.5038051635279456	0.3167547903549080	T	T	T
0.5959023338143723	0.5000000000000000	0.1619665696173342	F	F	F
0.5932969270067986	0.7431127760527646	0.2850229050969701	T	T	T
0.6136609047274552	0.5047440878871813	0.4188698812224079	T	T	T
0.6952193894500951	0.8473499999999987	0.1121865696173359	F	F	F
0.6969148633817286	0.5943454166079232	0.2385922056949168	T	T	T
0.7004147047852006	0.8416238137416167	0.3662381971261163	T	T	T
0.6952193894500951	0.6526500000000013	0.1121865696173359	F	F	F
0.6964170451752937	0.9046624347681382	0.2389983485223294	T	T	T
0.7024713816260273	0.6562454480211147	0.3685222265928540	T	T	T
0.7945364450858250	0.0000000000000000	0.0624065696173304	F	F	F
0.7900060938657085	0.2506594403513004	0.1856934608603143	T	T	T
0.7975873499467749	0.0005110340642715	0.3177306814381912	T	T	T
0.7945364450858250	0.0000000000000000	0.1619665696173342	F	F	F
0.7923820883622812	0.2471782446335092	0.2864481124881079	T	T	T
0.7990911188217154	0.9917880022796695	0.4175253411955174	T	T	T
0.8938535007215549	0.3473499999999987	0.1121865696173359	F	F	F
0.8966698117486657	0.0946479781569163	0.2374526139711713	T	T	T
0.9012743493270727	0.3460305771278902	0.3673225848182974	T	T	T
0.8938535007215549	0.1526500000000013	0.1121865696173359	F	F	F
0.8974489227969364	0.4050936741270202	0.2372405667535615	T	T	T
0.8994081889835370	0.1576644718560420	0.3682654928513321	T	T	T
0.7945364450858250	0.5000000000000000	0.0624065696173304	F	F	F
0.7999329453122183	0.7500836398886881	0.1854885604325305	T	T	T
0.8055894397488332	0.5063605429930168	0.3140354393006646	T	T	T
0.7945364450858250	0.5000000000000000	0.1619665696173342	F	F	F
0.8031885942850592	0.7491736875491414	0.2854312018033262	T	T	T
0.8038728660784182	0.5029799751537731	0.4121563648319373	T	T	T
0.8938535007215549	0.8473499999999987	0.1121865696173359	F	F	F
0.8984336915596621	0.6009690563597763	0.2355749382418214	T	T	T
0.8972989399602658	0.8453242340414752	0.3678733227417683	T	T	T
0.8938535007215549	0.6526500000000013	0.1121865696173359	F	F	F
0.8970189394340036	0.8999174366057915	0.2369659606367323	T	T	T
0.8996014196946356	0.6594722514405227	0.3693190876813083	T	T	T
0.3324290233747639	0.1565304994384411	0.4535304613636060	T	T	T
0.3495202021849816	0.3484116863373635	0.4510881422598248	T	T	T
0.3922866594090408	0.2349288328441211	0.5367688218404170	T	T	T

0.4881552145471020	0.3677097424108563	0.4986599479049973	T	T	T
0.3344379429795085	0.9477925578237276	0.4592801237094798	T	T	T
0.4064361108066123	0.0327428682975118	0.5422014059092776	T	T	T
0.5321456576685332	0.0088143015311001	0.4830950911858227	T	T	T
0.5130059490181829	0.1937601883879033	0.4546910189264713	T	T	T
0.5984633051180791	0.2400932352323059	0.5344015458189421	T	T	T
0.6371330139857011	0.0545749190956619	0.5490897673703878	T	T	T
0.6903991918182810	0.2039015724807685	0.4536968082882993	T	T	T
0.5033710232348473	0.1454420830357957	0.5973142267020042	T	T	T
0.6363619705976959	0.3834142640621254	0.4691477015038236	T	T	T
0.7540033685850880	0.0433196426915400	0.4852565934457960	T	T	T
0.3781541402552307	0.5511079974814818	0.4494880564680501	T	T	T
0.6146668430305348	0.5681570672250292	0.4384259344351983	T	T	T
0.2236540366601986	0.9296133900647643	0.4687868365249881	T	T	T
0.1873023828084818	1.0047482372993055	0.4116895787566219	T	T	T
0.2633678992750788	0.9958761815551453	0.6158548138001970	T	T	T
0.3160121121025508	0.0150749328039250	0.5870823640827249	T	T	T

O_TS
Ti O Pt O C
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16.1999999999999993 0.0000000000000000 0.0000000000000000
0.0000000000000008 13.1883981985216998 0.0000000000000000
0.0000000000000015 0.0000000000000015 25.7900218205815008
Ti O Pt O C
60 119 14 3 1
Selective dynamics
Direct

0.0000000000000000	0.2500000000000000	0.1121865696173359	F	F	F
0.9988159159389056	0.0000953072262683	0.2362965432486752	T	T	T
0.9974609458662012	0.2498666790591791	0.3647352156143751	T	T	T
0.0993170556357299	0.0000000000000000	0.1121865696173359	F	F	F
0.0944906223554777	0.2503503910083456	0.2361933661959939	T	T	T
0.1052718101174583	0.9994411366907610	0.3674705374290433	T	T	T
0.1986341112714598	0.2500000000000000	0.1121865696173359	F	F	F
0.1972733308626654	0.0003803806869000	0.2371963690588255	T	T	T
0.1956838034313911	0.2520279074594746	0.3576769023377371	T	T	T
0.2979511669071826	0.0000000000000000	0.1121865696173359	F	F	F
0.2986041451245199	0.2502021563910546	0.2360388790649494	T	T	T
0.2956357545201740	0.0035799831411637	0.3698694814546645	T	T	T
0.0000000000000000	0.7500000000000000	0.1121865696173359	F	F	F
0.9987480658875664	0.5005284132786196	0.2362834897155114	T	T	T
0.9972682357195700	0.7514577570401766	0.3563774344557665	T	T	T
0.0993170556357299	0.5000000000000000	0.1121865696173359	F	F	F
0.0979994096291043	0.7503473297996068	0.2350970394982800	T	T	T
0.1050406659429115	0.5023098597214345	0.3673951525415143	T	T	T
0.1986341112714598	0.7500000000000000	0.1121865696173359	F	F	F
0.1972921196492473	0.5002860185200684	0.2371400066360977	T	T	T
0.1980461805833391	0.7502458875965390	0.3577736407710660	T	T	T
0.2979511669071826	0.5000000000000000	0.1121865696173359	F	F	F
0.2974007883750879	0.7502419937089403	0.2342489679707934	T	T	T
0.2955261420863503	0.4990768411459663	0.3694871449725749	T	T	T
0.3972682225429125	0.2500000000000000	0.1121865696173359	F	F	F
0.3970158225719311	0.9999580724651118	0.2374266120606847	T	T	T
0.3956863556780437	0.2476315297327817	0.3628840137095711	T	T	T
0.4965852781786424	0.0000000000000000	0.1121865696173359	F	F	F
0.4957348140886075	0.2495629560812187	0.2371883899152023	T	T	T
0.4889241352973027	0.0005402369919884	0.3671223325305720	T	T	T
0.5959023338143723	0.2500000000000000	0.1121865696173359	F	F	F
0.5958474956305355	0.9996229389052091	0.2372111626844986	T	T	T
0.5998962012468250	0.2423379634440070	0.3591129402951599	T	T	T
0.6952193894500951	0.0000000000000000	0.1121865696173359	F	F	F
0.6982743386216232	0.2503191561970429	0.2363171607854019	T	T	T
0.6931136640826715	0.9971126535783253	0.3631047876748007	T	T	T
0.3972682225429125	0.7500000000000000	0.1121865696173359	F	F	F
0.3971783359089793	0.5003321564931651	0.2375376026923145	T	T	T
0.3939147243710738	0.7541783559481964	0.3582177129079687	T	T	T
0.4965852781786424	0.5000000000000000	0.1121865696173359	F	F	F
0.4963296777263305	0.7503938347291955	0.2355214198195232	T	T	T
0.4883214704431025	0.5114246002755972	0.3684430295756257	T	T	T
0.5959023338143723	0.7500000000000000	0.1121865696173359	F	F	F
0.5953205446191011	0.5003926156579948	0.2372148478998381	T	T	T
0.5978288493841888	0.7530016354478892	0.3575814783445266	T	T	T
0.6952193894500951	0.5000000000000000	0.1121865696173359	F	F	F
0.6958369028776201	0.7501378110305358	0.2340776567315171	T	T	T
0.6913702371358514	0.5004877657185645	0.3631685974955838	T	T	T
0.7945364450858250	0.2500000000000000	0.1121865696173359	F	F	F
0.7967593903699772	0.0006290570158661	0.2370861456104960	T	T	T
0.7979509077428345	0.2523128927326416	0.3639506238888313	T	T	T
0.8938535007215549	0.0000000000000000	0.1121865696173359	F	F	F
0.8958715395090335	0.2503298452257173	0.2387146823076786	T	T	T
0.9011047038221218	0.9994718464204376	0.3613994089578643	T	T	T

0.7945364450858250	0.7500000000000000	0.1121865696173359	F	F	F
0.7965050259040074	0.4998163047997344	0.2371765059527207	T	T	T
0.7977641263971618	0.7485314509480731	0.3567307431560003	T	T	T
0.8938535007215549	0.5000000000000000	0.1121865696173359	F	F	F
0.8966914650071656	0.7502498760158099	0.2333279142660246	T	T	T
0.9008619759050316	0.5016787514470691	0.3612941692160466	T	T	T
0.0000000000000000	0.0000000000000000	0.0624065696173304	F	F	F
0.9968512332135360	0.2502507566153879	0.1858460816136936	T	T	T
0.9960724227614068	0.9976063863485501	0.3146051388647225	T	T	T
0.0000000000000000	0.0000000000000000	0.1619665696173342	F	F	F
0.9969156614310228	0.2504274661165434	0.2852074618764024	T	T	T
0.9980949155550244	0.9930001048449805	0.4124516187672443	T	T	T
0.0993170556357299	0.3473499999999987	0.1121865696173359	F	F	F
0.0972121279277029	0.1008196104996641	0.2378130907103735	T	T	T
0.0966462894906033	0.3457518181550858	0.3681728197065642	T	T	T
0.0993170556357299	0.1526500000000013	0.1121865696173359	F	F	F
0.0972770930330688	0.3999320678829180	0.2379023991355715	T	T	T
0.0966309335328580	0.1561561649489388	0.3682520511497958	T	T	T
0.1986341112714598	0.0000000000000000	0.0624065696173304	F	F	F
0.1973194788490010	0.2503206256853407	0.1861621525315282	T	T	T
0.1975769957922108	-0.0000209113437710	0.3153187602621822	T	T	T
0.1986341112714598	0.0000000000000000	0.1619665696173342	F	F	F
0.1964532858877779	0.2506309497432326	0.2844395501425613	T	T	T
0.1959386763889853	0.9973699170205113	0.4126304238867270	T	T	T
0.2979511669071826	0.3473499999999987	0.1121865696173359	F	F	F
0.2967862532036368	0.0999784028103991	0.2376825846020908	T	T	T
0.2889098908387637	0.3462026109378261	0.3693531406651712	T	T	T
0.2979511669071826	0.1526500000000013	0.1121865696173359	F	F	F
0.2971829979664800	0.4006961912269907	0.2380650700301062	T	T	T
0.2881923717579893	0.1560854962549973	0.3695976894412046	T	T	T
0.0000000000000000	0.5000000000000000	0.0624065696173304	F	F	F
0.9939065604540080	0.7500631954283628	0.1846614804447715	T	T	T
0.9959851786480461	0.5033323078218157	0.3145735461319855	T	T	T
0.0000000000000000	0.5000000000000000	0.1619665696173342	F	F	F
0.9919602109723817	0.7505002319490879	0.2849692464151773	T	T	T
0.9979621597578975	0.5085228065009199	0.4122682513765799	T	T	T
0.0993170556357299	0.8473499999999987	0.1121865696173359	F	F	F
0.0977903822543268	0.5955074329001629	0.2378647697820787	T	T	T
0.0971378475408061	0.8434060889655122	0.3667374982880746	T	T	T
0.0993170556357299	0.6526500000000013	0.1121865696173359	F	F	F
0.0977809495080289	0.9051444752933162	0.2379672067653640	T	T	T
0.0973053083563631	0.6583316548086426	0.3667458635478482	T	T	T
0.1986341112714598	0.5000000000000000	0.0624065696173304	F	F	F
0.2016813273001739	0.7501726969827947	0.1854359308574187	T	T	T
0.1976200776546262	0.5019706255456117	0.3152251081742407	T	T	T
0.1986341112714598	0.5000000000000000	0.1619665696173342	F	F	F
0.2023513978120767	0.7505475221905634	0.2862817379177680	T	T	T
0.1960651214279395	0.5047251895947816	0.4123799276887103	T	T	T
0.2979511669071826	0.8473499999999987	0.1121865696173359	F	F	F
0.2973990962955073	0.5990013807148197	0.2375859424741384	T	T	T
0.2967466747210544	0.8450998731355825	0.3700373374317752	T	T	T
0.2979511669071826	0.6526500000000013	0.1121865696173359	F	F	F
0.2972848353639208	0.9017266340163669	0.2375875734066472	T	T	T
0.2966944903980419	0.6587438916527629	0.3697412398214393	T	T	T
0.3972682225429125	0.0000000000000000	0.0624065696173304	F	F	F
0.3974526957346526	0.2500683562477668	0.1862673279135054	T	T	T
0.3952722912392565	1.0000252553715985	0.3153755108293719	T	T	T
0.3972682225429125	0.0000000000000000	0.1619665696173342	F	F	F
0.3958066609088146	0.2492196494052752	0.2839402212413404	T	T	T
0.3967495368841218	0.0067592358835173	0.4118912329648786	T	T	T
0.4965852781786424	0.3473499999999987	0.1121865696173359	F	F	F
0.4976438224295719	0.1000140124079559	0.2383363766620793	T	T	T
0.4965852781786424	0.1526500000000013	0.1121865696173359	F	F	F
0.4971415656841354	0.3999567778934821	0.2386489103372806	T	T	T

0.5067096966318728	0.1485220543506452	0.3618228368459059	T	T	T
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0.5964402982036587	0.2501575062507287	0.1864221772667559	T	T	T
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0.5975255407830585	0.2505362794035982	0.2847439959004280	T	T	T
0.5999375171885379	0.9954260755696638	0.4148005503494333	T	T	T
0.6952193894500951	0.3473499999999987	0.1121865696173359	F	F	F
0.6968884590502591	0.0990179734750830	0.2382042685516892	T	T	T
0.6957683644794125	0.3454506216014412	0.3647176273168848	T	T	T
0.6952193894500951	0.1526500000000013	0.1121865696173359	F	F	F
0.6965847717294213	0.4015454460740791	0.2382953205555293	T	T	T
0.6969273227497791	0.1530336528856613	0.3635350107638530	T	T	T
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0.3934702787140897	0.7501550269299786	0.1855382886950325	T	T	T
0.3964208777429074	0.5032248161854610	0.3156537382985647	T	T	T
0.3972682225429125	0.5000000000000000	0.1619665696173342	F	F	F
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0.3962831039153675	0.5021980346725339	0.4120286948013442	T	T	T
0.4965852781786424	0.8473499999999987	0.1121865696173359	F	F	F
0.4966993037525488	0.5954349099763331	0.2382628477450099	T	T	T
0.4962583569845732	0.8449018995557375	0.3681736314911002	T	T	T
0.4965852781786424	0.6526500000000013	0.1121865696173359	F	F	F
0.4965653935086324	0.9051985910000871	0.2383663021336882	T	T	T
0.4961514850010986	0.6610924683582891	0.3688459494557177	T	T	T
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0.6001062306057687	0.7501297926260144	0.1855484372376437	T	T	T
0.5971229552111171	0.5056036141593245	0.3156420399749454	T	T	T
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0.6014719546096819	0.7509235550893979	0.2863187612638085	T	T	T
0.5971390646489469	0.5057447693390938	0.4144726118689352	T	T	T
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0.6965044849774871	0.6000536574864990	0.2373243605973198	T	T	T
0.6979730997909056	0.8421853879019130	0.3684914367340108	T	T	T
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0.6971793287389022	0.9000691210273428	0.2369447433597731	T	T	T
0.6966118689431606	0.6578990949228473	0.3679379962851873	T	T	T
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0.7959053527790119	0.2502485925082499	0.1866668049753481	T	T	T
0.7973070508228720	0.9948373853494027	0.3148754738526351	T	T	T
0.7945364450858250	0.0000000000000000	0.1619665696173342	F	F	F
0.7963579135233264	0.2505974782264216	0.2850050424986727	T	T	T
0.7983680877399377	0.9909512141199813	0.4105267829359692	T	T	T
0.8938535007215549	0.3473499999999987	0.1121865696173359	F	F	F
0.8962332203460976	0.0990718711896309	0.2374564065827500	T	T	T
0.8960698919369257	0.3474012175225391	0.3629305120088889	T	T	T
0.8938535007215549	0.1526500000000013	0.1121865696173359	F	F	F
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0.7964078457514563	0.5049615089998246	0.3149425213764995	T	T	T
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0.7976176952766464	0.5104905555908814	0.4102533953010050	T	T	T
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0.8963986654310426	0.6002541097444990	0.2364399076631341	T	T	T
0.8970054393308476	0.8425527332076244	0.3673011909012732	T	T	T
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0.8970469359632782	0.6578203421701759	0.3671034669195215	T	T	T
0.6293569700596492	0.2521661984538917	0.4907938954858403	T	T	T
0.6435117001669963	0.4436329122397891	0.4807058491900907	T	T	T
0.7242494616948738	0.3611737078580884	0.5581344874211115	T	T	T

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0.6439499746933639	0.0609682970567620	0.4802543290459242	T	T	T
0.7243470850578279	0.1440995659716403	0.5575873269625705	T	T	T
0.8007757936014492	0.0598622551484406	0.4775437308073040	T	T	T
0.7908060295785210	0.2515295208144590	0.4664698364351814	T	T	T
0.8877553176367712	0.3534497291874045	0.5532777752042377	T	T	T
0.8880635940160639	0.1485800842265556	0.5535838902112276	T	T	T
0.9578872766920401	0.2507158532001494	0.4671857877533465	T	T	T
0.8051701516773300	0.2518086455864905	0.6253240630871738	T	T	T
0.9586848108621840	0.4382626915559638	0.4765312757464432	T	T	T
0.9589403937223714	0.0631683646753152	0.4768142433814169	T	T	T
0.4864946307985288	0.3112926231907262	0.4124367385268743	T	T	T
0.5037550089884314	0.3513278815867425	0.3602298809447934	T	T	T
0.4537910748086467	0.2592320151026740	0.5314524264179089	T	T	T
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Ti Pt O C
60 14 121 1
Selective dynamics
Direct

0.0000000000000000	0.2500000000000000	0.1121865699999987	F	F	F
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0.9979617511062074	0.2497629292594577	0.3562183239822863	T	T	T
0.0993170559999967	0.0000000000000000	0.1121865699999987	F	F	F
0.1027514637859018	0.2497138278492148	0.2370605734132219	T	T	T
0.0897650577291117	0.0012336037467012	0.3676489495535581	T	T	T
0.1986341109999969	0.2500000000000000	0.1121865699999987	F	F	F
0.1977072996316825	0.0000160173090089	0.2373202743613406	T	T	T
0.1991723309880254	0.2501800367987019	0.3669940295173482	T	T	T
0.2979511670000008	0.0000000000000000	0.1121865699999987	F	F	F
0.2981348041749026	0.2495473615425503	0.2384567149477324	T	T	T
0.2917441531776997	0.9984834597091244	0.3629115353764496	T	T	T
0.0000000000000000	0.7500000000000000	0.1121865699999987	F	F	F
0.9975779569592070	0.4994803225244425	0.2362340951700097	T	T	T
0.9973933230649684	0.7503288136183974	0.3558817209176852	T	T	T
0.0993170559999967	0.5000000000000000	0.1121865699999987	F	F	F
0.0993033281019498	0.7502937473653870	0.2341039008793035	T	T	T
0.0870107005824684	0.4999035790615423	0.3673196983516308	T	T	T
0.1986341109999969	0.7500000000000000	0.1121865699999987	F	F	F
0.1974111200127733	0.4999958527372354	0.2358728222686985	T	T	T
0.1953734486134079	0.7512072098228698	0.3569809797028323	T	T	T
0.2979511670000008	0.5000000000000000	0.1121865699999987	F	F	F
0.3020824857630524	0.7506002610760313	0.2368185511292369	T	T	T
0.2853785716420190	0.4999950504772138	0.3585680154005897	T	T	T
0.3972682229999975	0.2500000000000000	0.1121865699999987	F	F	F
0.3973651360056505	-0.0001743569038055	0.2376682918823529	T	T	T
0.3994087374020687	0.2502752712003108	0.3622643636323482	T	T	T
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0.4972070511269756	0.2492397015671139	0.2385004533525457	T	T	T
0.5011899119283851	0.9924481892573438	0.3632396110586389	T	T	T
0.5959023340000016	0.2500000000000000	0.1121865699999987	F	F	F
0.5968423250730156	0.9992052165702072	0.2378392798520547	T	T	T
0.5967327094028271	0.2479834897445612	0.3669751143307657	T	T	T
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0.7075604105327470	-0.0019407882676941	0.3685850586493128	T	T	T
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0.3969830145620803	0.7438753369246854	0.3652075026856186	T	T	T
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0.5114664942563850	0.5017617595048030	0.3594662640865404	T	T	T
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0.5976596293112688	0.4997013844991672	0.2364071121395351	T	T	T
0.6014867746033580	0.7479663615344385	0.3627697082915824	T	T	T
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0.8997507873317582	0.4983423657392168	0.3684314031216979	T	T	T
0.2389682129664219	0.2629159329636283	0.4654174696765672	T	T	T
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0.4024246257225720	0.4716251670204683	0.4565427572860242	T	T	T
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0.3160694997451953	0.1667048215208352	0.5510091654492997	T	T	T
0.3966850227197979	0.0759731218832921	0.4738066520521540	T	T	T
0.3994539902215613	0.2737797005702760	0.4601356730246945	T	T	T
0.4825526234669764	0.3612279079121479	0.5493332892195608	T	T	T
0.4802579138400155	0.1618898606252512	0.5507518647037499	T	T	T
0.5594711344393913	0.2572415867213357	0.4654596311023007	T	T	T
0.3997161830007940	0.2626697664729744	0.6230293315541634	T	T	T
0.5574538991065162	0.4473187236505276	0.4746635506497152	T	T	T
0.5543824465568193	0.0667988064673205	0.4759919080639446	T	T	T
0.0000000000000000	0.0000000000000000	0.0624065700000003	F	F	F
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0.9968978901192457	0.0003082027699732	0.4119443216586840	T	T	T
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0.0978044417780272	0.4009877485941382	0.2367658618551545	T	T	T
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0.1941658778413708	0.0013853178153779	0.4132112737146847	T	T	T
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0.3970336895013561	0.7502286753797215	0.2840410205944084	T	T	T
0.4965852779999977	0.8473499999999987	0.1121865699999987	F	F	F
0.4969230989301675	0.5977088817054057	0.2389416385473765	T	T	T
0.4950427462482190	0.8431640714629164	0.3697693142476136	T	T	T
0.4965852779999977	0.6526500000000013	0.1121865699999987	F	F	F
0.4969949996314543	0.9007558442374078	0.2373834038947168	T	T	T
0.5959023340000016	0.5000000000000000	0.0624065700000003	F	F	F
0.5958451767994288	0.7491622486496802	0.1859986142187831	T	T	T
0.6043286233650870	0.5014288202014939	0.3133858917540315	T	T	T
0.5959023340000016	0.5000000000000000	0.1619665699999970	F	F	F
0.5979708849580647	0.7499224331542700	0.2829596486081176	T	T	T
0.6074400091210345	0.5076885530519089	0.4100690213900881	T	T	T
0.6952193890000018	0.8473499999999987	0.1121865699999987	F	F	F
0.6980940566456945	0.5987815327473496	0.2370566958452036	T	T	T
0.7058167021228623	0.8427968280186575	0.3690211927995002	T	T	T
0.6952193890000018	0.6526500000000013	0.1121865699999987	F	F	F
0.6974877123279060	0.9005005958559514	0.2372768540743087	T	T	T
0.7114552862085430	0.6535880097384220	0.3673388115336548	T	T	T
0.7945364449999985	0.0000000000000000	0.0624065700000003	F	F	F
0.7952527164994068	0.2495333296523475	0.1862865303586465	T	T	T
0.7988838250070708	-0.0007189850002732	0.3143601736692501	T	T	T
0.7945364449999985	0.0000000000000000	0.1619665699999970	F	F	F
0.7976582383636911	0.2494775061626020	0.2836752343361999	T	T	T
0.8006020111262447	0.0005306238584147	0.4120394928074123	T	T	T
0.8938535010000024	0.3473499999999987	0.1121865699999987	F	F	F
0.8973143065754191	0.0997989158762974	0.2363072195092598	T	T	T
0.8987874596290751	0.3416085980014593	0.3668822105830380	T	T	T
0.8938535010000024	0.1526500000000013	0.1121865699999987	F	F	F
0.8976352358048788	0.3996699750483870	0.2357056500588149	T	T	T
0.8983653424831771	0.1563304465619101	0.3669541065754670	T	T	T
0.7945364449999985	0.5000000000000000	0.0624065700000003	F	F	F
0.7953228799272191	0.7499725667640589	0.1860545746632481	T	T	T

0.8020082994229232	0.4975874795219281	0.3139189055636529	T	T	T
0.7945364449999985	0.5000000000000000	0.1619665699999970	F	F	F
0.7982338273425263	0.7504637813407227	0.2831178857065819	T	T	T
0.8035182512723493	0.4967899065958469	0.4125439091168866	T	T	T
0.8938535010000024	0.8473499999999987	0.1121865699999987	F	F	F
0.8973964928320997	0.5998241842038690	0.2359209591429325	T	T	T
0.9002884783290904	0.8434799521865016	0.3672454546678811	T	T	T
0.8938535010000024	0.6526500000000013	0.1121865699999987	F	F	F
0.8972862768799043	0.9001264035609811	0.2360974620595899	T	T	T
0.9004398885324221	0.6563755826161689	0.3666803892004910	T	T	T
0.3981815178933330	0.6709282794139412	0.4578522233908925	T	T	T
0.5035407428828224	0.6495748700497819	0.3681065811656000	T	T	T
0.3870357496560839	0.6272734809269860	0.5457731690046075	T	T	T
0.3929574508509479	0.6293941637008903	0.4998746275303400	T	T	T

H_FS
Ti O Pt H O C
1.00000000000000
16.1999999999999993 0.0000000000000000 0.0000000000000000
0.0000000000000008 13.1883981985216909 0.0000000000000000
0.0000000000000015 0.0000000000000015 25.7900218205815115
Ti O Pt H O C
60 119 14 2 3 1
Selective dynamics
Direct

0.0000000000000000	0.2500000000000000	0.1121865696173359	F	F	F
0.9790075001549602	-0.0069045331358126	0.2331673588957598	T	T	T
0.0005928424988049	0.2475438739678586	0.3503361419753558	T	T	T
0.0993170556357299	0.0000000000000000	0.1121865696173359	F	F	F
0.0986899436391198	0.2445302114613627	0.2295258236214237	T	T	T
0.0854782064064924	-0.0003850469833271	0.3684109939652072	T	T	T
0.1986341112714598	0.2500000000000000	0.1121865696173359	F	F	F
0.1768117516356565	-0.0064998523164146	0.2333572549861189	T	T	T
0.1911815120531082	0.2572855800918105	0.3527589665912118	T	T	T
0.2979511669071826	0.0000000000000000	0.1121865696173359	F	F	F
0.3022830720311688	0.2491003456773714	0.2379180031429909	T	T	T
0.2667723893438261	0.9948250825891779	0.3600902021423905	T	T	T
0.0000000000000000	0.7500000000000000	0.1121865696173359	F	F	F
0.9801228275872457	0.4890618973685199	0.2333466627772515	T	T	T
0.0038679940357946	0.7475241083592420	0.3503096349571352	T	T	T
0.0993170556357299	0.5000000000000000	0.1121865696173359	F	F	F
0.0985678208048911	0.7432269250309136	0.2328210545815684	T	T	T
0.0827686028959231	0.5010812266111748	0.3649734105054527	T	T	T
0.1986341112714598	0.7500000000000000	0.1121865696173359	F	F	F
0.1805714530957450	0.4914402633946514	0.2342376915447691	T	T	T
0.1972146171342022	0.7517900285447596	0.3535899344761504	T	T	T
0.2979511669071826	0.5000000000000000	0.1121865696173359	F	F	F
0.2979100755530495	0.7497314243776763	0.2316540507913168	T	T	T
0.2623476253593280	0.5012326219693246	0.3666650081504825	T	T	T
0.3972682225429125	0.2500000000000000	0.1121865696173359	F	F	F
0.3821209339716113	0.9984699761208303	0.2347137294693515	T	T	T
0.4184897734721735	0.2597965492324182	0.3650516118054712	T	T	T
0.4965852781786424	0.0000000000000000	0.1121865696173359	F	F	F
0.4886657434867434	0.2565942560918162	0.2381303931480410	T	T	T
0.4910629248457483	0.9786423013944232	0.3522318575963281	T	T	T
0.5959023338143723	0.2500000000000000	0.1121865696173359	F	F	F
0.5804435400945586	0.0075212899518576	0.2354538144580756	T	T	T
0.6083112775826103	0.2616323590727191	0.3643572258294419	T	T	T
0.6952193894500951	0.0000000000000000	0.1121865696173359	F	F	F
0.6833280387721493	0.2494639228503141	0.2378448241869781	T	T	T
0.7162969646070023	-0.0055219276696823	0.3597891405508313	T	T	T
0.3972682225429125	0.7500000000000000	0.1121865696173359	F	F	F
0.3772347735893447	0.5008479061217965	0.2343516049558959	T	T	T
0.3950102362487081	0.7462230938876560	0.3551163566893201	T	T	T
0.4965852781786424	0.5000000000000000	0.1121865696173359	F	F	F
0.4940646845946507	0.7537748304018039	0.2357501652302884	T	T	T
0.4939830428499127	0.5075051631449535	0.3516037336200438	T	T	T
0.5959023338143723	0.7500000000000000	0.1121865696173359	F	F	F
0.5802886811225534	0.5076307476489014	0.2343581225803962	T	T	T
0.6303668438605843	0.7886137473764951	0.3542820242003248	T	T	T
0.6952193894500951	0.5000000000000000	0.1121865696173359	F	F	F
0.6877534596991152	0.7506459342706626	0.2328805779897515	T	T	T
0.7172798818691229	0.5128327367374073	0.3627069181244680	T	T	T
0.7945364450858250	0.2500000000000000	0.1121865696173359	F	F	F
0.7810099125478843	0.0018596860846270	0.2345550339765632	T	T	T
0.8129730829977168	0.2426856887457112	0.3591049322264765	T	T	T
0.8938535007215549	0.0000000000000000	0.1121865696173359	F	F	F
0.8842340910547198	0.2450134219842414	0.2335669267066992	T	T	T
0.9054755008188662	0.9908181170466135	0.3622360836684636	T	T	T

0.7945364450858250	0.7500000000000000	0.1121865696173359	F	F	F
0.7771580069291582	0.4987620451150670	0.2342327622231984	T	T	T
0.8131415743853940	0.7413107071322536	0.3479259964766951	T	T	T
0.8938535007215549	0.5000000000000000	0.1121865696173359	F	F	F
0.8942758052319414	0.7417714549964405	0.2258942539432249	T	T	T
0.9029072975736048	0.4983689369231183	0.3656324041073327	T	T	T
0.0000000000000000	0.0000000000000000	0.0624065696173304	F	F	F
0.9981637163157883	0.2489500008148755	0.1825737324697256	T	T	T
0.9935153627394780	0.9956924064566037	0.3116981164396179	T	T	T
0.0000000000000000	0.0000000000000000	0.1619665696173342	F	F	F
0.9971035804699422	0.2475275566262443	0.2800713467810156	T	T	T
0.9922843772072918	0.9955155146482122	0.4097822839673969	T	T	T
0.0993170556357299	0.3473499999999987	0.1121865696173359	F	F	F
0.0984252978273381	0.1012800692359345	0.2342886439817906	T	T	T
0.0887267625716930	0.3435212945924252	0.3640102992441176	T	T	T
0.0993170556357299	0.1526500000000013	0.1121865696173359	F	F	F
0.0937368939696929	0.3983030190437043	0.2339993528918052	T	T	T
0.0862266449970756	0.1523271230396432	0.3637445118398020	T	T	T
0.1986341112714598	0.0000000000000000	0.0624065696173304	F	F	F
0.1984689522407737	0.2496213974393983	0.1842480485200087	T	T	T
0.1861749869900645	0.9918434120473621	0.3098635573488477	T	T	T
0.1986341112714598	0.0000000000000000	0.1619665696173342	F	F	F
0.1913740036286482	0.2520972301801598	0.2809709763632234	T	T	T
0.2979511669071826	0.3473499999999987	0.1121865696173359	F	F	F
0.3036954252908042	0.1037718934377679	0.2386410829337995	T	T	T
0.2754407705017060	0.3526642421973100	0.3615932921946715	T	T	T
0.2979511669071826	0.1526500000000013	0.1121865696173359	F	F	F
0.2931575515332074	0.4020319668324087	0.2373144524912852	T	T	T
0.2633747427603543	0.1426366769364998	0.3596597166389910	T	T	T
0.0000000000000000	0.5000000000000000	0.0624065696173304	F	F	F
0.0006817798177619	0.7481196501149870	0.1829878324484041	T	T	T
0.9943210473043812	0.4987179183005359	0.3111719085191862	T	T	T
0.0000000000000000	0.5000000000000000	0.1619665696173342	F	F	F
0.0001474590830491	0.7472385169669542	0.2797780973607352	T	T	T
0.9924627050923477	0.4997495354276257	0.4095011155978443	T	T	T
0.0993170556357299	0.8473499999999987	0.1121865696173359	F	F	F
0.1029416162470411	0.6027315863838836	0.2343480339699053	T	T	T
0.0927388154491703	0.8411260089454925	0.3642670899786944	T	T	T
0.0993170556357299	0.6526500000000013	0.1121865696173359	F	F	F
0.0939641037073248	0.8979072043463001	0.2336121054994935	T	T	T
0.0929747523972801	0.6542719233665908	0.3631781514303077	T	T	T
0.1986341112714598	0.5000000000000000	0.0624065696173304	F	F	F
0.1989657383716112	0.7518334916511472	0.1843745170039857	T	T	T
0.1860952585684476	0.5019943125911095	0.3113406336167583	T	T	T
0.1986341112714598	0.5000000000000000	0.1619665696173342	F	F	F
0.1968155144439058	0.7533134757855662	0.2827051273431750	T	T	T
0.1777837422267972	0.5011316409499421	0.4109684627599715	T	T	T
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0.2978181739201654	0.6040293452634503	0.2358906174043671	T	T	T
0.2900774430758341	0.8424718813505553	0.3668050610403132	T	T	T
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0.2979734266593179	0.9005776404947669	0.2369031820910021	T	T	T
0.2824615359444164	0.6528138793579455	0.3650647911376836	T	T	T
0.3972682225429125	0.0000000000000000	0.0624065696173304	F	F	F
0.3973957615419578	0.2522933078999072	0.1861891269871560	T	T	T
0.3914345161454569	0.9970334148193086	0.3192685312190186	T	T	T
0.3972682225429125	0.0000000000000000	0.1619665696173342	F	F	F
0.3972469243959952	0.2548801650131329	0.2901119842626880	T	T	T
0.4692777097888183	0.9799582081448631	0.4249271928825226	T	T	T
0.4965852781786424	0.3473499999999987	0.1121865696173359	F	F	F
0.4972665513300804	0.1024919163162339	0.2390890574011623	T	T	T
0.5059222090110937	0.3583762518455174	0.3623733254113143	T	T	T
0.4965852781786424	0.1526500000000013	0.1121865696173359	F	F	F
0.5013564310193976	0.3992306702700193	0.2358564534880213	T	T	T

0.5050550414416703	0.1604537248675928	0.3684858227932920	T	T	T
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0.5974733987206936	0.2489870134868700	0.1853058633663079	T	T	T
0.5954404051276496	0.9916725534482799	0.3168025545340578	T	T	T
0.5959023338143723	0.0000000000000000	0.1619665696173342	F	F	F
0.5987603023514019	0.2502462055456808	0.2860576918296737	T	T	T
0.6416575355200145	0.8917051884507798	0.4047293584588657	T	T	T
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0.6924212898440896	0.0967104936702498	0.2382077745434251	T	T	T
0.6954087325233709	0.3689617968627036	0.3605249398599835	T	T	T
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0.6972519114596804	0.3976487135506230	0.2380418438752805	T	T	T
0.7074540625774136	0.1545067850988734	0.3597312625346785	T	T	T
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0.3977335826239420	0.7532145118585387	0.1848464022336793	T	T	T
0.4065447969378292	0.4993811639482527	0.3069277428270071	T	T	T
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0.3722048368773457	0.4907961763527244	0.4120559058976549	T	T	T
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0.4932038144215001	0.8321885698373986	0.3576591896884073	T	T	T
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0.7040305089963382	0.8947682778591677	0.2352079105023233	T	T	T
0.7063406381521494	0.6769410212239746	0.3692991860066920	T	T	T
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0.8060166178938597	0.0084935212036374	0.3108152163797754	T	T	T
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0.7988284769703864	0.2466807190437173	0.2838036786675404	T	T	T
0.8008402505407404	-0.0113540706026904	0.4093666093679161	T	T	T
0.8938535007215549	0.3473499999999987	0.1121865696173359	F	F	F
0.8965662843366525	0.0985384665528907	0.2336735134976392	T	T	T
0.8969923210971242	0.3456522805281212	0.3638493623825076	T	T	T
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0.8945268713567921	0.3943557000315849	0.2345417388999195	T	T	T
0.9022401874304944	0.1543372427890134	0.3655929896649199	T	T	T
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0.7941654625563953	0.7469333043456107	0.1837850503993230	T	T	T
0.7988523143405949	0.5125993760066915	0.3097125841710001	T	T	T
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0.8084047357035202	0.7306157729703626	0.2779273925026494	T	T	T
0.8034713367469242	0.5106324261864454	0.4072382617245508	T	T	T
0.8938535007215549	0.8473499999999987	0.1121865696173359	F	F	F
0.9031560635384086	0.5986302685092575	0.2308126009530017	T	T	T
0.9002293144335973	0.8416133731293549	0.3615274612949559	T	T	T
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0.8984061351055066	0.8927681608132183	0.2330039944803849	T	T	T
0.9064350794289049	0.6553109675846350	0.3633721527764426	T	T	T
0.3251193754984987	0.1674352016380330	0.4286630026015176	T	T	T
0.3707146873938525	0.3528129650773034	0.4508858294160454	T	T	T
0.4092046613354359	0.2026302859768539	0.5130230711581377	T	T	T

0.5101628545654677	0.3510812623552736	0.4976478428688106	T	T	T
0.3848364935011790	0.0007244558567369	0.4791676945784163	T	T	T
0.5198168233460501	0.0529214112577828	0.5345778387107213	T	T	T
0.5886023991843786	-0.0069383031146957	0.4512253324240540	T	T	T
0.5440065030726422	0.1854824523814102	0.4465961665777854	T	T	T
0.6400851656208150	0.2490857915958483	0.5232330498165318	T	T	T
0.6694137536316631	0.0769119195536640	0.5613012016689607	T	T	T
0.7149187390739635	0.2025667377815467	0.4394828029814128	T	T	T
0.5219820516098451	0.2157824054809758	0.5895892704502217	T	T	T
0.6485551637818584	0.3794775950050843	0.4451303967848609	T	T	T
0.7395681122198906	0.0246869234456336	0.4784386107917867	T	T	T
0.3809146266681739	0.5490928605407835	0.4347634112172580	T	T	T
0.6032573273568792	0.5734562792470576	0.4382988672265724	T	T	T
0.2888140491731502	-0.0226066730593476	0.5334994219180272	T	T	T
0.1828290224499939	0.9908694166971298	0.4082571599750571	T	T	T
0.2944648521237938	0.8067525141124602	0.5055996571233728	T	T	T
0.3083696186256885	0.8956252008989886	0.5105403088367246	T	T	T

O_FS
Ti O Pt O C
1.00000000000000
16.1999999999999993 0.0000000000000000 0.0000000000000000
0.0000000000000008 13.1883981985216909 0.0000000000000000
0.0000000000000015 0.0000000000000015 25.7900218205815115
Ti O Pt O C
60 119 14 3 1
Selective dynamics
Direct

0.0000000000000000	0.2500000000000000	0.1121865696173359	F	F	F
0.9991368923355298	0.0003889982025510	0.2364113336547198	T	T	T
0.9979920141111973	0.2509070043576557	0.3657825407050117	T	T	T
0.0993170556357299	0.0000000000000000	0.1121865696173359	F	F	F
0.0946821476027627	0.2505655536446078	0.2367302445731250	T	T	T
0.1074067108676336	0.0004397437998284	0.3678688529529377	T	T	T
0.1986341112714598	0.2500000000000000	0.1121865696173359	F	F	F
0.1976579105499554	0.0005443045681582	0.2372580603968636	T	T	T
0.1993964248371842	0.2508394264144785	0.3580398916539128	T	T	T
0.2979511669071826	0.0000000000000000	0.1121865696173359	F	F	F
0.2990499463288893	0.2504976737012335	0.2359236252985314	T	T	T
0.2988728173138251	0.0019880699490742	0.3695476214310470	T	T	T
0.0000000000000000	0.7500000000000000	0.1121865696173359	F	F	F
0.9991096239242861	0.5008078224801313	0.2364064148036813	T	T	T
0.9983641722818586	0.7508743934170388	0.3565721072388513	T	T	T
0.0993170556357299	0.5000000000000000	0.1121865696173359	F	F	F
0.0986231065172653	0.7505587575702168	0.2352029151016128	T	T	T
0.1073779222180585	0.5013369106088303	0.3678246786699513	T	T	T
0.1986341112714598	0.7500000000000000	0.1121865696173359	F	F	F
0.1976369082862348	0.5004474692947394	0.2372359465049070	T	T	T
0.1993147065464699	0.7508573893061651	0.3579470951836774	T	T	T
0.2979511669071826	0.5000000000000000	0.1121865696173359	F	F	F
0.2978233940390692	0.7504821907137569	0.2343626287507855	T	T	T
0.2987442172497421	0.4999352909836653	0.3695387658664785	T	T	T
0.3972682225429125	0.2500000000000000	0.1121865696173359	F	F	F
0.3976678142956916	0.0001780724327239	0.2373466397195907	T	T	T
0.4019010092065878	0.2509061106270725	0.3629422993766316	T	T	T
0.4965852781786424	0.0000000000000000	0.1121865696173359	F	F	F
0.4979069316236842	0.2504916349630040	0.2374866784485073	T	T	T
0.4904184705808172	-0.0001913627239282	0.3671270113853614	T	T	T
0.5959023338143723	0.2500000000000000	0.1121865696173359	F	F	F
0.5960724583918746	0.0002512228321615	0.2371148949430403	T	T	T
0.5997988174677371	0.2509687250760109	0.3599291009818347	T	T	T
0.6952193894500951	0.0000000000000000	0.1121865696173359	F	F	F
0.6986828008098958	0.2505735615775702	0.2361265679925117	T	T	T
0.6933139453688734	-0.0005579301412531	0.3624084221861328	T	T	T
0.3972682225429125	0.7500000000000000	0.1121865696173359	F	F	F
0.3976675337255739	0.5007310337763592	0.2373540108543815	T	T	T
0.3964604146736614	0.7510586678879511	0.3579798607873989	T	T	T
0.4965852781786424	0.5000000000000000	0.1121865696173359	F	F	F
0.4967394861015209	0.7505304075474062	0.2353297909493966	T	T	T
0.4902504286596441	0.5021096354439241	0.3671528613529534	T	T	T
0.5959023338143723	0.7500000000000000	0.1121865696173359	F	F	F
0.5959986322907622	0.5007914124801893	0.2371067001917081	T	T	T
0.5975273258343585	0.7509186917483273	0.3573489296677778	T	T	T
0.6952193894500951	0.5000000000000000	0.1121865696173359	F	F	F
0.6961618671247390	0.7505252929749886	0.2341365184826279	T	T	T
0.6931795521331847	0.5023732558138223	0.3624225097071725	T	T	T
0.7945364450858250	0.2500000000000000	0.1121865696173359	F	F	F
0.7970957550784797	0.0010146012899208	0.2371757154625129	T	T	T
0.7983338787354711	0.2508076728771136	0.3618625541209897	T	T	T
0.8938535007215549	0.0000000000000000	0.1121865696173359	F	F	F
0.8973041278553381	0.2505815868325181	0.2382480988596853	T	T	T
0.9028605073749084	-0.0000031073336541	0.3619516704283529	T	T	T

0.7945364450858250	0.7500000000000000	0.1121865696173359	F	F	F
0.7971028905903931	0.5000647386504253	0.2371868828358071	T	T	T
0.7981581538931620	0.7508197310188867	0.3567264506684991	T	T	T
0.8938535007215549	0.5000000000000000	0.1121865696173359	F	F	F
0.8972337297069165	0.7505837473565442	0.2333591939457338	T	T	T
0.9028245788136879	0.5017396860657355	0.3618950076493824	T	T	T
0.0000000000000000	0.0000000000000000	0.0624065696173304	F	F	F
0.9975622621699333	0.2503494192674598	0.1858997367415601	T	T	T
0.9972238001620699	0.9983173694040314	0.3146044492863401	T	T	T
0.0000000000000000	0.0000000000000000	0.1619665696173342	F	F	F
0.9978985953678974	0.2505792048307632	0.2851818521636075	T	T	T
-0.0004469259682869	0.9950629156991596	0.4124145821795045	T	T	T
0.0993170556357299	0.3473499999999987	0.1121865696173359	F	F	F
0.0980426853514246	0.1011259016716407	0.2378767435582411	T	T	T
0.1004071216851599	0.3447342376592168	0.3688935125356393	T	T	T
0.0993170556357299	0.1526500000000013	0.1121865696173359	F	F	F
0.0980369682449282	0.3999299158423853	0.2379964081269957	T	T	T
0.1004148751061274	0.1570890738032755	0.3689656002131161	T	T	T
0.1986341112714598	0.0000000000000000	0.0624065696173304	F	F	F
0.1982501508397369	0.2503769206851413	0.1865247633822152	T	T	T
0.1993385552226431	0.0015074475481482	0.3153725728433797	T	T	T
0.1986341112714598	0.0000000000000000	0.1619665696173342	F	F	F
0.1978011819235151	0.2505745111623809	0.2853087092386451	T	T	T
0.1990416040508036	-0.0002386122135390	0.4123707194225645	T	T	T
0.2979511669071826	0.3473499999999987	0.1121865696173359	F	F	F
0.2979510937082974	0.1010074267385576	0.2379357887047594	T	T	T
0.2981217992340304	0.3438253800884231	0.3685094915573016	T	T	T
0.2979511669071826	0.1526500000000013	0.1121865696173359	F	F	F
0.2979380782210836	0.3999855442775617	0.2380374276214619	T	T	T
0.2981492451093140	0.1579881474136818	0.3685778192316775	T	T	T
0.0000000000000000	0.5000000000000000	0.0624065696173304	F	F	F
0.9943854828779378	0.7503127614908002	0.1847190011994167	T	T	T
0.9972687745877137	0.5033426090612049	0.3145960828400520	T	T	T
0.0000000000000000	0.5000000000000000	0.1619665696173342	F	F	F
0.9927308591987449	0.7506404750073888	0.2851522561704664	T	T	T
-0.0003407931751798	0.5069110659943399	0.4123164790007082	T	T	T
0.0993170556357299	0.8473499999999987	0.1121865696173359	F	F	F
0.0985873329503238	0.5956037916919555	0.2380051710730120	T	T	T
0.0989863841871873	0.8438450152650511	0.3670541033636134	T	T	T
0.0993170556357299	0.6526500000000013	0.1121865696173359	F	F	F
0.0985980655391149	0.9054515505851224	0.2381453853757346	T	T	T
0.0989922214963649	0.6579832125926702	0.3670997812414629	T	T	T
0.1986341112714598	0.5000000000000000	0.0624065696173304	F	F	F
0.2020261469695425	0.7503223549366128	0.1854508789299981	T	T	T
0.1993491421558442	0.5001828896282441	0.3153651414516496	T	T	T
0.1986341112714598	0.5000000000000000	0.1619665696173342	F	F	F
0.2030374333734304	0.7505741614264648	0.2864067677610508	T	T	T
0.1990171498511734	0.5020815410171310	0.4123750580758373	T	T	T
0.2979511669071826	0.8473499999999987	0.1121865696173359	F	F	F
0.2976610254020759	0.5988858191008892	0.2375549255374726	T	T	T
0.2982630751111255	0.8442484459461475	0.3698709647898097	T	T	T
0.2979511669071826	0.6526500000000013	0.1121865696173359	F	F	F
0.2976403053825891	0.9020895215543978	0.2376409121229821	T	T	T
0.2982623699861661	0.6576534280802026	0.3699564899499381	T	T	T
0.3972682225429125	0.0000000000000000	0.0624065696173304	F	F	F
0.3979188923258959	0.2503145449302865	0.1869699441494285	T	T	T
0.3966167905519212	-0.0004355422478595	0.3152529234914210	T	T	T
0.3972682225429125	0.0000000000000000	0.1619665696173342	F	F	F
0.3978764357771323	0.2506046977976837	0.2869702958697419	T	T	T
0.3986593827607858	0.0025194919861844	0.4120022890635757	T	T	T
0.4965852781786424	0.3473499999999987	0.1121865696173359	F	F	F
0.4974726493942296	0.1008957724907255	0.2382642462731296	T	T	T
0.4965852781786424	0.1526500000000013	0.1121865696173359	F	F	F
0.4974281387425383	0.4001140100013634	0.2383503638134517	T	T	T

0.5005759563848222	0.1554930443627833	0.3636725957399873	T	T	T
0.5959023338143723	0.0000000000000000	0.0624065696173304	F	F	F
0.5966651692381078	0.2503429910717633	0.1864532142635604	T	T	T
0.5984951962271073	-0.0037194604709781	0.3148329044622236	T	T	T
0.5959023338143723	0.0000000000000000	0.1619665696173342	F	F	F
0.5982106136574994	0.2506545109005405	0.2845732314783537	T	T	T
0.5965685229294001	-0.0045475681769888	0.4128128910492639	T	T	T
0.6952193894500951	0.3473499999999987	0.1121865696173359	F	F	F
0.6973361389387528	0.0993585835945729	0.2379437856215253	T	T	T
0.6966572709371098	0.3474188058611115	0.3624376464373911	T	T	T
0.6952193894500951	0.1526500000000013	0.1121865696173359	F	F	F
0.6973366611972394	0.4016768654627815	0.2380347633343401	T	T	T
0.6966557839561001	0.1543803158628347	0.3624495765501488	T	T	T
0.3972682225429125	0.5000000000000000	0.0624065696173304	F	F	F
0.3936197681955187	0.7502972697378916	0.1854754796961453	T	T	T
0.3965873569643500	0.5021806177423811	0.3152711904650888	T	T	T
0.3972682225429125	0.5000000000000000	0.1619665696173342	F	F	F
0.3926013135225240	0.7506756258781657	0.2864375819548228	T	T	T
0.3985727317017416	0.4993889917611387	0.4120297155555416	T	T	T
0.4965852781786424	0.8473499999999987	0.1121865696173359	F	F	F
0.4969797799612032	0.5954922673213841	0.2380208409867691	T	T	T
0.4971399502455585	0.8437576268078657	0.3675626571538571	T	T	T
0.4965852781786424	0.6526500000000013	0.1121865696173359	F	F	F
0.4970179960514888	0.9055100283971307	0.2381674636880594	T	T	T
0.4970881143732295	0.6581705861332710	0.3675870365273879	T	T	T
0.5959023338143723	0.5000000000000000	0.0624065696173304	F	F	F
0.6004747206690476	0.7503060426658273	0.1854753935143066	T	T	T
0.5984382355399547	0.5053095720333803	0.3148242012155145	T	T	T
0.5959023338143723	0.5000000000000000	0.1619665696173342	F	F	F
0.6017797176201399	0.7506232410082755	0.2859837511193887	T	T	T
0.5965310141686281	0.5066119029960179	0.4127873970465169	T	T	T
0.6952193894500951	0.8473499999999987	0.1121865696173359	F	F	F
0.6971147543459355	0.6004132055335636	0.2371701628923945	T	T	T
0.6978268271309046	0.8431909804245122	0.3677670657606466	T	T	T
0.6952193894500951	0.6526500000000013	0.1121865696173359	F	F	F
0.6971356017427429	0.9006120481226195	0.2372615120463374	T	T	T
0.6977860083786722	0.6586621012351668	0.3677890107732227	T	T	T
0.7945364450858250	0.0000000000000000	0.0624065696173304	F	F	F
0.7963720730942063	0.2503762561679666	0.1863735795464734	T	T	T
0.7976162747115900	0.9955933198802398	0.3146814921862385	T	T	T
0.7945364450858250	0.0000000000000000	0.1619665696173342	F	F	F
0.7972958259738175	0.2506090410300787	0.2840307038889959	T	T	T
0.7974394661306921	0.9913633974991749	0.4099864338639154	T	T	T
0.8938535007215549	0.3473499999999987	0.1121865696173359	F	F	F
0.8969411080301237	0.0993079367694923	0.2372743266588413	T	T	T
0.8973503744982593	0.3474927387882740	0.3620527025836378	T	T	T
0.8938535007215549	0.1526500000000013	0.1121865696173359	F	F	F
0.8969714245061964	0.4017459229562148	0.2373904559833118	T	T	T
0.8973155473363464	0.1542416993020109	0.3621050151997300	T	T	T
0.7945364450858250	0.5000000000000000	0.0624065696173304	F	F	F
0.7958974763064698	0.7503542053114139	0.1865821579726240	T	T	T
0.7976304857622105	0.5059839656977965	0.3146626713884802	T	T	T
0.7945364450858250	0.5000000000000000	0.1619665696173342	F	F	F
0.7976742686001956	0.7505797514907063	0.2845082238530880	T	T	T
0.7974274942631200	0.5106016187114603	0.4098951527300572	T	T	T
0.8938535007215549	0.8473499999999987	0.1121865696173359	F	F	F
0.8972023374978642	0.6005925198140162	0.2363602308361055	T	T	T
0.8981844246965520	0.8433307295655030	0.3673834296849444	T	T	T
0.8938535007215549	0.6526500000000013	0.1121865696173359	F	F	F
0.8971776517784866	0.9004395657839533	0.2364243039460390	T	T	T
0.8982167520212996	0.6584654992285158	0.3674149403076115	T	T	T
0.6229306101194841	0.2515312164063436	0.4814469946122217	T	T	T
0.6390059684516423	0.4441112545704226	0.4793185990880182	T	T	T
0.7161784006189975	0.3546997237767523	0.5547912097792309	T	T	T

0.7957663009688536	0.4417451757159367	0.4770419640641769	T	T	T
0.6388927989154811	0.0589319156421092	0.4791527322787956	T	T	T
0.7160500092516170	0.1480492622878706	0.5548184636380721	T	T	T
0.7956696730886946	0.0606535306916187	0.4770514626270763	T	T	T
0.7864791991273390	0.2511432143939357	0.4614073339199542	T	T	T
0.8810582540913059	0.3522093083647286	0.5529520464365716	T	T	T
0.8809587251589814	0.1503414334571322	0.5529399223401562	T	T	T
0.9505168371677620	0.2510284314028321	0.4667687947578650	T	T	T
0.7988368314132110	0.2512450443913976	0.6249898075776722	T	T	T
0.9540866005808596	0.4397842416931843	0.4764876922057366	T	T	T
0.9539626733779066	0.0622863429271497	0.4766225920002710	T	T	T
0.4301244331141502	0.2506662622794063	0.4461220411777359	T	T	T
0.5005125100723460	0.3463268808587983	0.3637401735344632	T	T	T
0.4957049494996048	0.2533350613131031	0.5247695595612946	T	T	T
0.4881930033529016	0.2518212430059808	0.4770357078772148	T	T	T

CO2_desorption_2
R
Ti Pt O C
1.00000000000000
16.1999999999999993 0.0000000000000000 0.0000000000000000
0.0000000000000008 13.1883981985216909 0.0000000000000000
0.0000000000000015 0.0000000000000015 25.7900218205815115
Ti Pt O C
60 14 120 1
Selective dynamics
Direct

0.0000000000000000	0.2500000000000000	0.1121865699999987	F	F	F
0.9977651818134164	-0.0002805685319515	0.2364916011449217	T	T	T
0.9959048191200672	0.2493025029910111	0.3565417524604287	T	T	T
0.0993170559999967	0.0000000000000000	0.1121865699999987	F	F	F
0.1010708397620843	0.2494723547698746	0.2366101511043577	T	T	T
0.0858064657859721	0.9979019399879668	0.3676226962124832	T	T	T
0.1986341109999969	0.2500000000000000	0.1121865699999987	F	F	F
0.1963083925039191	0.9988668718051453	0.2374816696415379	T	T	T
0.1965158385380952	0.2505033941366567	0.3635129758430001	T	T	T
0.2979511670000008	0.0000000000000000	0.1121865699999987	F	F	F
0.2976907617796679	0.2489009690972491	0.2374603000626023	T	T	T
0.2927770612553514	0.9969868386744997	0.3625496360910099	T	T	T
0.0000000000000000	0.7500000000000000	0.1121865699999987	F	F	F
0.9966197460899047	0.4998937874756701	0.2348304016047924	T	T	T
0.9938937038465767	0.7508191647557342	0.3574681797762586	T	T	T
0.0993170559999967	0.5000000000000000	0.1121865699999987	F	F	F
0.0991876298290221	0.7499367753947941	0.2367686502568783	T	T	T
0.0778342062594432	0.5010612288906690	0.3608189801443610	T	T	T
0.1986341109999969	0.7500000000000000	0.1121865699999987	F	F	F
0.1970883965432795	0.5003895363427969	0.2373330014525355	T	T	T
0.1965562347349220	0.7477397856859620	0.3657310884848787	T	T	T
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0.2926575376686703	0.7505118770465080	0.2382984215879926	T	T	T
0.3011700317672057	0.4971808760948453	0.3598515339950636	T	T	T
0.3972682229999975	0.2500000000000000	0.1121865699999987	F	F	F
0.3967166106476040	-0.0004703846670355	0.2372961376651005	T	T	T
0.3961282740441188	0.2483131297204754	0.3599230843666622	T	T	T
0.4965852779999977	0.0000000000000000	0.1121865699999987	F	F	F
0.4974093038763944	0.2490332834743766	0.2378168054545420	T	T	T
0.5007353926197284	0.0000888628563810	0.3637522411410306	T	T	T
0.5959023340000016	0.2500000000000000	0.1121865699999987	F	F	F
0.5974108748349868	0.9997156057154667	0.2375690288109160	T	T	T
0.5960963847941511	0.2507331146106062	0.3659157157587146	T	T	T
0.6952193890000018	0.0000000000000000	0.1121865699999987	F	F	F
0.6924226078966507	0.2498162410083110	0.2368915353564474	T	T	T
0.7035927731548004	0.0012339853476290	0.3689743017731918	T	T	T
0.3972682229999975	0.7500000000000000	0.1121865699999987	F	F	F
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0.4965852779999977	0.5000000000000000	0.1121865699999987	F	F	F
0.4949236904994052	0.7502648291464974	0.2339612734868562	T	T	T
0.5113121130645994	0.4998258661451524	0.3609737259212584	T	T	T
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0.6962773797062236	0.7501050513003898	0.2353406683237846	T	T	T
0.7072271008806671	0.5021417844146323	0.3671584832898576	T	T	T
0.7945364449999985	0.2500000000000000	0.1121865699999987	F	F	F
0.7955260499053320	0.9998178291219727	0.2375383967238899	T	T	T
0.7964015770523747	0.2511856584018968	0.3571301173667116	T	T	T
0.8938535010000024	0.0000000000000000	0.1121865699999987	F	F	F
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0.7975880201251730	0.7518044994351809	0.3573239131061437	T	T	T
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0.2290732974640995	0.2734385416797308	0.4600250733460695	T	T	T
0.2282736112655578	0.4677158183520978	0.4569332187782844	T	T	T
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0.3857295871470807	0.4690627913995862	0.4524959759203616	T	T	T
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0.3902336343864036	0.2739773137596117	0.4564191142517978	T	T	T
0.4665101363698313	0.3762320995555301	0.5461471165396842	T	T	T
0.4699979111249185	0.1773469043486823	0.5507318116355990	T	T	T
0.5500475405499254	0.2672785302195277	0.4652336750000340	T	T	T
0.3738848228733001	0.2878105202212185	0.6170156815121204	T	T	T
0.5410520131884495	0.4580892157727591	0.4712584369120631	T	T	T
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0.9940596065987430	0.0028354659818602	0.4123908767080170	T	T	T
0.0993170559999967	0.3473499999999987	0.1121865699999987	F	F	F
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0.0917912077504907	0.3464357213344817	0.3662783495233425	T	T	T
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0.1975292116909568	0.9951923250529209	0.3147882933447332	T	T	T
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0.1935891526542791	0.9942117939227554	0.4120940382370793	T	T	T
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0.9910570073947764	0.7485037994293373	0.2853921610874235	T	T	T
0.9944310875289688	0.4983126561693619	0.4115242574909911	T	T	T
0.0993170559999967	0.8473499999999987	0.1121865699999987	F	F	F
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0.0870266556528595	0.8440660661702800	0.3681443608744117	T	T	T
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0.1951694534571768	0.5047012583648777	0.3240043212102613	T	T	T
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0.1170871449157453	0.6805247350761134	0.5333189060169908	T	T	T
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0.3974737453866048	0.9950389016042906	0.3152592444360152	T	T	T
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0.3957128131118004	0.9965918925146193	0.4115437981387928	T	T	T
0.4965852779999977	0.3473499999999987	0.1121865699999987	F	F	F
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0.5003374185939151	0.3484013927857804	0.3594179806515218	T	T	T
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0.4964388885228035	0.1545311692063344	0.3618575935969164	T	T	T
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0.5958625777324089	0.2502849487216785	0.1863838792419733	T	T	T
0.5959307370164756	0.9976445929039537	0.3158723984856620	T	T	T
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0.5974720301090246	0.2498567401635117	0.2850657281439714	T	T	T
0.5959806066315947	0.0027371902852764	0.4151243458150068	T	T	T
0.6952193890000018	0.3473499999999987	0.1121865699999987	F	F	F
0.6961126103902553	0.1001639457218745	0.2379969694175241	T	T	T
0.6998347394952582	0.3453358326550593	0.3678956469900977	T	T	T
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0.6967627218554728	0.3999746654713042	0.2375987683500005	T	T	T
0.6991664001245796	0.1574796195189707	0.3689819962503936	T	T	T
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0.3965692263731018	0.7487787643829812	0.1864385471802983	T	T	T
0.4030025075673279	0.5031502818699033	0.3191721992616551	T	T	T
0.3972682229999975	0.5000000000000000	0.1619665699999970	F	F	F
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0.4965852779999977	0.8473499999999987	0.1121865699999987	F	F	F
0.4964258451990551	0.5982936108527033	0.2380586117882657	T	T	T
0.4985129660169958	0.8426634170895194	0.3695318919671538	T	T	T
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0.6021338020633550	0.5027575445340250	0.3139902594926141	T	T	T
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0.5910045542867625	0.7495621613830891	0.2861144605378595	T	T	T
0.6055037806445712	0.5127502442342822	0.4107429981923564	T	T	T
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0.6973060334920131	0.5948180156881883	0.2377050481641023	T	T	T
0.6960805543991102	0.8449373098863174	0.3682366024620182	T	T	T
0.6952193890000018	0.6526500000000013	0.1121865699999987	F	F	F
0.6964522686118479	0.9051520758201808	0.2383530892496346	T	T	T
0.6996164596153516	0.6587722748479776	0.3662866928957429	T	T	T
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0.7947176661898430	0.2499479435104301	0.1863444018090509	T	T	T
0.7963434061100003	0.0013584490917288	0.3153325444206375	T	T	T
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0.7966957183154739	0.2504742075441301	0.2842744311021349	T	T	T
0.7965276741866039	0.0005790313503905	0.4125494238356341	T	T	T
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0.8938535010000024	0.1526500000000013	0.1121865699999987	F	F	F
0.8968350934153343	0.3994275348732242	0.2360206427144605	T	T	T
0.8958113081909715	0.1579722518896313	0.3677721573901127	T	T	T

0.7945364449999985	0.5000000000000000	0.0624065700000003	F	F	F
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0.7991447844621010	0.5003626801288678	0.3153464987789399	T	T	T
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0.8023023680864960	0.7506484962127671	0.2855191822180541	T	T	T
0.7970931515434180	0.5006085146702196	0.4139331650920263	T	T	T
0.8938535010000024	0.8473499999999987	0.1121865699999987	F	F	F
0.8966250443062399	0.5979351403406744	0.2356510870903130	T	T	T
0.8955067799513893	0.8448267703424998	0.3691592603566892	T	T	T
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0.8966426162891670	0.9020269107165847	0.2366541561686348	T	T	T
0.8937409583167572	0.6574863720716418	0.3703210700845709	T	T	T
0.1893878530465415	0.7408465365708674	0.4605087534305042	T	T	T
0.1526265529986900	0.7097771566672536	0.4968257699005220	T	T	T

H
Ti O Pt H C
1.00000000000000
16.1999999999999993 0.0000000000000000 0.0000000000000000
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Ti O Pt H C
60 121 14 2 1
Selective dynamics
Direct

0.0000000000000000	0.2500000000000000	0.1121865696173359	F	F	F
0.0132853512183240	0.0059293725680739	0.2338097937041259	T	T	T
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0.0993170556357299	0.0000000000000000	0.1121865696173359	F	F	F
0.1121632225655139	0.2518626615711481	0.2373190714382012	T	T	T
0.1012425101247983	0.9987035571539794	0.3604219713741392	T	T	T
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0.2135799088263411	0.0048772685422443	0.2351205296524589	T	T	T
0.1912236645573772	0.2492799652325112	0.3674670436474470	T	T	T
0.2979511669071826	0.0000000000000000	0.1121865696173359	F	F	F
0.3071854568245910	0.2515598227203659	0.2368436747682332	T	T	T
0.3027560138631694	-0.0023858393227254	0.3686764213340509	T	T	T
0.0000000000000000	0.7500000000000000	0.1121865696173359	F	F	F
0.0170461721823439	0.5024198842062904	0.2324408691942755	T	T	T
0.0127126605567836	0.7462132237237039	0.3522536635623594	T	T	T
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0.1002141701018752	0.7559003409571855	0.2309022138380627	T	T	T
0.0921675780223221	0.4968845692768643	0.3572237931273747	T	T	T
0.1986341112714598	0.7500000000000000	0.1121865696173359	F	F	F
0.2133808928247360	0.5047465262495496	0.2334508618103080	T	T	T
0.2005346116385071	0.7512268372454004	0.3524421684603568	T	T	T
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0.2989939408193579	0.7552837762831928	0.2310657918141533	T	T	T
0.2961682259366347	0.4974974242280943	0.3533837682554495	T	T	T
0.3972682225429125	0.2500000000000000	0.1121865696173359	F	F	F
0.4128175844334778	0.0024626981083492	0.2351116716185217	T	T	T
0.3741725679027703	0.2409524004382404	0.3582113151976655	T	T	T
0.4965852781786424	0.0000000000000000	0.1121865696173359	F	F	F
0.5071281655494966	0.2519427979834719	0.2387307007349549	T	T	T
0.4980237488892293	0.0073681679235709	0.3509815142265604	T	T	T
0.5959023338143723	0.2500000000000000	0.1121865696173359	F	F	F
0.6140836348338925	-0.0008798736702324	0.2346996860616221	T	T	T
0.5853617973404445	0.2629520526863571	0.3623202546538536	T	T	T
0.6952193894500951	0.0000000000000000	0.1121865696173359	F	F	F
0.6981172271946402	0.2470225292943330	0.2353826284098518	T	T	T
0.7142120931650595	0.9882842996489607	0.3644309235944286	T	T	T
0.3972682225429125	0.7500000000000000	0.1121865696173359	F	F	F
0.4095746346481367	0.4990336182576237	0.2331484144034377	T	T	T
0.3905594401492384	0.7447864712399154	0.3523182560533782	T	T	T
0.4965852781786424	0.5000000000000000	0.1121865696173359	F	F	F
0.5019571097714528	0.7500531626526393	0.2299778936226341	T	T	T
0.5125682416721399	0.5160245477677023	0.3525038675272656	T	T	T
0.5959023338143723	0.7500000000000000	0.1121865696173359	F	F	F
0.6196400249071211	0.4994277824374731	0.2334142229849105	T	T	T
0.5774442184153926	0.7762568771893819	0.3519717361774783	T	T	T
0.6952193894500951	0.5000000000000000	0.1121865696173359	F	F	F
0.7052465833624146	0.7490967975769177	0.2361252015434385	T	T	T
0.7427294361354850	0.5105739761252511	0.3718065910241334	T	T	T
0.7945364450858250	0.2500000000000000	0.1121865696173359	F	F	F
0.8136184042534692	0.9979032194308883	0.2354960228111850	T	T	T
0.7989830190613304	0.2507545023334444	0.3549928084316491	T	T	T
0.8938535007215549	0.0000000000000000	0.1121865696173359	F	F	F
0.8980885401299863	0.2480640995088873	0.2295970736308778	T	T	T
0.9160408770349816	0.9877348563328742	0.3686305591928410	T	T	T

0.7945364450858250	0.7500000000000000	0.1121865696173359	F	F	F
0.8164583513777421	0.4995381911127297	0.2345787590933540	T	T	T
0.8305248258244059	0.7268431358419366	0.3544280487739476	T	T	T
0.8938535007215549	0.5000000000000000	0.1121865696173359	F	F	F
0.8969321877572999	0.7494239879734118	0.2312861548143590	T	T	T
0.9190371075161898	0.4838892901554263	0.3713423187071737	T	T	T
0.0000000000000000	0.0000000000000000	0.0624065696173304	F	F	F
0.9949928921541660	0.2500113862479945	0.1827644256852836	T	T	T
-0.0024014944163572	0.9946894404192809	0.3116324885106808	T	T	T
0.0000000000000000	0.0000000000000000	0.1619665696173342	F	F	F
0.9978761694406023	0.2452579409072224	0.2824815393793320	T	T	T
0.0041777653671197	0.9951276347310792	0.4093835524501465	T	T	T
0.0993170556357299	0.3473499999999987	0.1121865696173359	F	F	F
0.0974446530669677	0.1028620243547338	0.2346911904489536	T	T	T
0.1151681859087353	0.3553916870718565	0.3676183132573915	T	T	T
0.0993170556357299	0.1526500000000013	0.1121865696173359	F	F	F
0.0973001682006405	0.3977928675886986	0.2363012836069401	T	T	T
0.0946225380178164	0.1573499948778422	0.3666545395316644	T	T	T
0.1986341112714598	0.0000000000000000	0.0624065696173304	F	F	F
0.1990631047663929	0.2524174518406583	0.1844432206050719	T	T	T
0.1839819372078596	0.9974919978142607	0.3079498246189975	T	T	T
0.1986341112714598	0.0000000000000000	0.1619665696173342	F	F	F
0.1980254299521736	0.2515370895301688	0.2836925796568541	T	T	T
0.1930680123030572	0.9889522980108351	0.4063127970724837	T	T	T
0.2979511669071826	0.3473499999999987	0.1121865696173359	F	F	F
0.2966984666134708	0.1044327937466227	0.2355189339582083	T	T	T
0.2984316428699363	0.3526101682081991	0.3541842460513685	T	T	T
0.2979511669071826	0.1526500000000013	0.1121865696173359	F	F	F
0.2993701495182702	0.4039825882460386	0.2387954436871182	T	T	T
0.2905604147174707	0.1460799547674509	0.3525254886293306	T	T	T
0.0000000000000000	0.5000000000000000	0.0624065696173304	F	F	F
0.9989095618337057	0.7483042229595437	0.1836804795655308	T	T	T
0.0036763494002798	0.4916026932250474	0.3125130089814874	T	T	T
0.0000000000000000	0.5000000000000000	0.1619665696173342	F	F	F
0.0031775246582426	0.7468493329288677	0.2822872475709940	T	T	T
0.0132321085866448	0.4929300035201854	0.4105427411286223	T	T	T
0.0993170556357299	0.8473499999999987	0.1121865696173359	F	F	F
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0.1040694236320409	0.8386492396608636	0.3644807546122618	T	T	T
0.0993170556357299	0.6526500000000013	0.1121865696173359	F	F	F
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0.1078710969622672	0.6497488586241652	0.3661568182684269	T	T	T
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0.2002690797477457	0.5055931801557286	0.3149851688928531	T	T	T
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0.0283497922273138	0.2880913164500806	0.4865946406513951	T	T	T
0.2979511669071826	0.8473499999999987	0.1121865696173359	F	F	F
0.2967414620416737	0.6014858359345763	0.2362731119666477	T	T	T
0.2968646678835012	0.8416224875643062	0.3641760825220961	T	T	T
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0.2948356199307655	0.8991248704460515	0.2358401537565387	T	T	T
0.2968281525697159	0.6551495884042717	0.3666680154949410	T	T	T
0.3972682225429125	0.0000000000000000	0.0624065696173304	F	F	F
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0.3898164352728061	0.0030011097345340	0.3104317430108226	T	T	T
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0.3957789737729984	-0.0054707838917513	0.4085641621003827	T	T	T
0.4965852781786424	0.3473499999999987	0.1121865696173359	F	F	F
0.4958301495924083	0.1034665473799993	0.2373582573722466	T	T	T
0.5160379561251870	0.3728670983350258	0.3548582469297283	T	T	T
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0.4910130422563743	0.1682635185082241	0.3618073936483830	T	T	T
0.5959023338143723	0.0000000000000000	0.0624065696173304	F	F	F
0.5963296262001346	0.2517401278991415	0.1856974372683848	T	T	T
0.5950537581041985	0.0047335032136395	0.3110356881683959	T	T	T
0.5959023338143723	0.0000000000000000	0.1619665696173342	F	F	F
0.5995348020488769	0.2500580858880475	0.2861592769664290	T	T	T
0.5550829583517762	-0.0077357211056025	0.4110172525245213	T	T	T
0.6952193894500951	0.3473499999999987	0.1121865696173359	F	F	F
0.6966733049216627	0.1000800849843175	0.2360123566490188	T	T	T
0.7196463123465785	0.3583423289987462	0.3659228329130116	T	T	T
0.6952193894500951	0.1526500000000013	0.1121865696173359	F	F	F
0.6996304297155711	0.3994562608220993	0.2385516349239005	T	T	T
0.7150276607434511	0.1499228015888970	0.3682210486413435	T	T	T
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0.3965299418724275	0.7537285487357056	0.1841582612102440	T	T	T
0.4029629899084551	0.5141317149523001	0.3216690642084669	T	T	T
0.3972682225429125	0.5000000000000000	0.1619665696173342	F	F	F
0.3921777686553347	0.7460285912088972	0.2828864452083128	T	T	T
0.2428893647247493	0.5042882733380686	0.4236025278868749	T	T	T
0.4965852781786424	0.8473499999999987	0.1121865696173359	F	F	F
0.4861338372672909	0.6073327747077027	0.2340342543101553	T	T	T
0.4820459807344316	0.8512822195042781	0.3531847883582335	T	T	T
0.4965852781786424	0.6526500000000013	0.1121865696173359	F	F	F
0.4938788243577859	0.8981643433803783	0.2365127812443293	T	T	T
0.4953933382468183	0.6661367930180019	0.3726294556504378	T	T	T
0.5959023338143723	0.5000000000000000	0.0624065696173304	F	F	F
0.5973167228173660	0.7480009544034770	0.1847270772163612	T	T	T
0.5923284364705615	0.5269660405249689	0.3052896011820354	T	T	T
0.5959023338143723	0.5000000000000000	0.1619665696173342	F	F	F
0.5937008513796378	0.7485339837596856	0.2829733873298503	T	T	T
0.6226232602714817	0.5242604760105389	0.4055174592395245	T	T	T
0.6952193894500951	0.8473499999999987	0.1121865696173359	F	F	F
0.7017806364349111	0.6009137828066287	0.2356851661862423	T	T	T
0.6693774093667368	0.8519152165372021	0.3688698229835033	T	T	T
0.6952193894500951	0.6526500000000013	0.1121865696173359	F	F	F
0.6943670020219864	0.8954637783348389	0.2360775914590873	T	T	T
0.7432587550480857	0.6585718787071541	0.3816268629487699	T	T	T
0.7945364450858250	0.0000000000000000	0.0624065696173304	F	F	F
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0.7916235321458550	0.9892375596949236	0.3104495963024945	T	T	T
0.7945364450858250	0.0000000000000000	0.1619665696173342	F	F	F
0.7982902688815354	0.2466189189190132	0.2845113324803686	T	T	T
0.8093297796554435	0.9736947879002779	0.4078490907071829	T	T	T
0.8938535007215549	0.3473499999999987	0.1121865696173359	F	F	F
0.8977366019444466	0.0980331615810576	0.2358272670956057	T	T	T
0.9086705270480179	0.3356692732947381	0.3664483140711213	T	T	T
0.8938535007215549	0.1526500000000013	0.1121865696173359	F	F	F
0.8945160306966061	0.3948335769759501	0.2356496911027029	T	T	T
0.9000709206937145	0.1457772115689516	0.3634912539401616	T	T	T
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0.7965757924736171	0.7490816485827346	0.1847392170432978	T	T	T
0.8113799839875706	0.5068492505425901	0.3149226117383277	T	T	T
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0.8018155632432057	0.7458251584144159	0.2855863296332805	T	T	T
0.8277579173208832	0.4935005968814234	0.4163445555116786	T	T	T
0.8938535007215549	0.8473499999999987	0.1121865696173359	F	F	F
0.9010493986162867	0.5977766387621981	0.2350259312233336	T	T	T
0.9152559391831255	0.8317285787012031	0.3676448898494732	T	T	T
0.8938535007215549	0.6526500000000013	0.1121865696173359	F	F	F
0.8947064377402387	0.8950679124320150	0.2350386176944486	T	T	T
0.9223606296704810	0.6428814926622357	0.3636156067727768	T	T	T
0.1088184049527937	0.4116021888194023	0.5288255564037402	T	T	T
0.2721208655139836	0.2453763396632686	0.4496612196061465	T	T	T

0.3287623376090088	0.4220822305145918	0.4693519817124874	T	T	T
0.4012189029981592	0.2846186780788920	0.5251521917430194	T	T	T
0.4867633677260829	0.4096209130012262	0.4679744917655734	T	T	T
0.2415963395048054	0.0625100192906922	0.4670415260165973	T	T	T
0.3602748393993961	0.0953595672356405	0.5256483482529721	T	T	T
0.4749321660960703	0.0317142516316837	0.4676234111409812	T	T	T
0.4606461018387108	0.2223118455184083	0.4369252713187737	T	T	T
0.5734842096193807	0.2599451917165425	0.5137768623729922	T	T	T
0.6014510410904261	0.0658189835635178	0.5221217264036776	T	T	T
0.6699019803225942	0.1839430774430889	0.4422380116837321	T	T	T
0.4894993048116089	0.1526476727599376	0.5797037210237076	T	T	T
0.6375303784093274	0.3705834685816137	0.4402222153599104	T	T	T
0.7241119512507873	0.0114202012857061	0.4667549946710612	T	T	T
0.2386718594916202	0.5739725664623408	0.4360908108963025	T	T	T
0.6207635390646974	0.5769898804011849	0.4320940775534681	T	T	T
0.0687685504994351	0.3500429461816824	0.5075055030958142	T	T	T

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Ti O C Pt
1.00000000000000
16.1999999999999993 0.0000000000000000 0.0000000000000000
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0.0000000000000015 0.0000000000000015 25.7900218205815115
Ti O C Pt
60 122 1 14
Selective dynamics
Direct

0.0000000000000000	0.2500000000000000	0.1121865696173359	F	F	F
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0.0993170556357299	0.0000000000000000	0.1121865696173359	F	F	F
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0.1052962456520043	-0.0003145563980811	0.3676099416022163	T	T	T
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0.1973990860404674	0.0004312303925209	0.2370744255809187	T	T	T
0.1958212428591390	0.2501102035114650	0.3569560836680336	T	T	T
0.2979511669071826	0.0000000000000000	0.1121865696173359	F	F	F
0.3011096688025555	0.2500181402793178	0.2361143534479760	T	T	T
0.2962095027649713	0.0021963319945841	0.3692568710929460	T	T	T
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0.9978452262049420	0.5002938187471430	0.2361284250403809	T	T	T
0.9985220396824456	0.7500420267093518	0.3581640130078596	T	T	T
0.0993170556357299	0.5000000000000000	0.1121865696173359	F	F	F
0.0966140539145862	0.7500103623602105	0.2346824249184818	T	T	T
0.1051965875983219	0.5005072566357121	0.3676192362642177	T	T	T
0.1986341112714598	0.7500000000000000	0.1121865696173359	F	F	F
0.1973907190303207	0.4996263952903451	0.2370599507049105	T	T	T
0.1986258050041333	0.7500878253520735	0.3580924954906769	T	T	T
0.2979511669071826	0.5000000000000000	0.1121865696173359	F	F	F
0.2964818443699822	0.7500255851071708	0.2350130904222519	T	T	T
0.2960545770049453	0.4980226179956750	0.3692415197076052	T	T	T
0.3972682225429125	0.2500000000000000	0.1121865696173359	F	F	F
0.3971405757723905	0.0006651939919394	0.2375219548473146	T	T	T
0.3963788326362104	0.2501180005822515	0.3653731785571365	T	T	T
0.4965852781786424	0.0000000000000000	0.1121865696173359	F	F	F
0.4979143434287844	0.2500264143799425	0.2395078409128493	T	T	T
0.4896733850891323	0.0021399267688352	0.3680664776094780	T	T	T
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0.5967529238391164	0.0005789879022422	0.2373355388060344	T	T	T
0.5985068741326115	0.2499545235656901	0.3663133036550629	T	T	T
0.6952193894500951	0.0000000000000000	0.1121865696173359	F	F	F
0.6955173533714967	0.2500206361389393	0.2374211199405703	T	T	T
0.6930802782113107	0.9992703055365957	0.3624957767049066	T	T	T
0.3972682225429125	0.7500000000000000	0.1121865696173359	F	F	F
0.3971275594472948	0.4994015375944237	0.2375263246293762	T	T	T
0.3970768190640176	0.7500614598734243	0.3579019514019841	T	T	T
0.4965852781786424	0.5000000000000000	0.1121865696173359	F	F	F
0.4964801335180897	0.7500298125105339	0.2347763097043277	T	T	T
0.4895484683431727	0.4979249195811644	0.3680835385742074	T	T	T
0.5959023338143723	0.7500000000000000	0.1121865696173359	F	F	F
0.5967425359962931	0.4994233548220596	0.2373349592632329	T	T	T
0.5959816141335782	0.7500013775812615	0.3573517175159229	T	T	T
0.6952193894500951	0.5000000000000000	0.1121865696173359	F	F	F
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0.6929931632204805	0.5007035081254368	0.3625110044986976	T	T	T
0.7945364450858250	0.2500000000000000	0.1121865696173359	F	F	F
0.7971976245615268	0.0000941531372584	0.2371160316377328	T	T	T
0.7973365114390379	0.2500177602236506	0.3612173091034995	T	T	T
0.8938535007215549	0.0000000000000000	0.1121865696173359	F	F	F
0.8964238356538800	0.2500199633271146	0.2375887455121004	T	T	T
0.9024351140406808	0.9990623734325483	0.3617147202366616	T	T	T

0.7945364450858250	0.7500000000000000	0.1121865696173359	F	F	F
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0.7974323833692557	0.7500130768971809	0.3569782447798886	T	T	T
0.8938535007215549	0.5000000000000000	0.1121865696173359	F	F	F
0.8986881851343940	0.7500120985100818	0.2335253129506842	T	T	T
0.9023603827787939	0.5010118801693558	0.3616987062314974	T	T	T
0.0000000000000000	0.0000000000000000	0.0624065696173304	F	F	F
0.9973423765420829	0.2500057079713552	0.1858228523020488	T	T	T
0.9975145102530563	0.9956985651447738	0.3143537647774031	T	T	T
0.0000000000000000	0.0000000000000000	0.1619665696173342	F	F	F
0.9976336937820511	0.2500225978996611	0.2843616865134648	T	T	T
-0.0009000065054935	0.9938081704823498	0.4123489890827085	T	T	T
0.0993170556357299	0.3473499999999987	0.1121865696173359	F	F	F
0.0977524718056029	0.0987965312427700	0.2376802622583484	T	T	T
0.0975621147295828	0.3447359376721348	0.3681774001397675	T	T	T
0.0993170556357299	0.1526500000000013	0.1121865696173359	F	F	F
0.0977494618289518	0.4012381743373627	0.2376832312799419	T	T	T
0.0975839351989226	0.1554194582807088	0.3682045028419647	T	T	T
0.1986341112714598	0.0000000000000000	0.0624065696173304	F	F	F
0.1981620210567441	0.2500084714983171	0.1861787160695239	T	T	T
0.1976232351080147	0.9984270825677957	0.3149200416329350	T	T	T
0.1986341112714598	0.0000000000000000	0.1619665696173342	F	F	F
0.1968048742107930	0.2500192530295007	0.2838093393738617	T	T	T
0.1974071817748498	0.9969030131714579	0.4122616888180215	T	T	T
0.2979511669071826	0.3473499999999987	0.1121865696173359	F	F	F
0.2975318696558201	0.0985930112208413	0.2378836159449445	T	T	T
0.2892823083977032	0.3448945118555974	0.3681588864306398	T	T	T
0.2979511669071826	0.1526500000000013	0.1121865696173359	F	F	F
0.2975101442954376	0.4014636093619644	0.2378966951949146	T	T	T
0.2895386880422545	0.1554294054365248	0.3681725020819351	T	T	T
0.0000000000000000	0.5000000000000000	0.0624065696173304	F	F	F
0.9981684019293018	0.7500142180621477	0.1912315204776655	T	T	T
0.9974836436704493	0.5043758631164227	0.3143477838107354	T	T	T
0.0000000000000000	0.5000000000000000	0.1619665696173342	F	F	F
0.9976355438624096	0.7500434489469634	0.2863302643053475	T	T	T
-0.0009688778032880	0.5063016098290286	0.4123436969718611	T	T	T
0.0993170556357299	0.8473499999999987	0.1121865696173359	F	F	F
0.0986477575096442	0.5998176906767702	0.2378468031860557	T	T	T
0.0988650263955262	0.8424144802134260	0.3681048309288423	T	T	T
0.0993170556357299	0.6526500000000013	0.1121865696173359	F	F	F
0.0986616821992234	0.9002322056756804	0.2378511376322612	T	T	T
0.0988143735192561	0.6577575357472560	0.3680999211022489	T	T	T
0.1986341112714598	0.5000000000000000	0.0624065696173304	F	F	F
0.1983395769538150	0.7500092550120812	0.1875380365877757	T	T	T
0.1975470385861463	0.5017596259225289	0.3149191109663951	T	T	T
0.1986341112714598	0.5000000000000000	0.1619665696173342	F	F	F
0.1983032169862917	0.7500557552598215	0.2855828529028509	T	T	T
0.1973019479433265	0.5033780778241582	0.4122715053657877	T	T	T
0.2979511669071826	0.8473499999999987	0.1121865696173359	F	F	F
0.2978325061916820	0.6003301476472743	0.2378741051566640	T	T	T
0.2980414330953205	0.8429322287175580	0.3683906634803036	T	T	T
0.2979511669071826	0.6526500000000013	0.1121865696173359	F	F	F
0.2978422157543830	0.8997274582132317	0.2378739891779224	T	T	T
0.2980130927793342	0.6572236298518243	0.3683846243767168	T	T	T
0.3972682225429125	0.0000000000000000	0.0624065696173304	F	F	F
0.3980281948860733	0.2500192671030163	0.1863626122497566	T	T	T
0.3971407111570304	0.0006187907266194	0.3151469289947214	T	T	T
0.3972682225429125	0.0000000000000000	0.1619665696173342	F	F	F
0.3974520766739429	0.2500329680166978	0.2840759229978588	T	T	T
0.3961254184283347	0.0035316326843116	0.4120059912946553	T	T	T
0.4965852781786424	0.3473499999999987	0.1121865696173359	F	F	F
0.4975110222295740	0.0975915164092007	0.2382934039077178	T	T	T
0.5022966366829756	0.3457620590995834	0.3695696699226094	T	T	T
0.4965852781786424	0.1526500000000013	0.1121865696173359	F	F	F

0.4974964479164182	0.4024441970749648	0.2382977143621123	T	T	T
0.5025040171308787	0.1542035328170377	0.3695499742186230	T	T	T
0.5959023338143723	0.0000000000000000	0.0624065696173304	F	F	F
0.5964066208650174	0.2500136676605408	0.1866350053642107	T	T	T
0.5974179760908672	0.9954890474724986	0.3148379443733075	T	T	T
0.5959023338143723	0.0000000000000000	0.1619665696173342	F	F	F
0.5967930103776363	0.2500387074696667	0.2855076369807756	T	T	T
0.5969628314297444	0.9926703436598958	0.4130792072924457	T	T	T
0.6952193894500951	0.3473499999999987	0.1121865696173359	F	F	F
0.6964514322616312	0.0978024326271314	0.2382783099178118	T	T	T
0.6991916547982409	0.3475407911554517	0.3621261595188632	T	T	T
0.6952193894500951	0.1526500000000013	0.1121865696173359	F	F	F
0.6964556112510036	0.4022299104389826	0.2382842459591714	T	T	T
0.6991910143402494	0.1524994273097199	0.3621274078678623	T	T	T
0.3972682225429125	0.5000000000000000	0.0624065696173304	F	F	F
0.3969639846462930	0.7500115216713873	0.1867028448952598	T	T	T
0.3970912650457604	0.4994531837326381	0.3151489540317946	T	T	T
0.3972682225429125	0.5000000000000000	0.1619665696173342	F	F	F
0.3971354742618228	0.7500376412291468	0.2850665075204596	T	T	T
0.3960302454439092	0.4965721556581938	0.4120123163174640	T	T	T
0.4965852781786424	0.8473499999999987	0.1121865696173359	F	F	F
0.4965030781714976	0.6008704027691359	0.2376463375961998	T	T	T
0.4960795107619138	0.8429198135313759	0.3682440761786324	T	T	T
0.4965852781786424	0.6526500000000013	0.1121865696173359	F	F	F
0.4965136307299311	0.8991705773950815	0.2376434685612666	T	T	T
0.4960490550738209	0.6571385531446698	0.3682348762096737	T	T	T
0.5959023338143723	0.5000000000000000	0.0624065696173304	F	F	F
0.5963041730289217	0.7500192432839075	0.1866776486308473	T	T	T
0.5973773133651483	0.5044930132802012	0.3148434729904647	T	T	T
0.5959023338143723	0.5000000000000000	0.1619665696173342	F	F	F
0.5961324392356671	0.7500144483901894	0.2848292083701410	T	T	T
0.5968809099225477	0.5072559813880991	0.4130830348697564	T	T	T
0.6952193894500951	0.8473499999999987	0.1121865696173359	F	F	F
0.6964352823729932	0.6009998078301427	0.2374080993330405	T	T	T
0.6963762652218120	0.8418952385394087	0.3669921796948054	T	T	T
0.6952193894500951	0.6526500000000013	0.1121865696173359	F	F	F
0.6964399802182238	0.8990229972868143	0.2374021911489114	T	T	T
0.6963480631874387	0.6581216285354121	0.3670056281998856	T	T	T
0.7945364450858250	0.0000000000000000	0.0624065696173304	F	F	F
0.7953435496202785	0.2500068357059501	0.1864469769193315	T	T	T
0.7975232741283866	0.9939746545460874	0.3144108640779189	T	T	T
0.7945364450858250	0.0000000000000000	0.1619665696173342	F	F	F
0.7972092602079912	0.2500108192576291	0.2835093996980415	T	T	T
0.7979554856695554	0.9887111410486377	0.4096871822479357	T	T	T
0.8938535007215549	0.3473499999999987	0.1121865696173359	F	F	F
0.8970070746497896	0.0981066304428670	0.2371900165985857	T	T	T
0.8974846941765804	0.3472971696852971	0.3615928092349533	T	T	T
0.8938535007215549	0.1526500000000013	0.1121865696173359	F	F	F
0.8969980370523338	0.4019246960276461	0.2371916233637590	T	T	T
0.8975094010478741	0.1527745938011479	0.3615990193730601	T	T	T
0.7945364450858250	0.5000000000000000	0.0624065696173304	F	F	F
0.7957558844437607	0.7500016274688417	0.1874069796518818	T	T	T
0.7974938579571130	0.5060784014653892	0.3144151945311651	T	T	T
0.7945364450858250	0.5000000000000000	0.1619665696173342	F	F	F
0.7972769027076935	0.7500176148331027	0.2849422820151514	T	T	T
0.7979155566809404	0.5112859829273430	0.4096931573081979	T	T	T
0.8938535007215549	0.8473499999999987	0.1121865696173359	F	F	F
0.8968081209992209	0.5999624001916268	0.2369158405062066	T	T	T
0.8981820839209298	0.8421369348475222	0.3673894073674221	T	T	T
0.8938535007215549	0.6526500000000013	0.1121865696173359	F	F	F
0.8968113637398928	0.9000704091880904	0.2369148474281725	T	T	T
0.8981787240246055	0.6579350925707592	0.3673862093881657	T	T	T
0.3861308951153196	0.2505226074678835	0.4575901228939850	T	T	T
0.4357612878494732	0.2537303649488049	0.5431203489990654	T	T	T

0.4115947516950781	0.2521752818247189	0.5004162211931734	T	T	T
0.6397925919728100	0.2500006582587680	0.4687469799312454	T	T	T
0.6415503450490370	0.4406117230629625	0.4780793108166665	T	T	T
0.7168610075012430	0.3510065637610352	0.5539598943383016	T	T	T
0.7986793319668294	0.4414051670439791	0.4767156324525244	T	T	T
0.6415961262488935	0.0593717927242118	0.4780618271592831	T	T	T
0.7168471026688806	0.1489748447564401	0.5539598087505824	T	T	T
0.7986894768758825	0.0586136721372106	0.4767044978010613	T	T	T
0.7992239147200995	0.2500053113904922	0.4610779675045040	T	T	T
0.8811432778942250	0.3508391402749731	0.5536213788205391	T	T	T
0.8811823824401017	0.1492271478671244	0.5536048131352668	T	T	T
0.9586281225385065	0.2500364031509926	0.4674257717761636	T	T	T
0.7994584413827152	0.2499847413446805	0.6256538322110490	T	T	T
0.9557247561606180	0.4404073795447966	0.4778595586031864	T	T	T
0.9557436281624987	0.0596432760851373	0.4778763952968200	T	T	T