

Supporting Information

Breaking H₂ with CeO₂: effect of the surface termination

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I. Cutoff Convergence Test

Two different set of pseudopotential were tested for PBE+U ($U=5.0$ eV):

- ✚ Setting 1: standard pseudopotentials for both cerium and oxygen,
- ✚ Setting 2: standard pseudopotential for cerium and soft pseudopotential for oxygen.

The optimized bulk cell parameter is converged for a cutoff of 300 eV for the setting 2 (Figure S2) while the setting 1 requires a cutoff of 450 eV to achieve the same accuracy (Figure S1).

Both of these settings lead to comparable results.

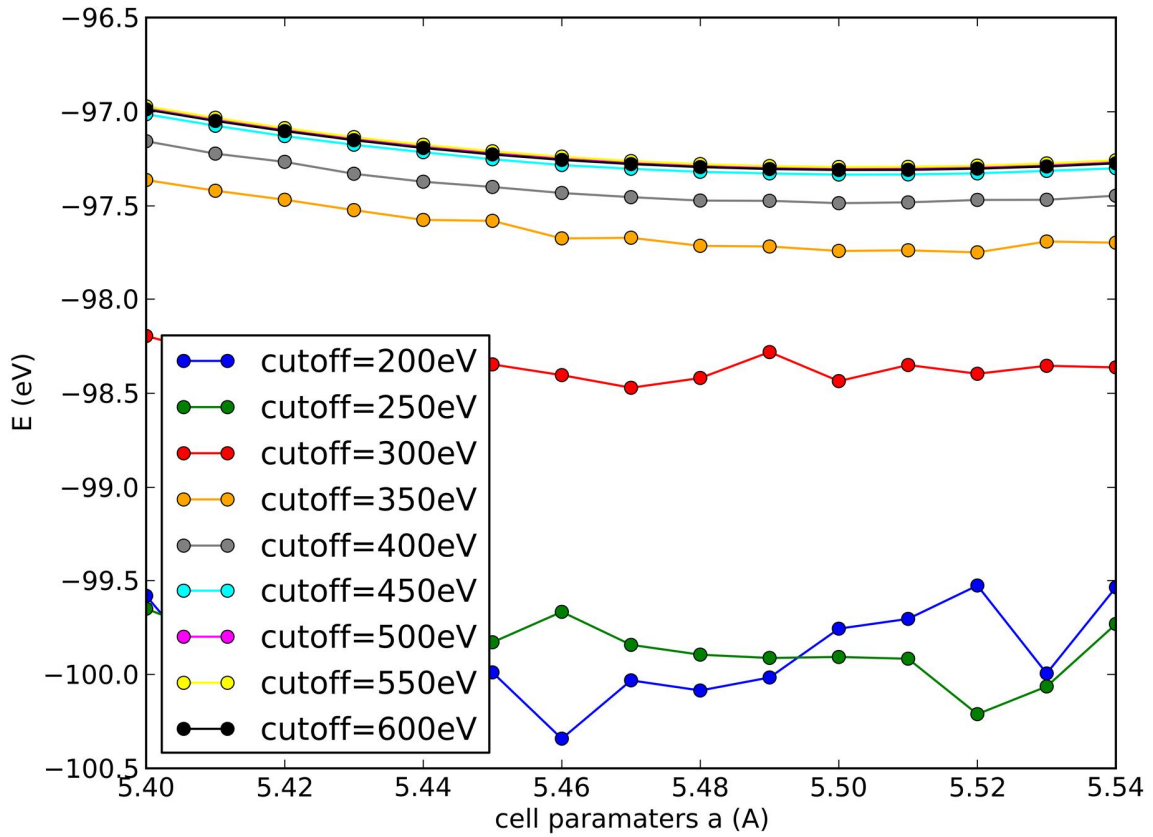


Figure S1. Cutoff convergence test for CeO_2 bulk cell parameter for setting 1.

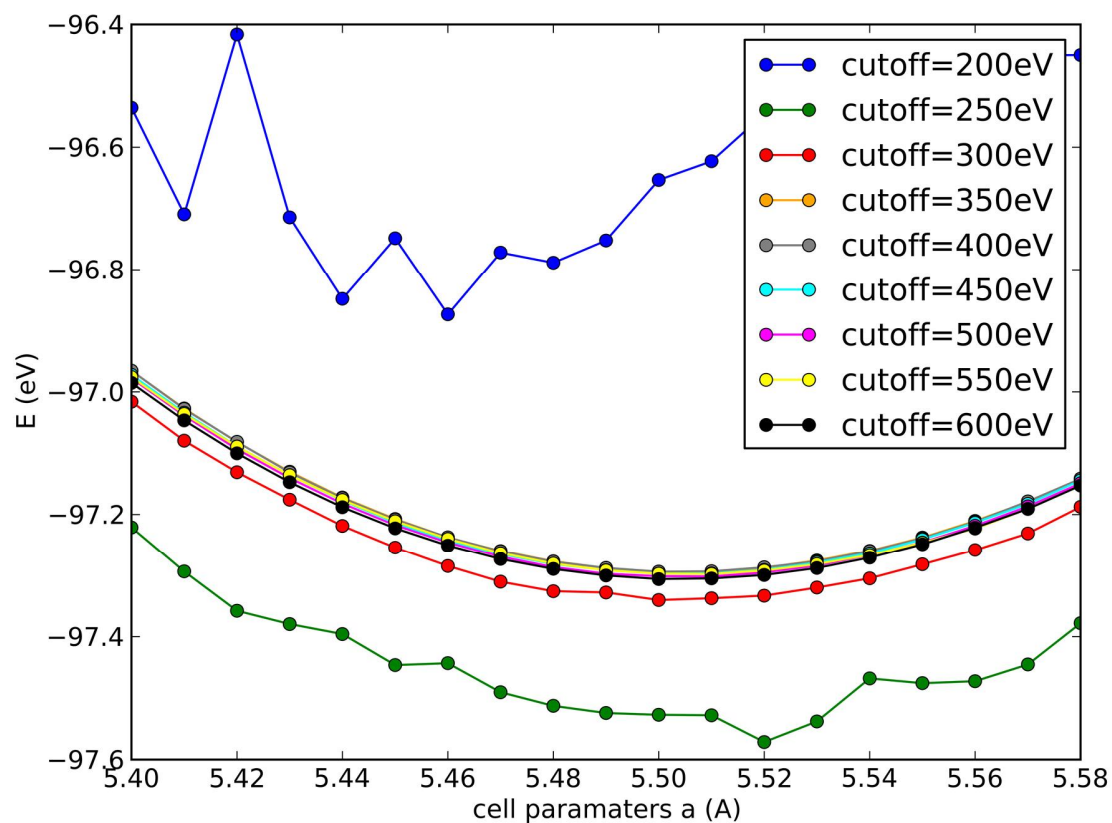


Figure S2. Cutoff convergence test for CeO₂ bulk cell parameter for setting 2.

II. Thermostatistics

The effect of the temperature was considered by calculating the Gibbs Free energy:

$$G(T, P) = U(T) - TS(T, P)$$

A. Gas Phase Molecule:

For gas phase molecule, a common approximation is to build the partition function by considering only the electronic, rotational, translational and vibrational terms. Thus, the partition function Z can be developed as:

$$Z = Z_{\text{elec}} \times Z_{\text{rot}} \times Z_{\text{trans}} \times Z_{\text{vib}}$$

Leading to the following expression for H and S :

$$G(T, P) = U(T) + TS(T, P) + TS(T, P) + TS(T, P) + TS(T, P) + TS(T, P)$$

$$\begin{aligned} \ln Z_{\text{rot}} &= \ln \left(\frac{1}{2} \frac{2\pi^2 I k_B T}{h^2} \right) \\ \ln Z_{\text{trans}} &= \ln \left(\frac{2\pi^2 m k_B T}{h^2} \right) \\ \ln Z_{\text{vib}} &= \ln \left(\frac{3}{2} \frac{2\pi^2 m k_B T}{h^2} \right) \\ \ln Z_{\text{elec}} &= \ln \left(\frac{3}{2} \frac{2\pi^2 m k_B T}{h^2} \right) \\ \ln Z_{\text{vib}} &= \ln \left(\frac{3}{2} \frac{2\pi^2 m k_B T}{h^2} \right) \\ \ln Z_{\text{elec}} &= \ln \left(\frac{3}{2} \frac{2\pi^2 m k_B T}{h^2} \right) \end{aligned}$$

$$G(T, P) = U(T) + TS(T, P) + TS(T, P) + TS(T, P) + TS(T, P) + TS(T, P)$$

$$\begin{aligned}
\frac{U_{vib}}{kT} &= \frac{U_{vib}^{(0)}}{kT} \times \frac{U_{vib}^{(1)}}{kT} + 1 \\
\frac{U_{vib}^{(0)}}{kT} &= \frac{8 \pi^2 k T}{h^2} \frac{I}{\sigma} \left(\frac{1}{2} + \frac{1}{4} \right) + 1 \\
\frac{U_{vib}^{(1)}}{kT} &= \frac{8 \pi^2 k T}{h^2} \frac{I}{\sigma} \left(\frac{1}{2} + \frac{1}{4} \right) \frac{1}{4} + \frac{3}{2} \\
\frac{U_{vib}^{(2)}}{kT} &= \frac{2 \pi^2 k T}{h^2} \frac{I}{\sigma} \frac{1}{2} + \frac{5}{2} \\
\frac{U_{vib}^{(3)}}{kT} &= \frac{2 \pi^2 k T}{h^2} \frac{I}{\sigma} \frac{1}{2} - \frac{1}{2}
\end{aligned}$$

B. Solid, Surface and Adsorbate:

In solid state, if we assume that the expansion term pV in $H = U + pV$ is negligible, which is a reasonable approximation, then Gibbs free energy can be approximate as the Helmholtz free energy:

$$G \approx H = U - TS$$

Therefore, for solid and adsorption system, a common and reasonable approximation is to consider only vibrational contributions in the partition function, leading to the following expressions for internal energy and entropy:

$$U_{vib} = U_{vib}^{(0)} + U_{vib}^{(1)} + U_{vib}^{(2)}$$

$$S_{vib} = S_{vib}^{(0)}$$

The expressions of vibrational internal energy (U_{vib}) and vibrational entropy (S_{vib}) can be developed as:

$$\begin{aligned}
U_{vib} &= \frac{U_{vib}^{(0)}}{kT} \frac{U_{vib}^{(1)}}{kT} \\
S_{vib} &= \frac{U_{vib}^{(0)}}{kT} \frac{U_{vib}^{(1)}}{kT} - 1
\end{aligned}$$

$$\frac{\partial}{\partial T} \ln Z = \frac{1}{Z} \frac{\partial Z}{\partial T} = \frac{1}{Z} \frac{\partial}{\partial T} \left(\int \exp \left(-\beta \left(\sum_{i,j} J_{ij} S_i S_j + \sum_i h_i S_i \right) \right) d\mathbf{S} \right)$$

Finally, Gibbs free energy is given by:

$$G = -k_B T \ln Z = -k_B T \ln \left(\int \exp \left(-\beta \left(\sum_{i,j} J_{ij} S_i S_j + \sum_i h_i S_i \right) \right) d\mathbf{S} \right)$$

III. Slab Thickness Convergence

The slab thickness was chosen in order to converge surface energy within 0.005 J/m^2 .

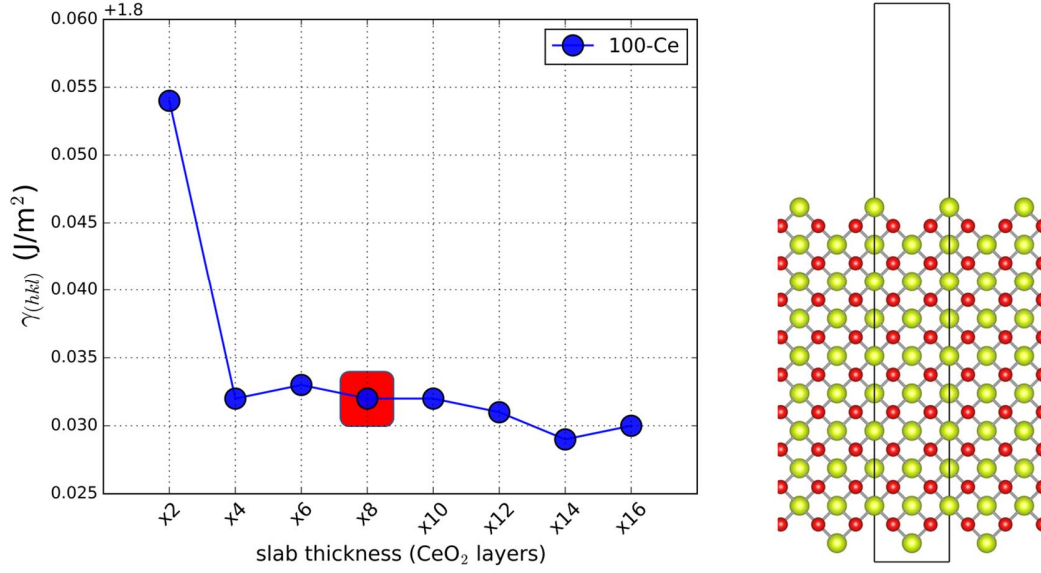


Figure S3. Slab thickness convergence for (100)-Ce surface model (left) and structure related to the red highlight (right).

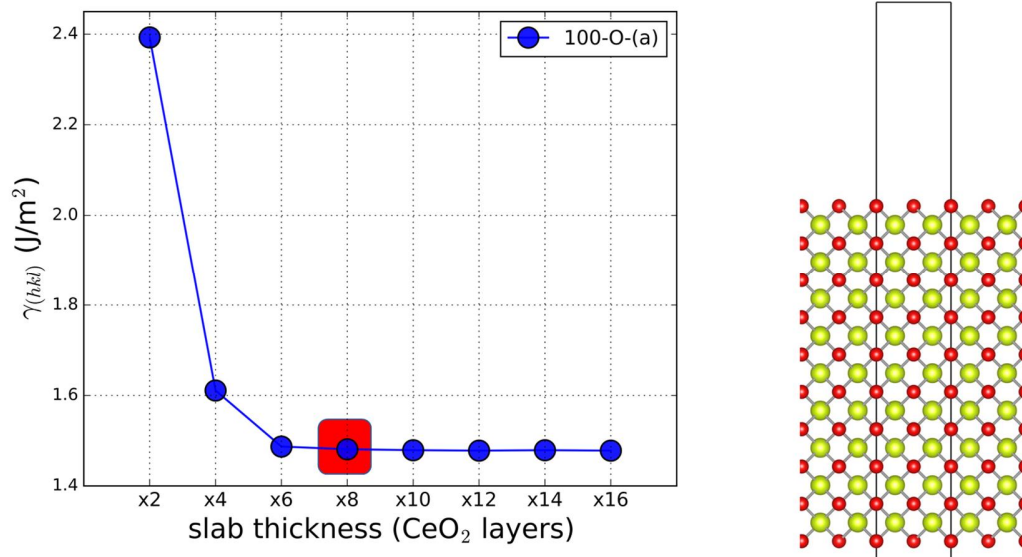


Figure S4. Slab thickness convergence for (100)-O-(a) surface model (left) and structure related to the red highlight (right).

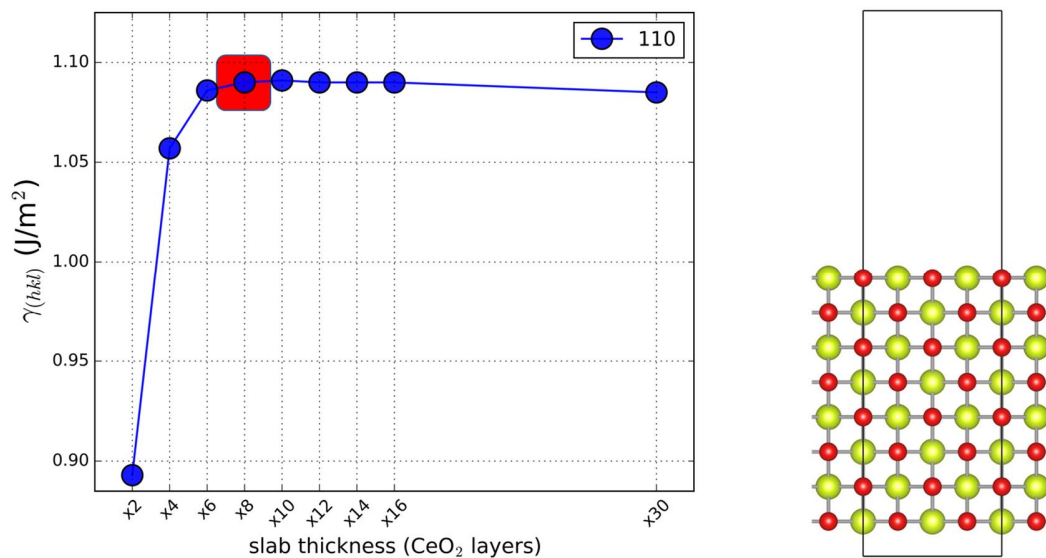


Figure S5. Slab thickness convergence for (110) surface model (at left) and structure related to the red highlight (right).

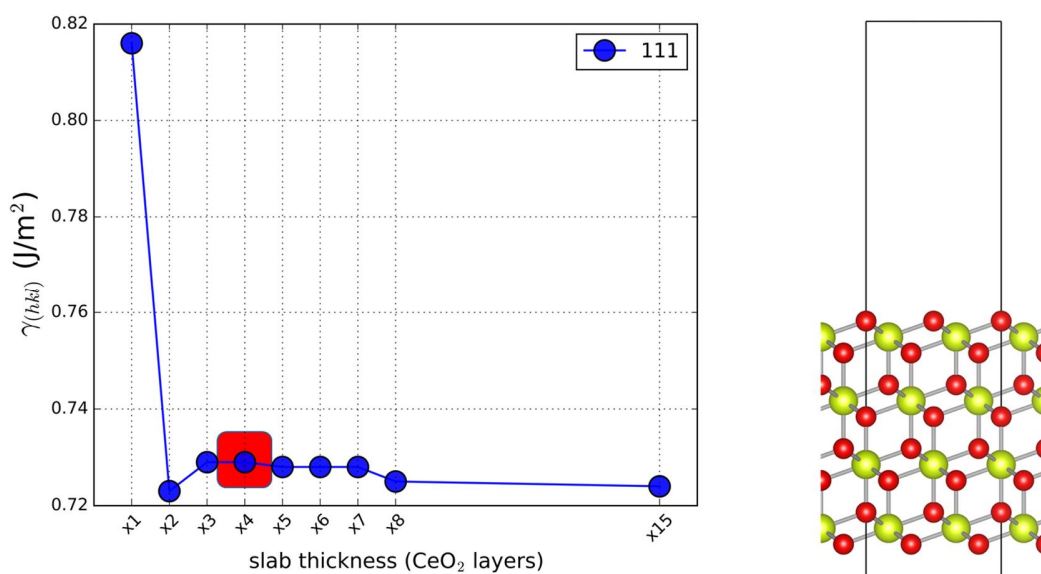


Figure S6. Slab thickness convergence for (111) surface model (left) and structure related to the red highlight (right).

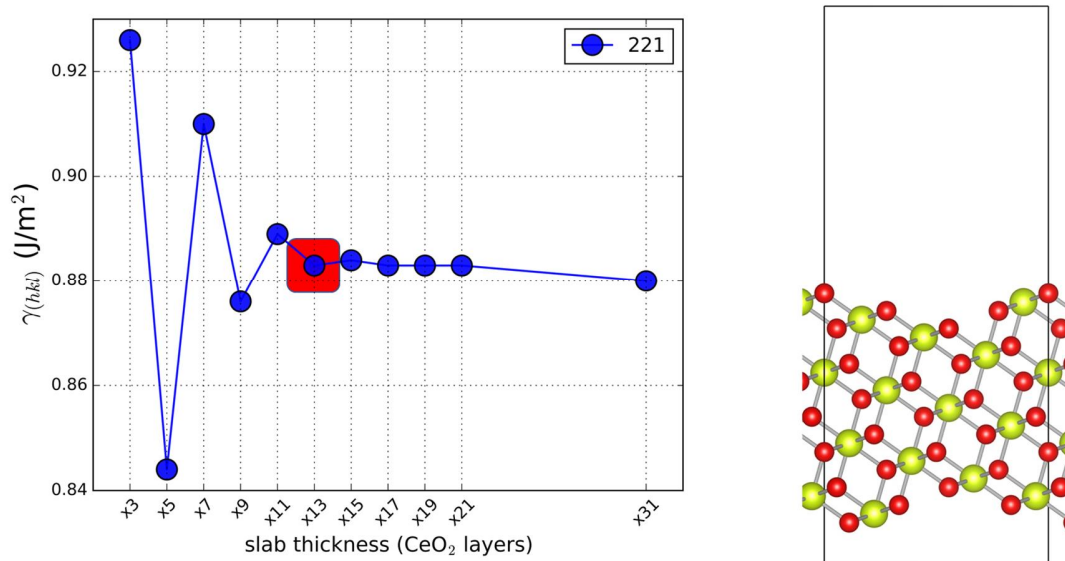


Figure S7. Slab thickness convergence for (221) surface model (left) and structure related to the red highlight (right).

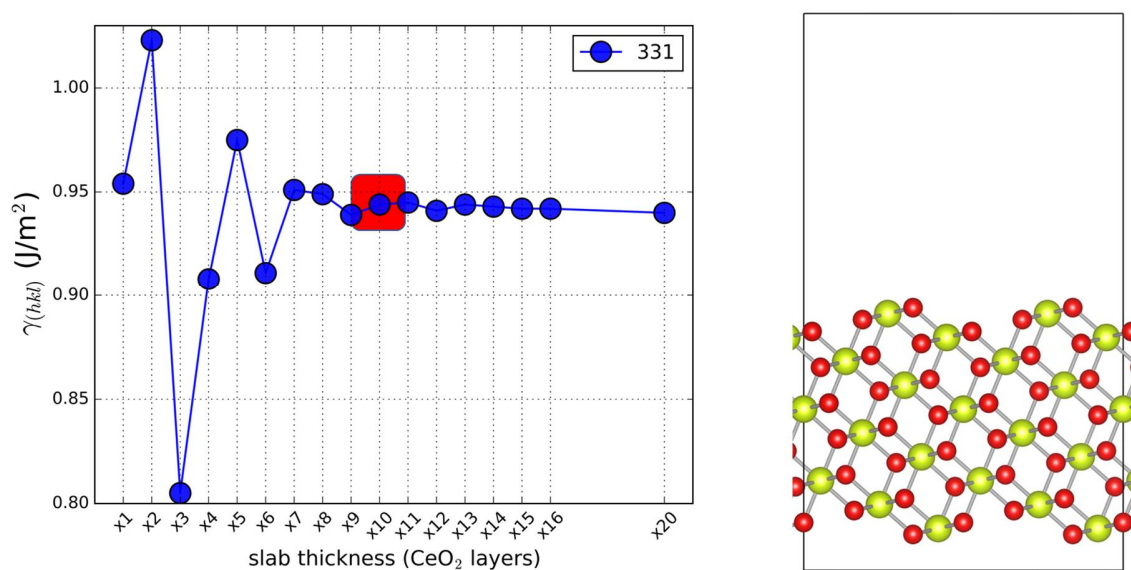


Figure S8. Slab thickness convergence for (331) surface model (left) and structure related to the red highlight (right).

IV. DOS

PDOS of bare slabs, H_2^* , TS and (H^+, H^-) systems for each terminations are given below. Surfaces of group I ((100)-Ce, (100)-O-(a) and (100)-O-(b)) shows a small energy difference between the Fermi level of (H^+, H^-) and slab. Moreover, for the surfaces of this group, the bands associated to the TS overlap with the band of the slab. At the contrary, surface of group II ((110), (111), (221) and (331)) show a large energy difference between the Fermi level of (H^+, H^-) and slab. For this group, the TS band does not overlap with the slab valance band.

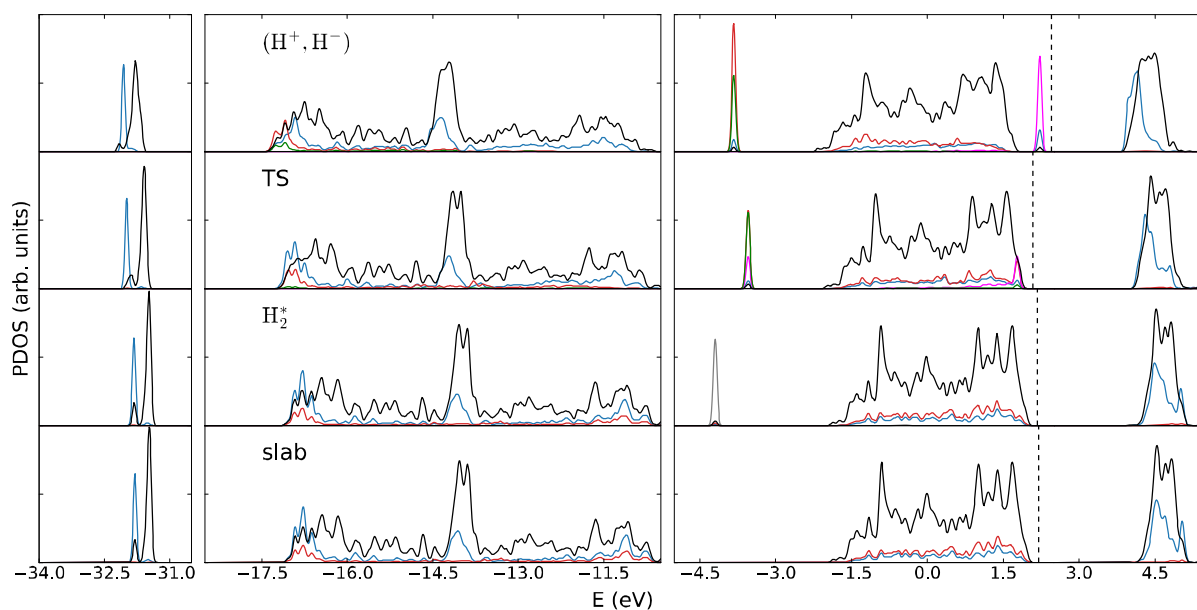


Figure S9. PDOS of the slab, H_2^* , TS and (H^+, H^-) for (100)-Ce. Only cerium and oxygen bond to hydrogen are projected. PDOS of cerium, oxygen, hydrogen molecule, hydride (x3), proton (x3) and total DOS are depicted in blue, red, grey, fuchsia, green and black, respectively. PDOS are given in arbitrary unit and the Fermi level was depicted with dashed line.

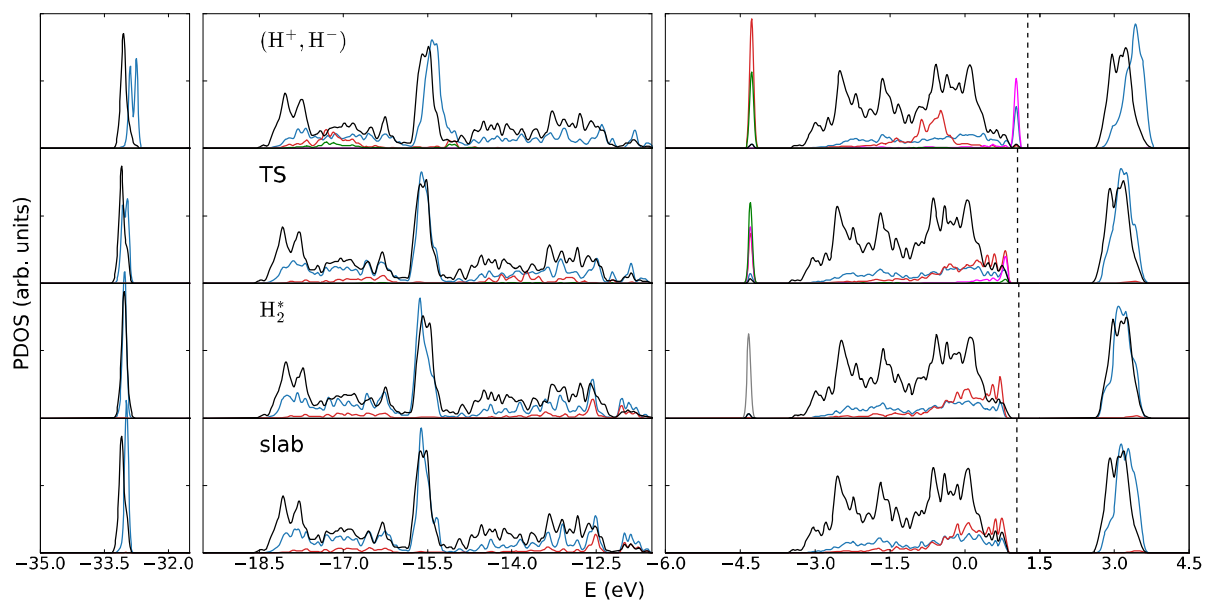


Figure S10. PDOS of the slab, H_2^* , TS and (H^+, H^-) for (100)-O-(a). Same legend as Figure S9.

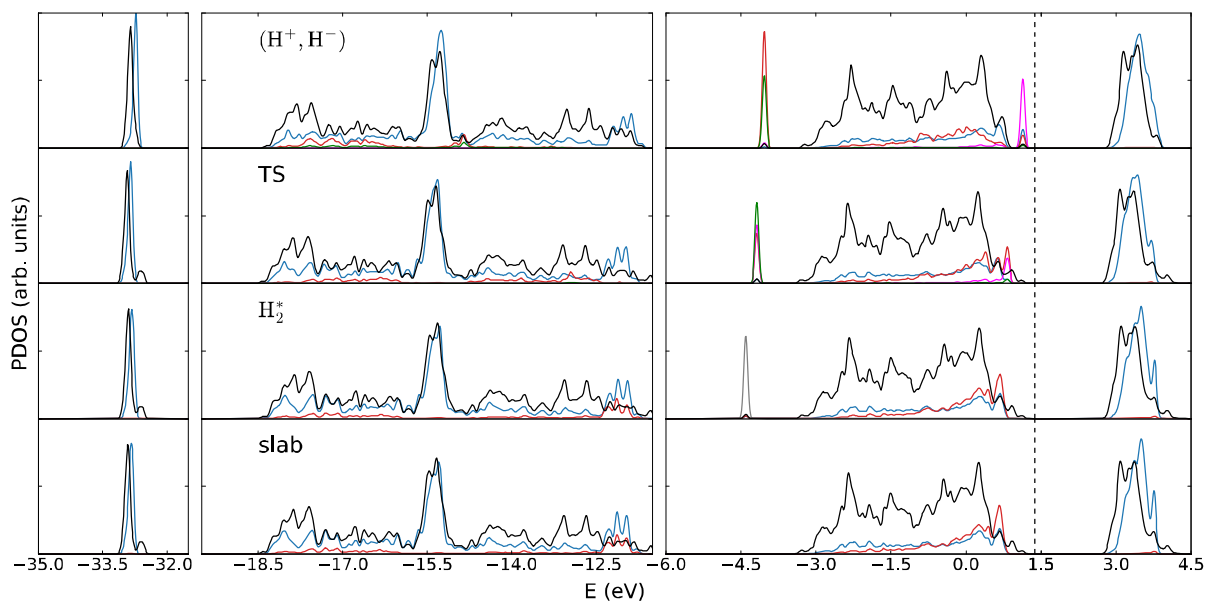


Figure S11. PDOS of the slab, H_2^* , TS and (H^+, H^-) for (100)-O-(b). Same legend as Figure S9.

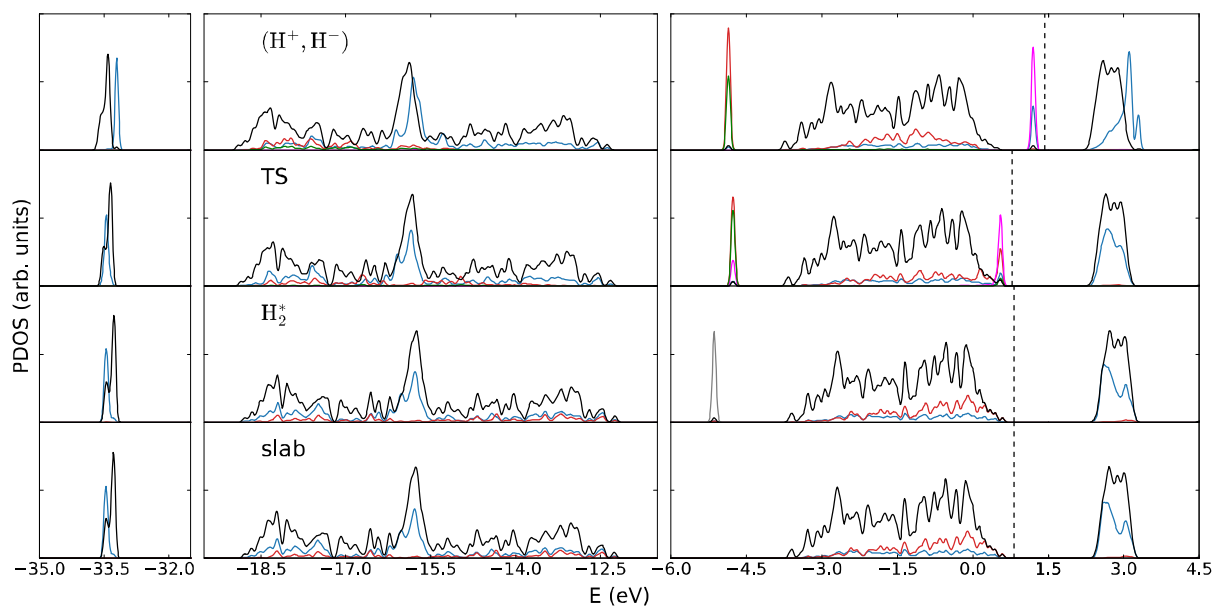


Figure S12. PDOS of the slab, H_2^* , TS and (H^+, H^-) for (110). Same legend as Figure S9.

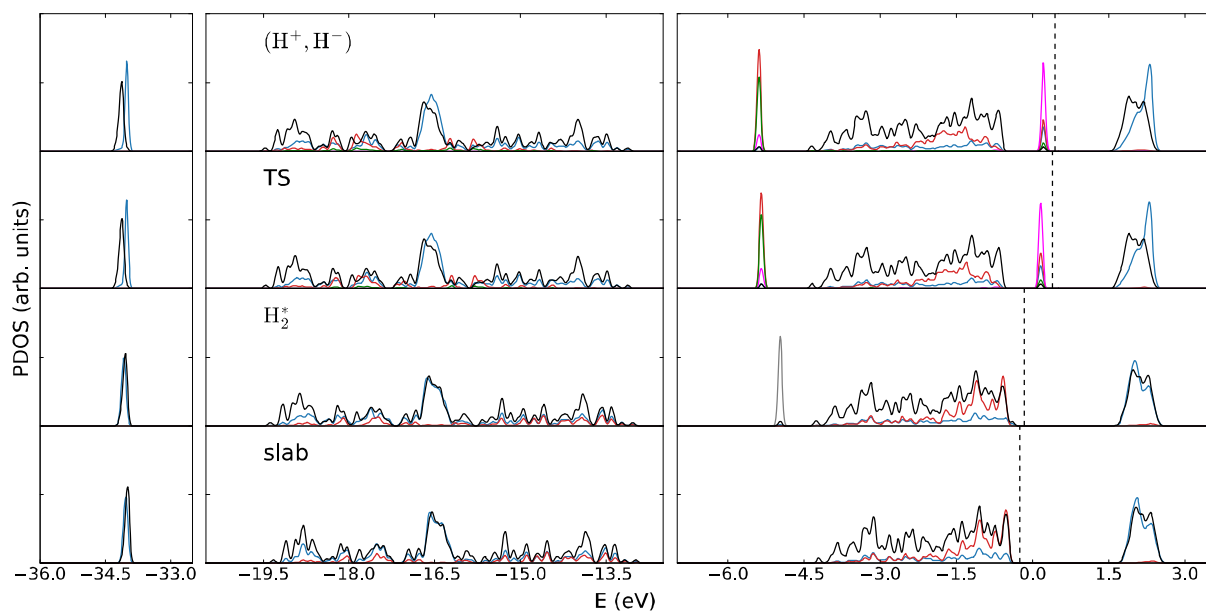


Figure S13. PDOS of the slab, H_2^* , TS and (H^+, H^-) for (111). Same legend as Figure S9.

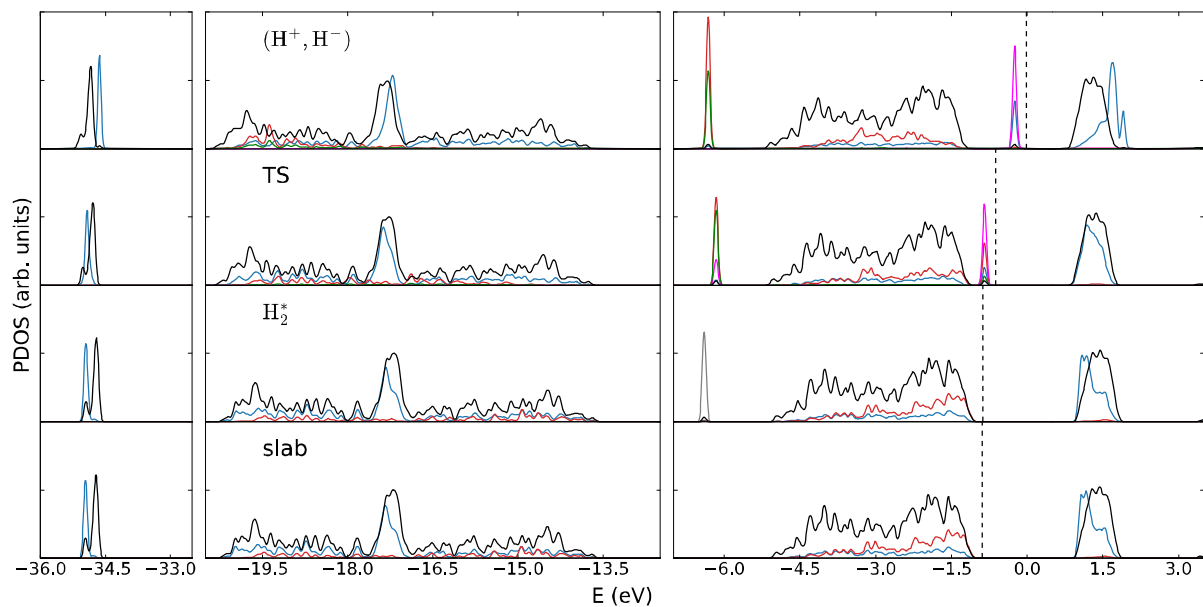


Figure S14. PDOS of the slab, H_2^* , TS and (H^+, H^-) for (221). Same legend as Figure S9.

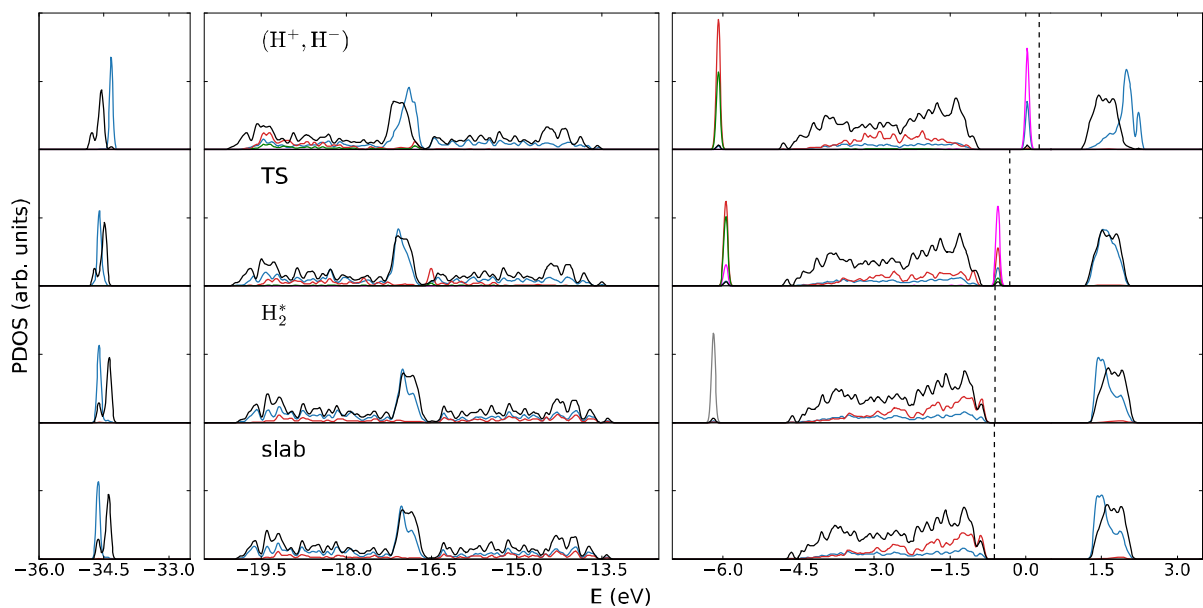


Figure S15. PDOS of the slab, H_2^* , TS and (H^+, H^-) for (331). Same legend as Figure S9.

V. Structures (POSCAR format)

A. Surfaces

 (100)-Ce

```
100-Ce
1.0000000000000000
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0.0000000000000000 11.0003118514999993 0.0000000000000000
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72 144
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0.1249999999602309	0.6250008345047533	0.3343499600942863
0.6249999999829541	0.1250008493906947	0.3343499600942863
0.6249999999829541	0.6250008345047533	0.3343499600942863
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0.6249999999829541	0.3749991655407001	0.3343499600942863
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72 144

Direct

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0.1249999999602309	0.8749999999943157	0.4013685881982880
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0.3749999999715925	0.3749999999715925	0.3343499600942863
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0.1249999999602309	0.6249999999829541	0.4684043228637549
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0.1249999999602309	0.3749999999715925	0.2673313319659627
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0.6249999999829541	0.3749999999715925	0.2673313319659627
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0.3749999999715925	0.6249999999829541	0.2673313319659627
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0.3749999999715925	0.6249999999829541	0.4013685881982880
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0.62499999999829541	0.37499999999715925	0.5356035828540371
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0.62499999999829541	0.12499999999602309	0.2002955824193009
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0.12499999999602309	0.12499999999602309	0.6034662723647557
0.12499999999602309	0.62499999999829541	0.6034662723647557
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0.7500000000340918	0.2500000000113616	0.4337290823399087
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0.7500000000340918	0.2500000000113616	0.5642693042861495
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0.0000000000000000	0.2500000000113616	0.5755983591169880
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0.5000000000227232	0.2500000000113616	0.2326220124930671
0.5000000000227232	0.7500000000340918	0.2326220124930671
0.2500000000113616	0.2500000000113616	0.2349708378243420
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0.7500000000340918	0.2500000000113616	0.2349708378243420
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0.5000000000227232	0.0000000000000000	0.3011814951791578
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100-o-b

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72 144

Direct

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0.2496468902117073	0.5001211114621711	0.4350685210494802
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0.7496365956409008	0.5001102294994766	0.4350575471838738
0.9996377979340139	0.2497126883765333	0.4344806509626054
0.9996225622313659	0.7497027258107494	0.4344916684367277
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0.4996154526889285	0.7496946041550814	0.4344852461473678
0.2496396176022913	0.2501099889289122	0.4344998059383371
0.2496037158109985	0.7500912658153496	0.4344989604292664
0.7496261758858367	0.2500948155952969	0.4344885328834351
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0.0043256166720980	0.0173024665686796	0.4834611713858976
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 (331)

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1.0000000000000000		
7.7783946990999997	0.0000000000000000	0.0000000000000000
-3.8891978593999998	16.9526194624999995	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.5109348296999983

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Direct

0.2070265015634618	0.4140530032108316	0.0802330004625205
0.7070264717951105	0.4140530032108316	0.0802330004625205
0.7070264717491739	0.9140530031960878	0.0802330004625205
0.2070265016460837	0.9140530031960878	0.0802330004625205
0.3682650995053578	0.7365301990932736	0.1193551106863637
0.8682651293894139	0.7365301990932736	0.1193551106863637
0.3682650995272283	0.2365302139729835	0.1193551106863637
0.8682651292827259	0.2365302139729835	0.1193551106863637
0.0273863223808632	0.5547726225118339	0.1557412350687173
0.5273863410800956	0.5547726225118339	0.1557412350687173
0.0273863223906972	0.0547726448240198	0.1557412350687173
0.5273863410899295	0.0547726448240198	0.1557412350687173
0.6848992130395430	0.8697984260817719	0.2046384621488073
0.1848991981971437	0.8697984260817719	0.2046384621488073
0.6848992130746367	0.3697983962486262	0.2046384621488073
0.1848991981036789	0.3697983962486262	0.2046384621488073
0.8412263810545966	0.6824527620334067	0.2462392074519855
0.3412263809967442	0.6824527620334067	0.2462392074519855
0.8412263809665532	0.1824527471242092	0.2462392074519855
0.3412263810372593	0.1824527471242092	0.2462392074519855
0.0008788883813438	0.5017577768398311	0.2882316487584475
0.5008788884391961	0.5017577768398311	0.2882316487584475
0.0008788884272874	0.0017577768545749	0.2882316487584475
0.5008788884851398	0.0017577768545749	0.2882316487584475
0.6572060564083131	0.8144121127767150	0.3298323940616257
0.6572060564542568	0.3144121127914588	0.3298323940616257
0.1572060563504607	0.8144121127767150	0.3298323940616257
0.1572060563964044	0.3144121127914588	0.3298323940616257
0.3147189283931411	0.6294378567835892	0.3787296062319854
0.3147189284204401	0.1294378865872403	0.3787296062319854
0.8147189284509935	0.6294378567835892	0.3787296062319854
0.8147189283497269	0.1294378865872403	0.3787296062319854
0.9738401401162875	0.9476803397652134	0.4151157231594738
0.4738401699492272	0.4476803099910498	0.4151157231594738
0.4738401698846388	0.9476803397652134	0.4151157231594738
0.9738401400523173	0.4476803099910498	0.4151157231594738
0.6350787380462677	0.7701575356623991	0.4542378557479125
0.1350787678146261	0.7701575356623991	0.4542378557479125
0.1350787678605627	0.2701575356771500	0.4542378557479125
0.6350787380922114	0.2701575356771500	0.4542378557479125
0.4170155525084169	0.3340311051074920	0.0655088778534036

0.9170155525203256	0.8340311050927411	0.0655088778534036
0.4170155525910317	0.8340311050927411	0.0655088778534036
0.9170155525662693	0.3340311051074920	0.0655088778534036
0.4942966404309388	0.4885932808233235	0.0841907432088149
0.9942966403730864	0.4885932808233235	0.0841907432088149
0.4942966404768825	0.9885932808380673	0.0841907432088149
0.9942966404190301	0.9885932808380673	0.0841907432088149
0.5822182161947609	0.6644364324788441	0.1077145937252553
0.0822182162654741	0.6644364324788441	0.1077145937252553
0.5822182162112099	0.1644364324346057	0.1077145937252553
0.0822182161533576	0.1644364324346057	0.1077145937252553
0.6592746315916642	0.8185492631434030	0.1309389510593064
0.1592746315338047	0.8185492631434030	0.1309389510593064
0.6592746316376079	0.3185492631581468	0.1309389510593064
0.1592746315797484	0.3185492631581468	0.1309389510593064
0.7370659089869349	0.9741318180618350	0.1485269180647961
0.2370659239707464	0.9741318180618350	0.1485269180647961
0.7370659090142269	0.4741318478654861	0.1485269180647961
0.2370659238694799	0.4741318478654861	0.1485269180647961
0.8149573701764936	0.1299147702407737	0.1703037661321218
0.3149573702472068	0.1299147702407737	0.1703037661321218
0.3149573702199078	0.6299147404371226	0.1703037661321218
0.8149573702777602	0.6299147404371226	0.1703037661321218
0.3940850536893024	0.2881700776004408	0.1928221267361536
0.8940850239209510	0.2881700776004408	0.1928221267361536
0.8940850238858573	0.7881701074335865	0.1928221267361536
0.3940850536542087	0.7881701074335865	0.1928221267361536
0.9739589497145928	0.9479179589618383	0.2131423800910923
0.4739589794829442	0.9479179589618383	0.2131423800910923
0.9739589496506227	0.4479179291876747	0.2131423800910923
0.4739589795475325	0.4479179291876747	0.2131423800910923
0.5528165044077191	0.6056330677945425	0.2345959120521002
0.0528165264880798	0.6056330677945425	0.2345959120521002
0.55281650441177289	0.1056330529443272	0.2345959120521002
0.0528165264295311	0.1056330529443272	0.2345959120521002
0.6314898388446792	0.7629797372592151	0.2566869992584984
0.1314898686130377	0.7629797372592151	0.2566869992584984
0.6314898388906229	0.2629797372739660	0.2566869992584984
0.1314898686589743	0.2629797372739660	0.2566869992584984
0.7106153709966989	0.4212308016140156	0.2777838569519346
0.7106153709507623	0.9212308015992718	0.2777838569519346
0.2106154008476722	0.9212308015992718	0.2777838569519346
0.2106154007650503	0.4212308016140156	0.2777838569519346
0.7892887653175151	0.5785774710786953	0.2998749441583328
0.2892887355620175	0.5785774710786953	0.2998749441583328
0.7892887653339642	0.0785774710344498	0.2998749441583328
0.2892887355784666	0.0785774710344498	0.2998749441583328
0.8681463197911086	0.7362925798966486	0.3213284761193407
0.3681462899070524	0.7362925798966486	0.3213284761193407
0.3681462899289230	0.2362925947763586	0.3213284761193407
0.8681463196844206	0.2362925947763586	0.3213284761193407
0.4480202157357951	0.8960404314249004	0.3416487145645561
0.9480202455185847	0.3960404612285515	0.3416487145645561
0.4480202157630870	0.3960404612285515	0.3416487145645561
0.9480202454912927	0.8960404314249004	0.3416487145645561
0.5271478992533289	0.5542957388583005	0.3641670900783112
0.5271478992631629	0.0542957611704864	0.3641670900783112
0.0271478805639305	0.0542957611704864	0.3641670900783112
0.0271478805540966	0.5542957388583005	0.3641670900783112
0.6050393603969439	0.2100786910224954	0.3859439232359065
0.1050393455545517	0.2100786910224954	0.3859439232359065
0.6050393603696520	0.7100786612188372	0.3859439232359065
0.1050393455272598	0.7100786612188372	0.3859439232359065
0.1828306230137997	0.8656612757150839	0.4035318902413962
0.6828306378561919	0.8656612757150839	0.4035318902413962
0.6828306378912856	0.3656612458819382	0.4035318902413962
0.1828306229203349	0.3656612458819382	0.4035318902413962
0.2598870532411794	0.5197741063943937	0.4267562624851777
0.7598870531527240	0.0197740877689512	0.4267562624851777
0.2598870532234301	0.0197740877689512	0.4267562624851777
0.7598870531704662	0.5197741063943937	0.4267562624851777
0.8478086290628539	0.6956172580499143	0.4502800906370297

0.3478086290050015	0.6956172580499143	0.4502800906370297
0.8478086289748106	0.1956172431407168	0.4502800906370297
0.3478086290455167	0.1956172431407168	0.4502800906370297
0.4250897169275234	0.8501794337657387	0.4689619709021642
0.9250897168568173	0.8501794337657387	0.4689619709021642
0.9250897169027610	0.3501794337804895	0.4689619709021642
0.4250897168449086	0.3501794337804895	0.4689619709021642

B. TS

TS-(100)-Ce

100-Ce-TS

1.0000000000000000		
11.0003119999999992	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.0003119999999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	41.1257400000000004

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Selective dynamics

Direct					
0.2500000000000000	0.0000000000000000	0.04312184999999986	F	F	F
0.2500000000000000	0.5000000000000000	0.04312184999999986	F	F	F
0.7500000000000000	0.0000000000000000	0.04312184999999986	F	F	F
0.7500000000000000	0.5000000000000000	0.04312184999999986	F	F	F
0.9985991939597625	0.2488754753111309	0.5686799967411531	T	T	T
0.9988023291501804	0.7491175402726213	0.5688767255258895	T	T	T
0.5003665499445518	0.2471145492797930	0.5683533007617072	T	T	T
0.4995154821214740	0.7489418581494860	0.5690418194786346	T	T	T
0.2490294250638385	0.9984281132835093	0.5686754768284317	T	T	T
0.2473373551677156	0.5001121819677721	0.5684166718551538	T	T	T
0.7492548896964806	0.9986161423556226	0.5688778505908090	T	T	T
0.7491612223571735	0.4993994949692464	0.5689902056051679	T	T	T
0.2490941591196645	0.2490083822430051	0.5017884138664641	T	T	T
0.2492660837073686	0.7493021651333009	0.5017470762784626	T	T	T
0.7494240267789891	0.2491719519277495	0.5017233483520442	T	T	T
0.7491692985616325	0.7491047509847562	0.5018800268330352	T	T	T
0.9991898356563169	0.9991122177771246	0.5017220607645783	T	T	T
0.9988601759294937	0.4991547890643204	0.5016597806380432	T	T	T
0.4992344141121592	0.9987199575986239	0.5016541934798582	T	T	T
0.4993166715079127	0.4992453123592071	0.5019058576336661	T	T	T
0.9995457756528268	0.2494402593465139	0.4347436357052885	T	T	T
0.9994194453738459	0.7494747025205371	0.4347834897637526	T	T	T
0.4995012684429767	0.2493918193711906	0.4348261267923874	T	T	T
0.4994420494848484	0.7492989078437589	0.4347981099896785	T	T	T
0.2494578808392447	0.9995168413526869	0.4347473934320476	T	T	T
0.2494161824025198	0.4994783099633651	0.4348305373440411	T	T	T
0.7494937901535863	0.9993970666546659	0.4347768668646026	T	T	T
0.7493254189307166	0.4994253795753707	0.4347966503111991	T	T	T
0.2498021371044317	0.2497997450372580	0.3678082784111254	T	T	T
0.2497866600152250	0.7497867520073669	0.3678124088731920	T	T	T
0.7497863312884334	0.2497889193179219	0.3678099716064906	T	T	T
0.7497997657220878	0.7497987200323379	0.3678110904393961	T	T	T
0.9997888289187813	0.9997882661894835	0.3677948323812785	T	T	T
0.9997963187309580	0.4997961422206103	0.3678130578831826	T	T	T
0.4997935240643727	0.9997975027824069	0.3678121738832587	T	T	T
0.4997798417101578	0.4997774342270631	0.3678219507144576	T	T	T
0.9995041820481347	0.9993351895026663	0.6254850688482207	T	T	T
0.0000464943211398	0.4985303721597987	0.6255626220779575	T	T	T
0.4986569328393813	0.0000063248730768	0.6255636988412192	T	T	T
0.5014907333332985	0.5009272530463065	0.6265166685879748	T	T	T
0.0000000000000000	0.2500000000000000	0.3008260100000015	F	F	F
0.0000000000000000	0.7500000000000000	0.3008260100000015	F	F	F
0.5000000000000000	0.2500000000000000	0.3008260100000015	F	F	F
0.5000000000000000	0.7500000000000000	0.3008260100000015	F	F	F
0.2500000000000000	0.0000000000000000	0.3008259200000012	F	F	F
0.2500000000000000	0.5000000000000000	0.3008259200000012	F	F	F

0.7500000000000000	0.0000000000000000	0.3008259200000012	F	F	F
0.7500000000000000	0.5000000000000000	0.3008259200000012	F	F	F
0.2500000000000000	0.2500000000000000	0.2337953799999966	F	F	F
0.2500000000000000	0.7500000000000000	0.2337953799999966	F	F	F
0.7500000000000000	0.2500000000000000	0.2337953799999966	F	F	F
0.7500000000000000	0.7500000000000000	0.2337953799999966	F	F	F
0.0000000000000000	0.0000000000000000	0.2337963399999978	F	F	F
0.0000000000000000	0.5000000000000000	0.2337963399999978	F	F	F
0.5000000000000000	0.0000000000000000	0.2337963399999978	F	F	F
0.5000000000000000	0.5000000000000000	0.2337963399999978	F	F	F
0.0000000000000000	0.0000000000000000	0.0997988199999966	F	F	F
0.0000000000000000	0.5000000000000000	0.0997988199999966	F	F	F
0.5000000000000000	0.0000000000000000	0.0997988199999966	F	F	F
0.5000000000000000	0.5000000000000000	0.0997988199999966	F	F	F
0.0000000000000000	0.2500000000000000	0.1667670499999971	F	F	F
0.0000000000000000	0.7500000000000000	0.1667670499999971	F	F	F
0.5000000000000000	0.2500000000000000	0.1667670499999971	F	F	F
0.5000000000000000	0.7500000000000000	0.1667670499999971	F	F	F
0.2500000000000000	0.0000000000000000	0.1668236300000032	F	F	F
0.2500000000000000	0.5000000000000000	0.1668236300000032	F	F	F
0.7500000000000000	0.0000000000000000	0.1668236300000032	F	F	F
0.7500000000000000	0.5000000000000000	0.1668236300000032	F	F	F
0.2500000000000000	0.2500000000000000	0.0997936999999993	F	F	F
0.2500000000000000	0.7500000000000000	0.0997936999999993	F	F	F
0.7500000000000000	0.2500000000000000	0.0997936999999993	F	F	F
0.7500000000000000	0.7500000000000000	0.0997936999999993	F	F	F
0.1244629365983698	0.1244287332866207	0.4683190225160629	T	T	T
0.1242402911985536	0.6243242291691331	0.4683160054663844	T	T	T
0.6243667752908451	0.1241903496845111	0.4683025133564698	T	T	T
0.6241901613833676	0.6241614103830528	0.4685083255061215	T	T	T
0.3744036929592340	0.124190779339141	0.4681026043618601	T	T	T
0.3744198342373011	0.6241497118216728	0.4682195939788159	T	T	T
0.8745104607224405	0.1242184878099479	0.4682097457759014	T	T	T
0.8742177186401321	0.6242510871703004	0.4682749921290466	T	T	T
0.1242511314004631	0.3743584538893785	0.4681171248186047	T	T	T
0.1242723299323742	0.8744490338787543	0.4682160164509881	T	T	T
0.6242040897149650	0.3743793142738454	0.4681983251904356	T	T	T
0.6242965617485510	0.8741617305526432	0.4682761811332909	T	T	T
0.3742398082529377	0.3742032181547401	0.4687716203083809	T	T	T
0.3742553507673421	0.8741588761297336	0.4683301154082997	T	T	T
0.8742230260981430	0.3742248030782989	0.4683202411937515	T	T	T
0.8741828070731330	0.8741521017713865	0.4683485395088027	T	T	T
0.1295997799999995	0.3796014699999972	0.0666311900000025	F	F	F
0.1295997799999995	0.8796014699999972	0.0666311900000025	F	F	F
0.6295997699999987	0.3796014699999972	0.0666311900000025	F	F	F
0.6295997699999987	0.8796014699999972	0.0666311900000025	F	F	F
0.3704001999999988	0.1203985399999965	0.0666311900000025	F	F	F
0.3704001999999988	0.6203985300000028	0.0666311900000025	F	F	F
0.8704001700000035	0.1203985399999965	0.0666311900000025	F	F	F
0.8704001700000035	0.6203985300000028	0.0666311900000025	F	F	F
0.1241485310064689	0.1240105862147658	0.5352132495457766	T	T	T
0.1237268478353286	0.6240005854088011	0.5352439737643664	T	T	T
0.6241831089389862	0.1235349152517671	0.5352124957920452	T	T	T
0.6237075418081233	0.6235841811007177	0.5356301432590627	T	T	T
0.3749917000000025	0.1249915799999997	0.2002911699999999	F	F	F
0.3749917000000025	0.6249915799999997	0.2002911699999999	F	F	F
0.8749917000000025	0.1249915799999997	0.2002911699999999	F	F	F
0.8749917000000025	0.6249915799999997	0.2002911699999999	F	F	F
0.3704001999999988	0.3796014699999972	0.0666311900000025	F	F	F
0.3704001999999988	0.8796014699999972	0.0666311900000025	F	F	F
0.8704001700000035	0.3796014699999972	0.0666311900000025	F	F	F
0.8704001700000035	0.8796014699999972	0.0666311900000025	F	F	F
0.3748354933339257	0.3746992706579064	0.5363790927122096	T	T	T
0.3743257703792651	0.8740582601849880	0.5353957869917920	T	T	T
0.874237018039014	0.3742063561845228	0.5353768030734614	T	T	T
0.8741138835416109	0.8739899193397704	0.5353200429193237	T	T	T
0.1295997799999995	0.1203985399999965	0.0666311900000025	F	F	F
0.1295997799999995	0.6203985300000028	0.0666311900000025	F	F	F
0.6295997699999987	0.1203985399999965	0.0666311900000025	F	F	F
0.6295997699999987	0.6203985300000028	0.0666311900000025	F	F	F
0.1196398297388868	0.1194608597381190	0.6017985491497768	T	T	T
0.1201672038763135	0.6194390816871049	0.6018479505558290	T	T	T

0.6196145699664797	0.1199957234087563	0.6018154420013531	T	T	T
0.6216744478235654	0.6213775096738416	0.6026575091446134	T	T	T
0.3792647017107242	0.1184571864780608	0.6010058360059674	T	T	T
0.3803196376044511	0.6154843130513825	0.6014140088375015	T	T	T
0.8788829854349274	0.1192404218119520	0.6017578842842966	T	T	T
0.8797732103339655	0.6190215533698264	0.6019075131555880	T	T	T
0.1186665978713108	0.3790877935838068	0.6010689753351244	T	T	T
0.1194037704217550	0.8787059136427402	0.6017561865841756	T	T	T
0.6159476589405202	0.3800409993702516	0.6013285164998763	T	T	T
0.6191485445980902	0.8796192106144574	0.6019322688426740	T	T	T
0.3720639477512009	0.3715208819211711	0.6038936156823738	T	T	T
0.3786731622871855	0.8778994613662832	0.6022929581558003	T	T	T
0.8780940219103215	0.3785316575220392	0.6022635014186832	T	T	T
0.8787483438675565	0.8785816711128120	0.6020523352715799	T	T	T
0.3742360975931618	0.1242376974689563	0.5347698378469445	T	T	T
0.3734305079863276	0.6245530209555810	0.5350501024991274	T	T	T
0.8739288552070121	0.1240362856876231	0.5351308857916379	T	T	T
0.8736274935636530	0.6241279165786651	0.5352480054666700	T	T	T
0.1243967193775148	0.3741019670254602	0.5348081460986478	T	T	T
0.1241405590943074	0.8737927448395411	0.5351298392207227	T	T	T
0.6247056544560152	0.3733015049726731	0.5349942228374971	T	T	T
0.6242172226218017	0.8734644399272113	0.5352662167241817	T	T	T
0.3746563873217923	0.3746634720454765	0.4014967948332639	T	T	T
0.3746631260807760	0.8746054252589701	0.4013474138691322	T	T	T
0.8746152191119307	0.3746591222546343	0.4013421269308495	T	T	T
0.8746326368675454	0.8746264911045358	0.4013352614629611	T	T	T
0.1246347988273016	0.3746011786820276	0.4012557365793370	T	T	T
0.1245557404000976	0.8745814047535490	0.4012852401749143	T	T	T
0.6245608369801090	0.3745839206973685	0.4012844925195367	T	T	T
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0.6250001299999965	0.6249996000000024	0.2673075399999973	F	F	F
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0.3749998700000035	0.6249996000000024	0.2673075399999973	F	F	F
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0.1250001200000028	0.3750004300000001	0.2673075399999973	F	F	F
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0.3750000000000000	0.8749996499999995	0.3343499599999973	F	F	F
0.8750000000000000	0.3749996499999995	0.3343499599999973	F	F	F
0.8750000000000000	0.8749996499999995	0.3343499599999973	F	F	F
0.1249694099999985	0.1250320299999998	0.1333152999999996	F	F	F
0.1249694099999985	0.6250320299999998	0.1333152999999996	F	F	F
0.6249694300000002	0.1250320299999998	0.1333152999999996	F	F	F
0.6249694300000002	0.6250320299999998	0.1333152999999996	F	F	F
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0.1246445756308390	0.6246183143236195	0.4013544664391873	T	T	T
0.6246219082179536	0.1246370824606231	0.4013482163836386	T	T	T
0.6245920766899360	0.6245957211164210	0.4013964562253776	T	T	T
0.3745975244507989	0.1246299250331759	0.4012493094176506	T	T	T
0.3745808651728666	0.6245623630604484	0.4012933153543230	T	T	T
0.8745846464109874	0.1245553639413046	0.4012830332330779	T	T	T
0.8745255675410206	0.6246011404094958	0.4013147645939767	T	T	T
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0.6250082999999975	0.6249915799999997	0.2002911699999999	F	F	F
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0.37500000000000000	0.62500035000000005	0.3343499599999973	F	F	F
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0.3671198966355789	0.3615285221237059	0.6588220175800288	T	T	T
0.3537792960059676	0.3504266674859693	0.6331799421720632	T	T	T

TS-(100)-O(a)

100-O-a-TS

1.0000000000000000		
11.000311999999992	0.0000000000000000	0.0000000000000000
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0.0000000000000000	0.0000000000000000	41.1257400000000004

Ce O H
72 144 2

Selective dynamics

Direct

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0.1250000000000000	0.6250000000000000	0.3343499599999973	F	F	F
0.6250000000000000	0.1250000000000000	0.3343499599999973	F	F	F
0.6250000000000000	0.6250000000000000	0.3343499599999973	F	F	F
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0.1256233710704180	0.8748214600284001	0.4013005390087017	T	T	T
0.6255220191555750	0.3749221626945811	0.4013271980248660	T	T	T
0.6256500849234570	0.8748582079396741	0.4013435841223085	T	T	T
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0.37500000000000000	0.87500000000000000	0.3343499599999973	F	F	F
0.87500000000000000	0.37500000000000000	0.3343499599999973	F	F	F
0.87500000000000000	0.87500000000000000	0.3343499599999973	F	F	F
0.1258229507156017	0.1243314161335789	0.4683060161691017	T	T	T
0.1263495725373431	0.6246491707660695	0.4681962699264020	T	T	T
0.6260789189562175	0.1250317562007695	0.4683098330321869	T	T	T
0.6263543479243907	0.6249664508567321	0.4684476660005785	T	T	T
0.12500000000000000	0.37500000000000000	0.2673391499999980	F	F	F
0.12500000000000000	0.87500000000000000	0.2673391499999980	F	F	F
0.62500000000000000	0.37500000000000000	0.2673391499999980	F	F	F
0.62500000000000000	0.87500000000000000	0.2673391499999980	F	F	F
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0.37500000000000000	0.62500000000000000	0.2673391499999980	F	F	F
0.87500000000000000	0.12500000000000000	0.2673391499999980	F	F	F
0.87500000000000000	0.62500000000000000	0.2673391499999980	F	F	F
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0.3761890723935366	0.8746807246550716	0.4683101560647742	T	T	T
0.8756762843324779	0.3746604208266362	0.4683162527298421	T	T	T
0.8763073255387326	0.8747468099059645	0.4683995151772891	T	T	T
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0.8750000000000000	0.3750000000000000	0.2003054999999989	F	F	F
0.8750000000000000	0.8750000000000000	0.2003054999999989	F	F	F
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0.8755982955215629	0.6248534537626966	0.4013301726818241	T	T	T
0.3760864984765888	0.1247304475694193	0.5353090555834541	T	T	T
0.3766469609370731	0.6239018177704665	0.5354881938149632	T	T	T
0.8761332642816413	0.1246157196189799	0.5355235546613955	T	T	T
0.8775775880094372	0.6241078755036824	0.5356998684915553	T	T	T
0.1254526671541072	0.3753029836528725	0.5351495294521342	T	T	T
0.1275394755053654	0.8729686758141213	0.5356669590053329	T	T	T
0.6256418818932374	0.3753186728725524	0.5357700694410781	T	T	T
0.6266134442223716	0.8751356431701041	0.5354426870257285	T	T	T
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0.1250000000000000	0.6250000000000000	0.2003054999999989	F	F	F
0.6250000000000000	0.1250000000000000	0.2003054999999989	F	F	F
0.6250000000000000	0.6250000000000000	0.2003054999999989	F	F	F
0.3750000000000000	0.3750000000000000	0.0652280199999993	F	F	F
0.3750000000000000	0.8750000000000000	0.0652280199999993	F	F	F
0.8750000000000000	0.3750000000000000	0.0652280199999993	F	F	F
0.8750000000000000	0.8750000000000000	0.0652280199999993	F	F	F
0.3750000000000000	0.1250000000000000	0.1330989599999981	F	F	F
0.3750000000000000	0.6250000000000000	0.1330989599999981	F	F	F
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0.8770904608901091	0.8736616818788434	0.6030525163829381	T	T	T
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0.1327561802556119	0.6253353606710306	0.6047634753431836	T	T	T
0.6277767025832617	0.1271455394968797	0.6032831311251172	T	T	T
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0.1250000000000000	0.3750000000000000	0.1330989599999981	F	F	F
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0.6250000000000000	0.3750000000000000	0.1330989599999981	F	F	F
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0.1250000000000000	0.1250000000000000	0.0652280199999993	F	F	F
0.1250000000000000	0.6250000000000000	0.0652280199999993	F	F	F
0.6250000000000000	0.1250000000000000	0.0652280199999993	F	F	F
0.6250000000000000	0.6250000000000000	0.0652280199999993	F	F	F
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0.0008802699963084	0.5048779515758071	0.6284429713288304	T	T	T
0.5037239451602034	0.0040447430784667	0.6286389961915404	T	T	T
0.4893692631203095	0.5176943671331315	0.6304027060069188	T	T	T
0.0008192839335877	0.9997518794308107	0.4337144622277833	T	T	T
0.0007440864585178	0.4997866603898942	0.4336184932091669	T	T	T
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0.5008692281180700	0.4998888570106885	0.4338546823990370	T	T	T
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0.2509243949232101	0.4996722169773662	0.4357378822976088	T	T	T
0.7509359676036595	0.9998239376525859	0.4360138559239957	T	T	T
0.7507784283585792	0.4998443356626154	0.4360505509324142	T	T	T
0.0006890274898907	0.2496656284465431	0.4359591128169242	T	T	T
0.0009719318827308	0.7498112677552840	0.4359991938000931	T	T	T
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0.5010603588502818	0.7497261036840399	0.4359751820537952	T	T	T
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0.2510006361740622	0.7498063597720304	0.4336987770692886	T	T	T
0.7506866097754923	0.2499300425553344	0.4336568960772311	T	T	T
0.7509536843841431	0.7498531049940382	0.4337626386364875	T	T	T
0.0017197813630290	0.9980771475388579	0.5642977509942639	T	T	T
0.9991403040293747	0.4965958936177728	0.5640051876461172	T	T	T
0.5019609159711393	0.0008824753193508	0.5640806364225881	T	T	T
0.5010699296412255	0.4993184018269190	0.5650745115422353	T	T	T
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0.2514394056156917	0.4994780121908065	0.5039579849608771	T	T	T
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0.7529108026933429	0.7502487446206985	0.5643852572582944	T	T	T
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0.2515275709163092	0.7492944756086359	0.4994745036660930	T	T	T
0.7508926804022096	0.2498342844462726	0.4993871489507669	T	T	T
0.7515478127361135	0.7499241279277626	0.4995232846803006	T	T	T
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0.5014463983475324	0.4996917157264065	0.4997454015845335	T	T	T
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0.2503361016041765	0.7498835580313852	0.3675193476354934	T	T	T
0.7502681281973196	0.2499213887394092	0.3675055434527437	T	T	T
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0.5000000000000000	0.2500000000000000	0.0931025300000030	F	F	F
0.5000000000000000	0.7500000000000000	0.0931025300000030	F	F	F
0.2500000000000000	0.2500000000000000	0.1044344100000032	F	F	F
0.2500000000000000	0.7500000000000000	0.1044344100000032	F	F	F
0.7500000000000000	0.2500000000000000	0.1044344100000032	F	F	F
0.7500000000000000	0.7500000000000000	0.1044344100000032	F	F	F
0.0000000000000000	0.0000000000000000	0.1692585199999996	F	F	F
0.0000000000000000	0.5000000000000000	0.1692585199999996	F	F	F
0.5000000000000000	0.0000000000000000	0.1692585199999996	F	F	F
0.5000000000000000	0.5000000000000000	0.1692585199999996	F	F	F
0.2500000000000000	0.0000000000000000	0.1640114400000030	F	F	F
0.2500000000000000	0.5000000000000000	0.1640114400000030	F	F	F
0.7500000000000000	0.0000000000000000	0.1640114400000030	F	F	F
0.7500000000000000	0.5000000000000000	0.1640114400000030	F	F	F
0.0000000000000000	0.2500000000000000	0.1640114400000030	F	F	F
0.0000000000000000	0.7500000000000000	0.1640114400000030	F	F	F
0.5000000000000000	0.2500000000000000	0.1640114400000030	F	F	F
0.5000000000000000	0.7500000000000000	0.1640114400000030	F	F	F
0.2500000000000000	0.2500000000000000	0.1692585199999996	F	F	F
0.2500000000000000	0.7500000000000000	0.1692585199999996	F	F	F
0.7500000000000000	0.2500000000000000	0.1692585199999996	F	F	F
0.7500000000000000	0.7500000000000000	0.1692585199999996	F	F	F
0.0000000000000000	0.0000000000000000	0.2349782499999975	F	F	F

0.0000000000000000	0.5000000000000000	0.2349782499999975	F	F	F
0.5000000000000000	0.0000000000000000	0.2349782499999975	F	F	F
0.5000000000000000	0.5000000000000000	0.2349782499999975	F	F	F
0.2500000000000000	0.0000000000000000	0.2326338900000025	F	F	F
0.2500000000000000	0.5000000000000000	0.2326338900000025	F	F	F
0.7500000000000000	0.0000000000000000	0.2326338900000025	F	F	F
0.7500000000000000	0.5000000000000000	0.2326338900000025	F	F	F
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0.5000000000000000	0.7500000000000000	0.2326338900000025	F	F	F
0.2500000000000000	0.2500000000000000	0.2349782499999975	F	F	F
0.2500000000000000	0.7500000000000000	0.2349782499999975	F	F	F
0.7500000000000000	0.2500000000000000	0.2349782499999975	F	F	F
0.7500000000000000	0.7500000000000000	0.2349782499999975	F	F	F
0.0000000000000000	0.0000000000000000	0.3011801099999971	F	F	F
0.0000000000000000	0.5000000000000000	0.3011801099999971	F	F	F
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0.2500000000000000	0.0000000000000000	0.3004992500000014	F	F	F
0.2500000000000000	0.5000000000000000	0.3004992500000014	F	F	F
0.7500000000000000	0.0000000000000000	0.3004992500000014	F	F	F
0.7500000000000000	0.5000000000000000	0.3004992500000014	F	F	F
0.0000000000000000	0.2500000000000000	0.3004992500000014	F	F	F
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0.5000000000000000	0.7500000000000000	0.3004992500000014	F	F	F
0.2500000000000000	0.2500000000000000	0.3011801099999971	F	F	F
0.2500000000000000	0.7500000000000000	0.3011801099999971	F	F	F
0.7500000000000000	0.2500000000000000	0.3011801099999971	F	F	F
0.7500000000000000	0.7500000000000000	0.3011801099999971	F	F	F
0.0003095440011265	0.9998621991374605	0.3675236850570442	T	T	T
0.0002699510241087	0.4998971913591603	0.3674815107812677	T	T	T
0.5003101029238337	0.9998839954328957	0.3675037999687447	T	T	T
0.50035246261195551	0.4998904187105921	0.3675611610865062	T	T	T
0.0002432987268008	0.2498969655030621	0.3681395438367403	T	T	T
0.0002985782512894	0.7499554777512785	0.3681705603904177	T	T	T
0.5002799743034032	0.2499950494648786	0.3681712958250714	T	T	T
0.50035246261195551	0.7499551802473690	0.3681474612582107	T	T	T
0.2503199053462595	0.2441392307765895	0.6283330721492817	T	T	T
0.2470141912699546	0.7661157717047757	0.6286190794551061	T	T	T
0.7492375773114475	0.2566540875760239	0.6285640902418521	T	T	T
0.7488498372754293	0.7514157915430388	0.6288166794050696	T	T	T
0.2871218881445543	0.5232484185802662	0.6399794245450110	T	T	T
0.3734088992236622	0.5356248781708643	0.6391468434314191	T	T	T

TS-(100)-O-(b)

100-o-b-TS

1.0000000000000000

11.0003119999999992

0.0000000000000000

0.0000000000000000

Ce O H

72 144 2

Selective dynamics

Direct

0.1250000000000000	0.1252832899999987	0.3343499599999973	F	F	F
0.1250000000000000	0.6252832600000033	0.3343499599999973	F	F	F
0.6250000000000000	0.1252832899999987	0.3343499599999973	F	F	F
0.6250000000000000	0.6252832600000033	0.3343499599999973	F	F	F
0.1259659468775141	0.3742322487203467	0.4013251034481016	T	T	T
0.1259643522818550	0.8741892957677990	0.4013413865176929	T	T	T
0.6259926778697462	0.3741021112819354	0.4012576075700096	T	T	T
0.6259207878144224	0.8741471803430869	0.4012918120443700	T	T	T
0.3750000000000000	0.3747167100000013	0.3343499599999973	F	F	F
0.3750000000000000	0.8747167399999967	0.3343499599999973	F	F	F
0.8750000000000000	0.3747167100000013	0.3343499599999973	F	F	F
0.8750000000000000	0.8747167399999967	0.3343499599999973	F	F	F

0.1270946090166305	0.1245869087931624	0.4683086805218863	T	T	T
0.1265071061678995	0.6246668902897383	0.4683540211600601	T	T	T
0.6270114578732304	0.1242736421735700	0.4682203879919200	T	T	T
0.6265971536336821	0.6242291538222133	0.4681250449632941	T	T	T
0.1250000000000000	0.3753026199999994	0.2672891799999988	F	F	F
0.1250000000000000	0.8753025899999969	0.2672891799999988	F	F	F
0.6250000000000000	0.3753026199999994	0.2672891799999988	F	F	F
0.6250000000000000	0.8753025899999969	0.2672891799999988	F	F	F
0.3750000000000000	0.1246973900000015	0.2672891799999988	F	F	F
0.3750000000000000	0.6246974100000031	0.2672891799999988	F	F	F
0.8750000000000000	0.1246973900000015	0.2672891799999988	F	F	F
0.8750000000000000	0.6246974100000031	0.2672891799999988	F	F	F
0.3769518744335443	0.3713423202193695	0.4681830656465280	T	T	T
0.3767971218325457	0.8714175855866984	0.4683484609622752	T	T	T
0.8770185484532718	0.3708752624113671	0.4682653688855325	T	T	T
0.8769523033140914	0.8708257680020068	0.4682308957166228	T	T	T
0.3750000000000000	0.3731640999999968	0.2002544899999990	F	F	F
0.3750000000000000	0.8731641299999993	0.2002544899999990	F	F	F
0.8750000000000000	0.3731640999999968	0.2002544899999990	F	F	F
0.8750000000000000	0.8731641299999993	0.2002544899999990	F	F	F
0.3760036484805127	0.1235616844333052	0.4013087867599765	T	T	T
0.3758413217331054	0.6236277732981179	0.4013014546336748	T	T	T
0.8760014888599983	0.1234836722414272	0.4013027837451020	T	T	T
0.8759352206193043	0.6234684461039492	0.4012899366532707	T	T	T
0.3779621923264003	0.1190110129562996	0.5354519553041399	T	T	T
0.3774244944267480	0.6174185116838657	0.5351831923468069	T	T	T
0.8782777424748289	0.1170686575597912	0.5352976706843791	T	T	T
0.8760106263896859	0.6167808192750854	0.5354312296329340	T	T	T
0.1279950422209026	0.3764667475465231	0.5354229674409083	T	T	T
0.1272921211887450	0.8768949555347731	0.5354869840502516	T	T	T
0.6274609042407135	0.3758193589640513	0.5352313085354510	T	T	T
0.6277889044869980	0.8756077485244376	0.5351136753561505	T	T	T
0.1250000000000000	0.1268359000000032	0.2002544899999990	F	F	F
0.1250000000000000	0.6268358700000007	0.2002544899999990	F	F	F
0.6250000000000000	0.1268359000000032	0.2002544899999990	F	F	F
0.6250000000000000	0.6268358700000007	0.2002544899999990	F	F	F
0.3750000000000000	0.3542213200000006	0.0669817100000003	F	F	F
0.3750000000000000	0.8542212899999981	0.0669817100000003	F	F	F
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0.8750000000000000	0.8542212899999981	0.0669817100000003	F	F	F
0.3750000000000000	0.1206602099999969	0.1330657299999984	F	F	F
0.3750000000000000	0.6206602299999986	0.1330657299999984	F	F	F
0.8750000000000000	0.1206602099999969	0.1330657299999984	F	F	F
0.8750000000000000	0.6206602299999986	0.1330657299999984	F	F	F
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0.3903570173337059	0.8547843174179093	0.6010412624440278	T	T	T
0.8900396558493000	0.3495110891634354	0.6017037858595700	T	T	T
0.8897017739091879	0.8497056680426667	0.6014351288905857	T	T	T
0.1427244134740917	0.1465771518205727	0.6020096216810771	T	T	T
0.1381351211109276	0.6397428376964811	0.6010065086869929	T	T	T
0.6428646147401622	0.1396405324610299	0.6013749353687174	T	T	T
0.6368346121592978	0.6413261418089320	0.6021173664320685	T	T	T
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0.1250000000000000	0.8793397700000014	0.1330657299999984	F	F	F
0.6250000000000000	0.3793397999999968	0.1330657299999984	F	F	F
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0.1250000000000000	0.1457786799999994	0.0669817100000003	F	F	F
0.1250000000000000	0.6457787100000019	0.0669817100000003	F	F	F
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0.0012864929296299	0.4981272640514902	0.4351045629707073	T	T	T
0.5012986437731897	0.9980983779208188	0.4350337079806437	T	T	T
0.5012471358798365	0.4981213567203753	0.4348229487442410	T	T	T
0.2515275816508904	0.9985677164442919	0.4351560483911712	T	T	T
0.2513649881660385	0.4986045043474121	0.4350761963446743	T	T	T
0.7515212988966269	0.9983233123148025	0.4350077289820220	T	T	T
0.7514623636955449	0.4983086052017924	0.4350551793224540	T	T	T
0.0016855415471042	0.2479533486229855	0.4345264275732532	T	T	T
0.0014932930525902	0.7479190981495876	0.4344588615391487	T	T	T
0.5016147044724164	0.2479867591566247	0.4344836651122819	T	T	T
0.5013763740636890	0.7480608769086103	0.4345022125882210	T	T	T

0.2514321637709429	0.2486349265704106	0.4345099301838857	T	T	T
0.2512554613872240	0.7487458933692110	0.4346032520693157	T	T	T
0.7514944527157752	0.2485159972241249	0.4344086284551238	T	T	T
0.7513407092047970	0.7484977000642985	0.4344294845442462	T	T	T
0.0039761862866641	0.9912451032257579	0.5718130405904773	T	T	T
0.0031336066748082	0.4926575974234666	0.5717340491494483	T	T	T
0.5037348922673885	0.9923885447147427	0.5712719467048117	T	T	T
0.5040637995028874	0.4912932366150145	0.5702299049168005	T	T	T
0.2522613694271953	0.9967953466766559	0.5027362965827393	T	T	T
0.2518776672023861	0.4965233217657783	0.5024776483110074	T	T	T
0.7524941775132490	0.9958659484340302	0.5023760045382701	T	T	T
0.7519353918149250	0.4959190198543553	0.5024966663830668	T	T	T
0.0026959196318614	0.2484403073174803	0.5010976551897741	T	T	T
0.0021507669292049	0.7486884017036672	0.5010068841402742	T	T	T
0.5023627527619396	0.2486938867385788	0.5010319898454938	T	T	T
0.5022596667266157	0.7486109550549997	0.5010273304563455	T	T	T
0.2553028181018036	0.2559700591097709	0.5662549537536776	T	T	T
0.2526848739005771	0.7545962623459488	0.5664738768883737	T	T	T
0.7546294128026787	0.2528283997202507	0.5656832862725309	T	T	T
0.7524638068106597	0.7527202864660296	0.5659338091711845	T	T	T
0.0048338717541796	0.2394901311291804	0.5660043532024517	T	T	T
0.0026094367083473	0.7392078002938831	0.5657313527894843	T	T	T
0.5053253191476159	0.2392075776060665	0.5660797664306969	T	T	T
0.5021710460090461	0.7397042282833866	0.5660160095335343	T	T	T
0.2525523010534130	0.2464886029943045	0.5011334139812078	T	T	T
0.2522942400062931	0.7464404773801050	0.5012476684096328	T	T	T
0.7529470434853209	0.2453963335570464	0.5008607884089642	T	T	T
0.7522338328982130	0.7456034871972932	0.5009504286782231	T	T	T
0.2544668257448208	0.0021689059581362	0.5721414830610598	T	T	T
0.2534147141494216	0.5028575960670949	0.5716814523477183	T	T	T
0.7540924622893144	0.9990194293693335	0.5712405116080106	T	T	T
0.7529338559478295	0.5004126310462169	0.5721464982171725	T	T	T
0.0025980819121756	0.9982079950283449	0.5025001066793422	T	T	T
0.0020293038027432	0.4980921383818355	0.5025857128556694	T	T	T
0.5023871832100895	0.9984780847443773	0.5024153550801600	T	T	T
0.5019339619141121	0.4984613171023469	0.5019666498395452	T	T	T
0.2505259620500553	0.2493714703240002	0.3677714864470474	T	T	T
0.2504796472854025	0.7494066492711866	0.3677864330609992	T	T	T
0.7505699396918288	0.2493039759978188	0.3677194816742002	T	T	T
0.7505175952408720	0.7493205755262977	0.3677396871041054	T	T	T
0.2504067686602980	0.9994642587144824	0.3678930458193364	T	T	T
0.2503494657905776	0.4994860143410662	0.3678652131279208	T	T	T
0.7504051871683544	0.9994383593233351	0.3678434497501257	T	T	T
0.7504151387498297	0.4994332982015308	0.3678470085928609	T	T	T
0.0000000000000000	0.2500000000000000	0.0387919900000000	F	F	F
0.0000000000000000	0.7500000000000000	0.0387919900000000	F	F	F
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0.5000000000000000	0.7500000000000000	0.0387919900000000	F	F	F
0.2500000000000000	0.2500000000000000	0.0387919900000000	F	F	F
0.2500000000000000	0.7500000000000000	0.0387919900000000	F	F	F
0.7500000000000000	0.2500000000000000	0.0387919900000000	F	F	F
0.7500000000000000	0.7500000000000000	0.0387919900000000	F	F	F
0.0000000000000000	0.0000000000000000	0.0958983599999996	F	F	F
0.0000000000000000	0.5000000000000000	0.0958983599999996	F	F	F
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0.2500000000000000	0.0000000000000000	0.0958983599999996	F	F	F
0.2500000000000000	0.5000000000000000	0.0958983599999996	F	F	F
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0.7500000000000000	0.5000000000000000	0.0958983599999996	F	F	F
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0.0000000000000000	0.7500000000000000	0.1029857400000012	F	F	F
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0.5000000000000000	0.7500000000000000	0.1029857400000012	F	F	F
0.2500000000000000	0.2500000000000000	0.1029857400000012	F	F	F
0.2500000000000000	0.7500000000000000	0.1029857400000012	F	F	F
0.7500000000000000	0.2500000000000000	0.1029857400000012	F	F	F
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0.0000000000000000	0.0000000000000000	0.1657462399999972	F	F	F
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0.0000000000000000	0.2500000000000000	0.1676434999999969	F	F	F
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0.5000000000000000	0.2500000000000000	0.1676434999999969	F	F	F
0.5000000000000000	0.7500000000000000	0.1676434999999969	F	F	F
0.2500000000000000	0.2500000000000000	0.1676434999999969	F	F	F
0.2500000000000000	0.7500000000000000	0.1676434999999969	F	F	F
0.7500000000000000	0.2500000000000000	0.1676434999999969	F	F	F
0.7500000000000000	0.7500000000000000	0.1676434999999969	F	F	F
0.0000000000000000	0.0000000000000000	0.2334133600000001	F	F	F
0.0000000000000000	0.5000000000000000	0.2334133600000001	F	F	F
0.5000000000000000	0.0000000000000000	0.2334133600000001	F	F	F
0.5000000000000000	0.5000000000000000	0.2334133600000001	F	F	F
0.2500000000000000	0.0000000000000000	0.2334133600000001	F	F	F
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0.7500000000000000	0.7500000000000000	0.2341147599999971	F	F	F
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0.7500000000000000	0.0000000000000000	0.3007607999999991	F	F	F
0.7500000000000000	0.5000000000000000	0.3007607999999991	F	F	F
0.0000000000000000	0.2500000000000000	0.3008723200000034	F	F	F
0.0000000000000000	0.7500000000000000	0.3008723200000034	F	F	F
0.5000000000000000	0.2500000000000000	0.3008723200000034	F	F	F
0.5000000000000000	0.7500000000000000	0.3008723200000034	F	F	F
0.2500000000000000	0.2500000000000000	0.3008723200000034	F	F	F
0.2500000000000000	0.7500000000000000	0.3008723200000034	F	F	F
0.7500000000000000	0.2500000000000000	0.3008723200000034	F	F	F
0.7500000000000000	0.7500000000000000	0.3008723200000034	F	F	F
0.0586267618711176	0.3052895260680444	0.6256764614978394	T	T	T
0.0563753789062034	0.7941074857971984	0.6258265574065760	T	T	T
0.5629407611344703	0.2955928883696615	0.6258862235159768	T	T	T
0.5530192527456634	0.8052533494823777	0.6255528989687065	T	T	T
0.0005697668576374	0.9994098102879931	0.3678654409572815	T	T	T
0.0005318830891454	0.4994132391105381	0.3678680348475751	T	T	T
0.5005093264533329	0.9994311145101946	0.3678442810705604	T	T	T
0.5004913842001173	0.4994430872101248	0.3677851246719825	T	T	T
0.0004254146916551	0.2495469739336968	0.3677750704876956	T	T	T
0.0004126590021087	0.7495370715940410	0.3677619760854540	T	T	T
0.5003926879200407	0.2494993591689436	0.3677576740518305	T	T	T
0.5003483854414483	0.7495611796211179	0.3677619083540264	T	T	T
0.3089331404217930	0.1949497532857976	0.6262732213884732	T	T	T
0.3108131649980450	0.6862542571521146	0.6264438877903729	T	T	T
0.8127258027417241	0.1868170428806195	0.6249327264477884	T	T	T
0.8020926023666775	0.6955646319496580	0.6261700822399163	T	T	T
0.4574020061363839	0.5425149576088231	0.6358910424267918	T	T	T
0.3971929025955774	0.6020836412081181	0.6328499748324390	T	T	T

 TS(110)

110-TS

1.0000000000000000	0.0000000000000000	0.0000000000000000
11.000311999999992	15.556789000000002	0.0000000000000000
0.0000000000000000		

0.0000000000000000	0.0000000000000000	30.556788999999984			
Ce	O	H			
64	128	2			
Selective dynamics					
Direct					
0.1250000000000000	0.0000000000000000	0.0690346700000006	F	F	F
0.1250000000000000	0.5000000000000000	0.0690346700000006	F	F	F
0.6250000000000000	0.0000000000000000	0.0690346700000006	F	F	F
0.6250000000000000	0.5000000000000000	0.0690346700000006	F	F	F
0.3735115999256564	0.1234608191594475	0.5035840367942228	T	T	T
0.3732328146184756	0.6291578539126377	0.5038480071879903	T	T	T
0.8732230566540551	0.1248017345236647	0.5035265584539914	T	T	T
0.8760048824704683	0.6249868898856334	0.5034982077036574	T	T	T
0.1233665733155291	0.2493193172722812	0.4485920419980829	T	T	T
0.1237656063406334	0.7504147661551102	0.4485355718086552	T	T	T
0.6238014872443642	0.2501390603312927	0.4489407174559901	T	T	T
0.6247160273454924	0.7501868257438744	0.4487152887287706	T	T	T
0.1234367193718455	0.9998587370525911	0.4486007676431001	T	T	T
0.1264497734236940	0.4994419887497799	0.4491823304980969	T	T	T
0.6240172656271241	0.9999635034851764	0.4485862336284541	T	T	T
0.6269077949628752	0.5006039042113528	0.4486118691998371	T	T	T
0.3746553485289610	0.3751655885428562	0.3814778665918439	T	T	T
0.3745063338335868	0.8750375968789683	0.3804229007584183	T	T	T
0.8749943144524650	0.3749385386271769	0.3805699622879430	T	T	T
0.8743638168032035	0.8749957151103445	0.3804035028268871	T	T	T
0.3742710689163573	0.1249200815866516	0.3805982067439970	T	T	T
0.3748122773800233	0.6250297743248296	0.3807658914714267	T	T	T
0.8741108589082387	0.1249867198725170	0.3804279900108796	T	T	T
0.8753067890966335	0.6248802878728767	0.3804726709614314	T	T	T
0.1251281660031793	0.2500268431501951	0.3189816973211990	T	T	T
0.1249879322570564	0.7499569269065915	0.3189189583121177	T	T	T
0.6247286611924281	0.2503687494377758	0.3190826112041449	T	T	T
0.6248545284767673	0.7498482433828428	0.3189780581139772	T	T	T
0.1247290414407445	0.0000299383864970	0.3189204384033815	T	T	T
0.1250360398272790	0.4997806845541461	0.3190820841305282	T	T	T
0.6246514447859681	0.0000453814974506	0.3189317525951338	T	T	T
0.6246610529293690	0.4998686142520867	0.3190190962046984	T	T	T
0.3750000000000000	0.1250000000000000	0.2536646300000029	F	F	F
0.3750000000000000	0.6250000000000000	0.2536646300000029	F	F	F
0.8750000000000000	0.1250000000000000	0.2536646300000029	F	F	F
0.8750000000000000	0.6250000000000000	0.2536646300000029	F	F	F
0.1250000000000000	0.2500000000000000	0.1920963900000032	F	F	F
0.1250000000000000	0.7500000000000000	0.1920963900000032	F	F	F
0.6250000000000000	0.2500000000000000	0.1920963900000032	F	F	F
0.6250000000000000	0.7500000000000000	0.1920963900000032	F	F	F
0.1250000000000000	0.0000000000000000	0.1920963900000032	F	F	F
0.1250000000000000	0.5000000000000000	0.1920963900000032	F	F	F
0.6250000000000000	0.0000000000000000	0.1920963900000032	F	F	F
0.6250000000000000	0.5000000000000000	0.1920963900000032	F	F	F
0.3750000000000000	0.3750000000000000	0.2536646300000029	F	F	F
0.3750000000000000	0.8750000000000000	0.2536646300000029	F	F	F
0.8750000000000000	0.3750000000000000	0.2536646300000029	F	F	F
0.8750000000000000	0.8750000000000000	0.2536646300000029	F	F	F
0.3707879335323270	0.3689542699455401	0.5059540959406235	T	T	T
0.3737117226444013	0.8759519970572782	0.5034748645484157	T	T	T
0.8748431762413134	0.3745845309725269	0.5035330000554197	T	T	T
0.8737092254667758	0.8750664372187629	0.5035459341963602	T	T	T
0.1250000000000000	0.2500000000000000	0.0690346700000006	F	F	F
0.1250000000000000	0.7500000000000000	0.0690346700000006	F	F	F
0.6250000000000000	0.2500000000000000	0.0690346700000006	F	F	F
0.6250000000000000	0.7500000000000000	0.0690346700000006	F	F	F
0.3750000000000000	0.1250000000000000	0.1237068800000003	F	F	F
0.3750000000000000	0.6250000000000000	0.1237068800000003	F	F	F
0.8750000000000000	0.1250000000000000	0.1237068800000003	F	F	F
0.8750000000000000	0.6250000000000000	0.1237068800000003	F	F	F
0.3750000000000000	0.3750000000000000	0.1237068800000003	F	F	F
0.3750000000000000	0.8750000000000000	0.1237068800000003	F	F	F
0.8750000000000000	0.3750000000000000	0.1237068800000003	F	F	F
0.8750000000000000	0.8750000000000000	0.1237068800000003	F	F	F
0.2548113160118959	0.9995490098509308	0.5083818466064471	T	T	T
0.2636189762818262	0.4993237986087280	0.5066034474138590	T	T	T
0.7551721735406858	0.9999335026501441	0.5082825295743447	T	T	T

0.7595118391525517	0.4990437140799244	0.5074967145334739	T	T	T
0.9918266189731924	0.9996930494385907	0.5083027116412708	T	T	T
0.9958727927971651	0.5002578828940401	0.5086568715664157	T	T	T
0.4921588770958323	0.9994868864444157	0.5085230018370197	T	T	T
0.5056398244650708	0.5122389124292965	0.5136120712961869	T	T	T
0.2476688737003698	0.3720788271905846	0.4455445959603992	T	T	T
0.2491083986530782	0.8751687208791594	0.4451142965852952	T	T	T
0.7492538267347513	0.3746809203420511	0.4451200976896530	T	T	T
0.7492626282934651	0.8749558193210447	0.4452622169471994	T	T	T
0.9986992743037888	0.3750465146836106	0.4454201701710119	T	T	T
0.9984636204092965	0.8749734822064568	0.4453308738636750	T	T	T
0.4984815786937347	0.3783860225431468	0.4482478159107401	T	T	T
0.4988969424237979	0.8753200153913312	0.4451650797292857	T	T	T
0.2433605599999993	0.1250000000000000	0.0641464600000035	F	F	F
0.2433605599999993	0.6250000000000000	0.0641464600000035	F	F	F
0.7433605599999993	0.1250000000000000	0.0641464600000035	F	F	F
0.7433605599999993	0.6250000000000000	0.0641464600000035	F	F	F
0.2495135059656874	0.0000843157355490	0.3819883962669053	T	T	T
0.2506857969571286	0.4999220545508081	0.3828297905659568	T	T	T
0.7494927140555747	0.9999971409454247	0.3820145027370145	T	T	T
0.750188613096041	0.5001868135704584	0.3823607199802694	T	T	T
0.2487327238590638	0.1246565348096667	0.4452991857797386	T	T	T
0.2489215942528844	0.6268476961635230	0.4455025887719657	T	T	T
0.7487684866900892	0.1250883238373390	0.4452993801845651	T	T	T
0.7499325298226935	0.6253008621163119	0.4454157858283594	T	T	T
0.9980514745526463	0.1245184692706260	0.4453120759425246	T	T	T
0.9994274358578963	0.6246997241270549	0.4452813206482489	T	T	T
0.4984884970216470	0.1236761217167199	0.4449748664054809	T	T	T
0.4984686616555223	0.6243473135624811	0.4457169991666419	T	T	T
0.9916649531128101	0.2496659450034855	0.5082049936957418	T	T	T
0.9926177948262449	0.7496315605854278	0.5082638715976984	T	T	T
0.4908089414759189	0.2462932889320300	0.5076018540811447	T	T	T
0.4921313132864285	0.7513175234356950	0.5081790131538213	T	T	T
0.0066394299999999	0.3750000000000000	0.0641464600000035	F	F	F
0.0066394299999999	0.8750000000000000	0.0641464600000035	F	F	F
0.5066394400000007	0.3750000000000000	0.0641464600000035	F	F	F
0.5066394400000007	0.8750000000000000	0.0641464600000035	F	F	F
0.2500772233000959	0.2493540949245485	0.3818354632553778	T	T	T
0.2500186502413726	0.7501686393483098	0.3818411297220408	T	T	T
0.7498445985928015	0.2498693520295276	0.3819018170043762	T	T	T
0.7499978027470462	0.7499079682105005	0.3820291284528423	T	T	T
0.9995426533714991	0.2499026165423786	0.3821244244795423	T	T	T
0.9996549668831065	0.7500082538517745	0.3820567324984623	T	T	T
0.4996845026759473	0.2516166054237843	0.3831455672676114	T	T	T
0.4998000731985854	0.7496927524434867	0.3822618076516875	T	T	T
0.2433605599999993	0.3750000000000000	0.0641464600000035	F	F	F
0.2433605599999993	0.8750000000000000	0.0641464600000035	F	F	F
0.7433605599999993	0.3750000000000000	0.0641464600000035	F	F	F
0.7433605599999993	0.8750000000000000	0.0641464600000035	F	F	F
0.0066394299999999	0.1250000000000000	0.0641464600000035	F	F	F
0.0066394299999999	0.6250000000000000	0.0641464600000035	F	F	F
0.5066394400000007	0.1250000000000000	0.0641464600000035	F	F	F
0.5066394400000007	0.6250000000000000	0.0641464600000035	F	F	F
0.2498003199999985	0.2500000000000000	0.1271687799999981	F	F	F
0.2498003199999985	0.7500000000000000	0.1271687799999981	F	F	F
0.7498002999999969	0.2500000000000000	0.1271687799999981	F	F	F
0.7498002999999969	0.7500000000000000	0.1271687799999981	F	F	F
0.9998887223031900	0.3748585275453706	0.3180055115156719	T	T	T
0.9996722675177523	0.8748961197537568	0.3180021144214393	T	T	T
0.4996252168525217	0.3749287541979101	0.3182708904501084	T	T	T
0.4997613742726088	0.8747005949207960	0.3179803644523247	T	T	T
0.0001536700000031	0.1250000000000000	0.1905233399999986	F	F	F
0.0001536700000031	0.6250000000000000	0.1905233399999986	F	F	F
0.5001536600000023	0.1250000000000000	0.1905233399999986	F	F	F
0.5001536600000023	0.6250000000000000	0.1905233399999986	F	F	F
0.2498463200000032	0.1250000000000000	0.1905233399999986	F	F	F
0.2498463200000032	0.6250000000000000	0.1905233399999986	F	F	F
0.7498463399999977	0.1250000000000000	0.1905233399999986	F	F	F
0.7498463399999977	0.6250000000000000	0.1905233399999986	F	F	F
0.0001996800000015	0.2500000000000000	0.1271687799999981	F	F	F
0.0001996800000015	0.7500000000000000	0.1271687799999981	F	F	F
0.5001997000000031	0.2500000000000000	0.1271687799999981	F	F	F

0.5001997000000031	0.7500000000000000	0.1271687799999981	F	F	F
0.0001536700000031	0.3750000000000000	0.1905233399999986	F	F	F
0.0001536700000031	0.8750000000000000	0.1905233399999986	F	F	F
0.5001536600000023	0.3750000000000000	0.1905233399999986	F	F	F
0.5001536600000023	0.8750000000000000	0.1905233399999986	F	F	F
0.2498463200000032	0.3750000000000000	0.1905233399999986	F	F	F
0.2498463200000032	0.8750000000000000	0.1905233399999986	F	F	F
0.7498463399999977	0.3750000000000000	0.1905233399999986	F	F	F
0.7498463399999977	0.8750000000000000	0.1905233399999986	F	F	F
0.0000256399999969	0.0000000000000000	0.2546287699999965	F	F	F
0.0000256399999969	0.5000000000000000	0.2546287699999965	F	F	F
0.5000256599999986	0.0000000000000000	0.2546287699999965	F	F	F
0.5000256599999986	0.5000000000000000	0.2546287699999965	F	F	F
0.9991531791466954	0.9998470758403855	0.3819894948182494	T	T	T
0.0001232445573649	0.4997759502726851	0.3819392397429979	T	T	T
0.4992225938580219	0.9997328011559858	0.3816870090229969	T	T	T
0.5005434900019381	0.4996164566325092	0.3823855458071961	T	T	T
0.2499743500000022	0.0000000000000000	0.2546287699999965	F	F	F
0.2499743500000022	0.5000000000000000	0.2546287699999965	F	F	F
0.7499743400000014	0.0000000000000000	0.2546287699999965	F	F	F
0.7499743400000014	0.5000000000000000	0.2546287699999965	F	F	F
0.2499743500000022	0.2500000000000000	0.2546287699999965	F	F	F
0.2499743500000022	0.7500000000000000	0.2546287699999965	F	F	F
0.7499743400000014	0.2500000000000000	0.2546287699999965	F	F	F
0.7499743400000014	0.7500000000000000	0.2546287699999965	F	F	F
0.2535270674988297	0.2479035367041860	0.5094506093216609	T	T	T
0.2547262306941036	0.7517901565355913	0.5088695270976800	T	T	T
0.7551446193212001	0.2498551521283474	0.5081753960595847	T	T	T
0.7560047102871792	0.7502260245235064	0.5082308581814488	T	T	T
0.2498003199999985	0.0000000000000000	0.1271687799999981	F	F	F
0.2498003199999985	0.5000000000000000	0.1271687799999981	F	F	F
0.7498002999999969	0.0000000000000000	0.1271687799999981	F	F	F
0.7498002999999969	0.5000000000000000	0.1271687799999981	F	F	F
0.9996337975933116	0.1250435424286351	0.3180517818264548	T	T	T
0.999673499266422	0.6249849304030022	0.3180275206440015	T	T	T
0.4996715405849557	0.1257895079465996	0.3183212707833007	T	T	T
0.4997405936019135	0.6248419664905214	0.3181687249821650	T	T	T
0.2497370116028677	0.1248232284634625	0.3178740702644447	T	T	T
0.2499325978482645	0.6246093520937492	0.3181983477119772	T	T	T
0.7494858579226076	0.1249930478635406	0.3179475897956294	T	T	T
0.7498769289620384	0.6248174272368630	0.3180582371736946	T	T	T
0.0001996800000015	0.0000000000000000	0.1271687799999981	F	F	F
0.0001996800000015	0.5000000000000000	0.1271687799999981	F	F	F
0.5001997000000031	0.0000000000000000	0.1271687799999981	F	F	F
0.5001997000000031	0.5000000000000000	0.1271687799999981	F	F	F
0.0000256399999969	0.2500000000000000	0.2546287699999965	F	F	F
0.0000256399999969	0.7500000000000000	0.2546287699999965	F	F	F
0.5000256599999986	0.2500000000000000	0.2546287699999965	F	F	F
0.5000256599999986	0.7500000000000000	0.2546287699999965	F	F	F
0.2500872161975920	0.3753021771896528	0.3184276612224934	T	T	T
0.2497082294016408	0.8750664833746882	0.3179186270900942	T	T	T
0.7497799536957857	0.3752175022954276	0.3180951474650229	T	T	T
0.7496211059555193	0.8749881445385483	0.3179986016523131	T	T	T
0.4678442102323714	0.4199437420361534	0.5687662177324455	T	T	T
0.4975467187138776	0.4699222146194089	0.5454995491914971	T	T	T

TS-(111)

111-TS

1.0000000000000000		
11.653295999999992	0.0000000000000000	0.0000000000000000
5.8266480000000005	10.0920520000000007	0.0000000000000000
0.0000000000000000	0.0000040000000000	26.0000000000000000

Ce O H

36 72 2

Selective dynamics

Direct

0.3333333100000004	0.0000000000000000	0.2309503299999989	F	F	F
0.3333333100000004	0.3333333400000029	0.2309503299999989	F	F	F

0.3333333100000004	0.6666666899999996	0.2309503299999989	F	F	F
0.6666666300000017	0.0000000000000000	0.2309503299999989	F	F	F
0.6666666300000017	0.3333333400000029	0.2309503299999989	F	F	F
0.6666666300000017	0.6666666899999996	0.2309503299999989	F	F	F
0.0000000000000000	0.0000000000000000	0.2309503299999989	F	F	F
0.0000000000000000	0.3333333400000029	0.2309503299999989	F	F	F
0.0000000000000000	0.6666666899999996	0.2309503299999989	F	F	F
0.2211684257334596	0.2230469945791000	0.3537128945195178	F	F	F
0.2216173224057272	0.5559585828488949	0.3534765119721612	F	F	F
0.2210491468129376	0.8895764359565632	0.3536839614369214	F	F	F
0.5547834063355523	0.2235120106708806	0.3544734594502685	F	F	F
0.5546691273073279	0.5553646211265857	0.3544434074040836	F	F	F
0.5555489349386988	0.8890192616866699	0.3539086602997088	F	F	F
0.8873754138153842	0.2231189888832503	0.3539538286722603	F	F	F
0.8881322598514743	0.5560579789830200	0.3533594418267185	F	F	F
0.8880288860698826	0.8894161063615087	0.3533869603534896	F	F	F
0.1111110800000006	0.1111111600000001	0.1094482800000023	F	F	F
0.1111110800000006	0.4444444800000014	0.1094482800000023	F	F	F
0.1111110800000006	0.7777778499999997	0.1094482800000023	F	F	F
0.4444444200000035	0.1111111600000001	0.1094482800000023	F	F	F
0.4444444200000035	0.4444444800000014	0.1094482800000023	F	F	F
0.4444444200000035	0.7777778499999997	0.1094482800000023	F	F	F
0.7777777299999968	0.1111111600000001	0.1094482800000023	F	F	F
0.7777777299999968	0.4444444800000014	0.1094482800000023	F	F	F
0.7777777299999968	0.7777778499999997	0.1094482800000023	F	F	F
0.1095876548909231	0.1122256483976827	0.4748823071259594	F	F	F
0.1090818697774765	0.4450689789226487	0.4751239240494769	F	F	F
0.1086433164372949	0.7800495647356271	0.4750444223628989	F	F	F
0.4429383550937374	0.1120183561954207	0.4754630472153636	F	F	F
0.4336518459433520	0.4503591094862074	0.4768536533337340	T	T	T
0.4425905391528886	0.7792356220496330	0.4753695980132449	F	F	F
0.7794227120954886	0.1074443607795530	0.4757549412058495	T	T	T
0.7796357007318520	0.4471575155110656	0.4756233304843818	T	T	T
0.7772424514493537	0.7782195436337744	0.4754078376472890	F	F	F
0.3333745810611859	0.0001334885642876	0.3238112151371411	F	F	F
0.3328623547531322	0.3330928500013997	0.3230493284637532	F	F	F
0.3327807609346252	0.6676256371813309	0.3230651982225439	F	F	F
0.6657380795217875	0.0004323621519546	0.3231700694141892	F	F	F
0.6658250739679445	0.3338575325217192	0.3235687022985445	F	F	F
0.6657050333142962	0.6673383121575966	0.3231711416437477	F	F	F
0.9991968048179416	0.0003664295670660	0.3230169494766955	F	F	F
0.9991822316030721	0.3340664160341902	0.3229833197386753	F	F	F
0.9994167854102614	0.6670416460909578	0.3229237294261580	F	F	F
0.2222221899999965	0.2222227000000032	0.0793340600000008	F	F	F
0.2222221899999965	0.5555555800000036	0.0793340600000008	F	F	F
0.2222221899999965	0.8888889500000019	0.0793340600000008	F	F	F
0.5555555199999986	0.2222227000000032	0.0793340600000008	F	F	F
0.5555555199999986	0.5555555800000036	0.0793340600000008	F	F	F
0.5555555199999986	0.8888889500000019	0.0793340600000008	F	F	F
0.8888888399999999	0.2222227000000032	0.0793340600000008	F	F	F
0.8888888399999999	0.5555555800000036	0.0793340600000008	F	F	F
0.8888888399999999	0.8888889500000019	0.0793340600000008	F	F	F
0.2202855478981078	0.2209249424672635	0.4436639434767997	F	F	F
0.2186860301769968	0.5574686598118319	0.4447621073358121	F	F	F
0.2196990940032748	0.8934167485953708	0.4434822005742447	F	F	F
0.5572645307081032	0.2273711087595132	0.4467012525584551	T	T	T
0.5568999797776044	0.5495880666829223	0.4466050371686521	T	T	T
0.5540644955172382	0.8898734696347148	0.4443146556109028	F	F	F
0.8842108946431182	0.2247832155721170	0.4447344164690747	T	T	T
0.8884398401042546	0.5563377236956484	0.4440633478009701	F	F	F
0.8880146113117107	0.8892770736190130	0.4441301486917268	F	F	F
0.2222221600000012	0.2222227000000032	0.2615932499999971	F	F	F
0.2222221600000012	0.5555555800000036	0.2615932499999971	F	F	F
0.2222221600000012	0.8888889500000019	0.2615932499999971	F	F	F
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0.5555555199999986	0.5555555800000036	0.2615932499999971	F	F	F
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0.8888888399999999	0.2222227000000032	0.2615932499999971	F	F	F
0.8888888399999999	0.5555555800000036	0.2615932499999971	F	F	F
0.8888888399999999	0.8888889500000019	0.2615932499999971	F	F	F
0.3333333400000029	0.0000000000000000	0.1403399000000007	F	F	F
0.3333333400000029	0.3333333400000029	0.1403399000000007	F	F	F

0.3333333400000029	0.6666666899999996	0.1403399000000007	F	F	F
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0.6666666899999996	0.3333333400000029	0.1403399000000007	F	F	F
0.6666666899999996	0.6666666899999996	0.1403399000000007	F	F	F
0.0000000000000000	0.0000000000000000	0.1403399000000007	F	F	F
0.0000000000000000	0.3333333400000029	0.1403399000000007	F	F	F
0.0000000000000000	0.6666666899999996	0.1403399000000007	F	F	F
0.3325990682390554	0.0005929674042378	0.5053743963506960	F	F	F
0.3269069580408228	0.3322836803004208	0.5040401192419850	T	T	T
0.3258323390822966	0.6760029111034314	0.5035791731220414	T	T	T
0.6666783410688737	0.9996674133618839	0.5052829622554071	F	F	F
0.6863301638603758	0.3244339550764508	0.5155725272720133	T	T	T
0.6670002154210124	0.6673865018962459	0.5051472436725177	F	F	F
0.9987780417592091	0.0002622788739686	0.5052147021932498	F	F	F
0.9991626540222569	0.3347008849674395	0.5051801399625830	F	F	F
0.9967723850656185	0.6684586545507472	0.5054622537495206	F	F	F
0.1111111049999981	0.1111111600000001	0.1997374099999973	F	F	F
0.1111111049999981	0.4444444800000014	0.1997374099999973	F	F	F
0.1111111049999981	0.7777778499999997	0.1997374099999973	F	F	F
0.4444443900000010	0.1111111600000001	0.1997374099999973	F	F	F
0.4444443900000010	0.4444444800000014	0.1997374099999973	F	F	F
0.4444443900000010	0.7777778499999997	0.1997374099999973	F	F	F
0.7777777299999968	0.1111111600000001	0.1997374099999973	F	F	F
0.7777777299999968	0.4444444800000014	0.1997374099999973	F	F	F
0.7777777299999968	0.7777778499999997	0.1997374099999973	F	F	F
0.1075118231645362	0.1133619035222324	0.3846893986341584	F	F	F
0.1105816766948848	0.4446946172498514	0.3847599710084566	F	F	F
0.1103664014192631	0.7784204865521076	0.3847544254056743	F	F	F
0.4451369964339165	0.1131076826202957	0.3858739957314086	F	F	F
0.4411735600563489	0.4461862976417592	0.3844051192339393	F	F	F
0.4449361969997341	0.7756385188681136	0.3858161446554220	F	F	F
0.7768895939718377	0.1107177658793574	0.3850680059365885	F	F	F
0.7768856337658292	0.4460254854613126	0.3850428737277909	F	F	F
0.7770139126178606	0.7782813295412083	0.3848620434748540	F	F	F
0.4939812503228325	0.4286178766094508	0.5597743426089394	T	T	T
0.6009602876277711	0.3711987576103013	0.5442603265902761	T	T	T

TS-(221)

221-TS

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Selective dynamics

Direct

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0.6766254300000014	0.2065023700000026	0.0961653299999981	F	F	F
0.4266253999999989	0.2065023700000026	0.0961653299999981	F	F	F
0.9266254300000014	0.2065023700000026	0.0961653299999981	F	F	F
0.2346029500000029	0.9384064500000022	0.1251644399999989	F	F	F
0.7346029599999966	0.9384064500000022	0.1251644399999989	F	F	F
0.4846029599999966	0.9384064500000022	0.1251644399999989	F	F	F
0.9846029599999966	0.9384064500000022	0.1251644399999989	F	F	F
0.2922178800000026	0.6688738400000034	0.1555735800000022	F	F	F
0.7922178800000026	0.6688738400000034	0.1555735800000022	F	F	F
0.0422178900000034	0.6688738400000034	0.1555735800000022	F	F	F
0.5422178800000026	0.6688738400000034	0.1555735800000022	F	F	F
0.0986668700000024	0.3946651799999970	0.1800825400000008	F	F	F
0.5986668800000032	0.3946651799999970	0.1800825400000008	F	F	F
0.3486668500000007	0.3946651799999970	0.1800825400000008	F	F	F
0.8486668199999983	0.3946651799999970	0.1800825400000008	F	F	F
0.4029683999999989	0.1118754800000019	0.2183137700000017	F	F	F
0.9029684300000014	0.1118754800000019	0.2183137700000017	F	F	F
0.1529683799999972	0.1118754800000019	0.2183137700000017	F	F	F
0.6529683699999964	0.1118754800000019	0.2183137700000017	F	F	F
0.4578611800000019	0.8314441899999991	0.2509747100000013	F	F	F

0.9578611800000019	0.8314441899999991	0.2509747100000013	F	F	F
0.2078611700000010	0.8314441899999991	0.2509747100000013	F	F	F
0.7078611800000019	0.8314441899999991	0.2509747100000013	F	F	F
0.0138888899999969	0.5555558000000036	0.2801990800000027	F	F	F
0.5138888999999978	0.5555558000000036	0.2801990800000027	F	F	F
0.2638888999999978	0.5555558000000036	0.2801990800000027	F	F	F
0.7638888999999978	0.5555558000000036	0.2801990800000027	F	F	F
0.0699949486578291	0.2799891085108044	0.3093788903426642	T	T	T
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0.3200530854930506	0.2800997812991710	0.3093590294594577	T	T	T
0.8198843205608028	0.2798576871055118	0.3093679553376489	T	T	T
0.1250985327818910	0.0001091078253666	0.3420548590438912	T	T	T
0.6249525418270849	0.9990712525649244	0.3427832468930632	T	T	T
0.3749195209628411	0.0000651740095776	0.3421827538773599	T	T	T
0.8750506396102935	0.9996555635044189	0.3422088369057334	T	T	T
0.1793385989971412	0.7177613031166246	0.3800516857167864	T	T	T
0.6795687269080517	0.7158056472086898	0.3797776149238956	T	T	T
0.4296845731179104	0.7183558829135919	0.3804290808958086	T	T	T
0.9297013456168770	0.7176360208790484	0.3801615080478271	T	T	T
0.2360904662799825	0.4442911620295789	0.4047382199625531	T	T	T
0.7360664787196143	0.4427316230551952	0.4048785463631290	T	T	T
0.485750812474002	0.4437568051179213	0.4047352307321859	T	T	T
0.9857191190029297	0.4432463743215678	0.4048380142350965	T	T	T
0.0441369215091498	0.1751085341722884	0.4351101985481662	T	T	T
0.5434549331707998	0.1749120231541426	0.4351857112167465	T	T	T
0.2936904965429861	0.1750377137957955	0.4351055916570274	T	T	T
0.7929465379293532	0.1726476062749924	0.4351286714655842	T	T	T
0.3499659667598465	0.9065663757853386	0.4643511949042178	T	T	T
0.8561203551546228	0.9075108105318463	0.4646894835582316	T	T	T
0.1027533517054664	0.9067369649518326	0.4643325564735648	T	T	T
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0.2734363100000010	0.0937380700000006	0.0769361300000000	F	F	F
0.7734363100000010	0.0937380700000006	0.0769361300000000	F	F	F
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0.5784225599999999	0.3136766900000012	0.1040784799999983	F	F	F
0.3284225900000024	0.3136766900000012	0.1040784799999983	F	F	F
0.8284225599999999	0.3136766900000012	0.1040784799999983	F	F	F
0.3327759299999968	0.8311121099999994	0.1087520100000035	F	F	F
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0.0827759100000023	0.8311121099999994	0.1087520100000035	F	F	F
0.5827759299999968	0.8311121099999994	0.1087520100000035	F	F	F
0.1382287899999994	0.0529157200000014	0.1411541800000009	F	F	F
0.6382288100000011	0.0529157200000014	0.1411541800000009	F	F	F
0.3882288100000011	0.0529157200000014	0.1411541800000009	F	F	F
0.8882288100000011	0.0529157200000014	0.1411541800000009	F	F	F
0.3914908599999976	0.5659549599999991	0.1386544200000017	F	F	F
0.8914908799999992	0.5659549599999991	0.1386544200000017	F	F	F
0.1414908599999976	0.5659549599999991	0.1386544200000017	F	F	F
0.6414908900000000	0.5659549599999991	0.1386544200000017	F	F	F
0.1942389100000028	0.2769545499999992	0.1681039200000001	F	F	F
0.6942389199999965	0.2769545499999992	0.1681039200000001	F	F	F
0.4442388900000012	0.2769545499999992	0.1681039200000001	F	F	F
0.9442388599999987	0.2769545499999992	0.1681039200000001	F	F	F
0.1950204500000012	0.7800809700000002	0.1728901600000015	F	F	F
0.6950204299999996	0.7800809700000002	0.1728901600000015	F	F	F
0.4450204600000021	0.7800809700000002	0.1728901600000015	F	F	F
0.9450204899999974	0.7800809700000002	0.1728901600000015	F	F	F
0.2498572200000027	0.9994266200000013	0.2024984600000010	F	F	F
0.7498572200000027	0.9994266200000013	0.2024984600000010	F	F	F
0.9997305300000008	0.4989176899999990	0.1994941399999988	F	F	F
0.4997305300000008	0.4989176899999990	0.1994941399999988	F	F	F
0.2497305400000016	0.4989176899999990	0.1994941399999988	F	F	F
0.7497305300000008	0.4989176899999990	0.1994941399999988	F	F	F
0.9998572200000027	0.9994266200000013	0.2024984600000010	F	F	F
0.4998572200000027	0.9994266200000013	0.2024984600000010	F	F	F
0.0559230499999970	0.2236992899999990	0.2314988400000004	F	F	F
0.5559230300000024	0.2236992899999990	0.2314988400000004	F	F	F
0.0550411899999972	0.7201730000000026	0.2335694699999991	F	F	F
0.5550411800000035	0.7201730000000026	0.2335694699999991	F	F	F
0.3059230599999978	0.2236992899999990	0.2314988400000004	F	F	F

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0.80504118000000035	0.72017300000000026	0.2335694699999991	F	F	F
0.11147713999999981	0.44589409999999967	0.26273590000000027	F	F	F
0.61147714999999989	0.44589409999999967	0.26273590000000027	F	F	F
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0.6665303798315563	0.6650812058224176	0.2977329274438105	T	T	T
0.4163191343941932	0.6655715343861957	0.2974586090014029	T	T	T
0.9164401139427625	0.6655548802259048	0.2975956274386888	T	T	T
0.16694078999999982	0.16776211999999990	0.29510300999999983	F	F	F
0.66694082000000007	0.16776211999999990	0.29510300999999983	F	F	F
0.41694076000000028	0.16776211999999990	0.29510300999999983	F	F	F
0.91694076000000028	0.16776211999999990	0.29510300999999983	F	F	F
0.2228815239806963	0.3915894376184568	0.3267955325853222	T	T	T
0.7230164134587653	0.3913929787876356	0.3268510201153774	T	T	T
0.4729161149315360	0.3915017634132880	0.3268332298251053	T	T	T
0.9727332333422680	0.3913360677636888	0.3268334106584234	T	T	T
0.2218151429183877	0.8884136266173712	0.3286400130524214	T	T	T
0.7215574450554811	0.8871215053099917	0.3289239789833047	T	T	T
0.4729049225169746	0.8869377213479268	0.3297123154730315	T	T	T
0.9717171613326130	0.8876758811013516	0.3291004743159078	T	T	T
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0.5275750034518225	0.1121673550724083	0.3576454141278091	T	T	T
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0.0280847008044276	0.6132887216667271	0.3607968599551867	T	T	T
0.5283844647752503	0.6139725170194907	0.3606141760022012	T	T	T
0.2786476871299186	0.6136901770423790	0.3608430969337846	T	T	T
0.7788423225296341	0.6133273749309041	0.3608048770213230	T	T	T
0.0843301311892546	0.8356602883759336	0.3922022883944578	T	T	T
0.5868103605783972	0.8344850088893949	0.3948984180794142	T	T	T
0.0832247977111606	0.3325815361963720	0.3874242256583571	T	T	T
0.5830457894211918	0.3316340823423261	0.3874016636773945	T	T	T
0.3330333575767170	0.3327615824786392	0.3873731452513169	T	T	T
0.8328395222084453	0.3312947025058932	0.3874440070999299	T	T	T
0.3324054195565012	0.8360565544596739	0.3919077952021652	T	T	T
0.8334564994044200	0.8362384623757038	0.3927711434681314	T	T	T
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0.6360855072918028	0.5451972214979577	0.4208612759138859	T	T	T
0.1401951681588400	0.0601830010714934	0.4191591492200857	T	T	T
0.6382238126344788	0.0616038909003862	0.4193794575441174	T	T	T
0.3868787941406140	0.5472151842313266	0.4215443029127357	T	T	T
0.8867835060498166	0.5463204210028039	0.4216303728524409	T	T	T
0.3899190223198943	0.0601877935008446	0.4193236526573898	T	T	T
0.8918703075355907	0.0605155927519547	0.4192207315766865	T	T	T
0.1957417018741552	0.2822647346506812	0.4515714015481080	T	T	T
0.6958254068137322	0.2820606731088873	0.4517935802581334	T	T	T
0.4464904988021559	0.8012981623659599	0.4553740616296267	T	T	T
0.9513001961697540	0.7996714221935477	0.4562138376227551	T	T	T
0.1992647644322219	0.7990366565037306	0.4566068706669881	T	T	T
0.7063386178289477	0.7835553947680722	0.4596068916640235	T	T	T
0.4451563587655940	0.2822049799229447	0.4515017973783912	T	T	T
0.9454830692854443	0.2814972389893953	0.4516014541132094	T	T	T
0.2544677726564188	0.0194391064248975	0.4834960849617644	T	T	T
0.7537579332846676	0.0142823491350015	0.4813935149702715	T	T	T
0.0059262950437500	0.0195768924835988	0.4839374080888632	T	T	T
0.5041923455480344	0.0201998747914942	0.4844870544312485	T	T	T
0.6595069933028483	0.7641627675825973	0.4923305336009420	T	T	T
0.6106589599368135	0.7727759185732950	0.5185634985971888	T	T	T

 TS-(331)

331-TS

1.0000000000000000				
7.7783949999999997	0.0000000000000000	0.0000000000000000		
-3.8891979999999999	16.9526199999999996	0.0000000000000000		
0.0000000000000000	0.0000000000000000	29.5109349999999999		

Ce O H

40 80 2

Selective dynamics

Direct

0.2069911399999995	0.4139822899999999	0.0802282100000014	F	F	F
0.7069911099999970	0.4139822899999999	0.0802282100000014	F	F	F
0.7069911099999970	0.9139822899999999	0.0802282100000014	F	F	F
0.2069911399999995	0.9139822899999999	0.0802282100000014	F	F	F
0.3682377200000033	0.7364754299999987	0.1193458999999990	F	F	F
0.8682377499999987	0.7364754299999987	0.1193458999999990	F	F	F
0.3682377200000033	0.2364754500000004	0.1193458999999990	F	F	F
0.8682377499999987	0.2364754500000004	0.1193458999999990	F	F	F
0.0273628300000013	0.5547256300000001	0.1557375800000003	F	F	F
0.5273628400000021	0.5547256300000001	0.1557375800000003	F	F	F
0.0273628300000013	0.0547256500000017	0.1557375800000003	F	F	F
0.5273628400000021	0.0547256500000017	0.1557375800000003	F	F	F
0.6848900299999983	0.8697800599999965	0.2046350700000019	F	F	F
0.1848900099999966	0.8697800599999965	0.2046350700000019	F	F	F
0.6848900299999983	0.3697800300000011	0.2046350700000019	F	F	F
0.1848900099999966	0.3697800300000011	0.2046350700000019	F	F	F
0.8412300700000017	0.6824601300000026	0.2462408600000003	F	F	F
0.3412300600000009	0.6824601300000026	0.2462408600000003	F	F	F
0.8412300600000009	0.1824601200000018	0.2462408600000003	F	F	F
0.3412300600000009	0.1824601200000018	0.2462408600000003	F	F	F
0.0009422598683102	0.5020265905468477	0.2880947671406773	T	T	T
0.5012618837935605	0.5021507404370738	0.2880887813656230	T	T	T
0.0005469219166585	0.0020064185900921	0.2880774208278822	T	T	T
0.5013569634773631	0.0020359356225015	0.2880884458456165	T	T	T
0.6576001909059244	0.8151565552729281	0.3298009146788985	T	T	T
0.6569533807444188	0.3149546924186879	0.3304274614935707	T	T	T
0.1576814027557063	0.8151804603878787	0.3298225690674172	T	T	T
0.1577008272303857	0.3151968525730808	0.3299644996245519	T	T	T
0.3158792835303288	0.6308652827416878	0.3786883370270786	T	T	T
0.3138614372426005	0.1294533827744786	0.3778100561470055	T	T	T
0.8153080085845374	0.6310162324296016	0.3787005519358857	T	T	T
0.8149857294187370	0.1312203511403780	0.3787434572973751	T	T	T
0.9741965732785971	0.9490247727384542	0.4150516925794960	T	T	T
0.4752268452495514	0.4489677340715303	0.4147747859375173	T	T	T
0.4750483146192863	0.9490825856865186	0.4150374172022282	T	T	T
0.9750385145243570	0.4503205605790512	0.4147242459333498	T	T	T
0.6359577714998892	0.7718715834633585	0.4543475605907190	T	T	T
0.1360881144077055	0.7717819037657350	0.4542710518689788	T	T	T
0.1313435527062055	0.2735084530388434	0.4546157716689905	T	T	T
0.6454135562836214	0.2739649115828726	0.4565797729247620	T	T	T
0.4170010300000015	0.3340020600000031	0.0655032800000015	F	F	F
0.9170010300000015	0.8340020600000031	0.0655032800000015	F	F	F
0.4170010300000015	0.8340020600000031	0.0655032800000015	F	F	F
0.9170010300000015	0.3340020600000031	0.0655032800000015	F	F	F
0.4942802300000011	0.4885604600000022	0.0841822599999986	F	F	F
0.9942802300000011	0.4885604600000022	0.0841822599999986	F	F	F
0.4942802300000011	0.9885604600000022	0.0841822599999986	F	F	F
0.9942802300000011	0.9885604600000022	0.0841822599999986	F	F	F
0.5822149299999992	0.6644298699999993	0.1077273499999976	F	F	F
0.0822149299999992	0.6644298699999993	0.1077273499999976	F	F	F
0.5822149299999992	0.1644298699999993	0.1077273499999976	F	F	F
0.0822149299999992	0.1644298699999993	0.1077273499999976	F	F	F
0.6592633200000009	0.8185266500000026	0.1309383199999985	F	F	F
0.1592633200000009	0.8185266500000026	0.1309383199999985	F	F	F
0.6592633200000009	0.3185266500000026	0.1309383199999985	F	F	F
0.1592633200000009	0.3185266500000026	0.1309383199999985	F	F	F
0.7370480599999993	0.9740961199999987	0.1485278500000007	F	F	F
0.2370480800000010	0.9740961199999987	0.1485278500000007	F	F	F
0.7370480599999993	0.4740961500000012	0.1485278500000007	F	F	F
0.2370480800000010	0.4740961500000012	0.1485278500000007	F	F	F
0.8149496600000035	0.1298993500000023	0.1703081100000006	F	F	F
0.3149496600000035	0.1298993500000023	0.1703081100000006	F	F	F
0.3149496600000035	0.6298993199999998	0.1703081100000006	F	F	F
0.8149496600000035	0.6298993199999998	0.1703081100000006	F	F	F

0.39407783000000005	0.2881556299999986	0.1928188500000019	F	F	F
0.8940777999999980	0.2881556299999986	0.1928188500000019	F	F	F
0.8940777999999980	0.7881556600000010	0.1928188500000019	F	F	F
0.39407783000000005	0.7881556600000010	0.1928188500000019	F	F	F
0.97394757000000000	0.9478951899999970	0.2131436000000022	F	F	F
0.47394760000000025	0.9478951899999970	0.2131436000000022	F	F	F
0.97394757000000000	0.44789516000000016	0.2131436000000022	F	F	F
0.47394760000000025	0.44789516000000016	0.2131436000000022	F	F	F
0.55282650000000019	0.60565306000000016	0.23459719000000023	F	F	F
0.05282652000000035	0.60565306000000016	0.23459719000000023	F	F	F
0.55282650000000019	0.10565304000000000	0.23459719000000023	F	F	F
0.05282652000000035	0.10565304000000000	0.23459719000000023	F	F	F
0.63149231999999996	0.76298469000000032	0.25670096999999971	F	F	F
0.13149235000000020	0.76298469000000032	0.25670096999999971	F	F	F
0.63149231999999996	0.26298469000000032	0.25670096999999971	F	F	F
0.13149235000000020	0.26298469000000032	0.25670096999999971	F	F	F
0.7099212477676460	0.4213783176940993	0.2778758557704251	T	T	T
0.7107590344617236	0.9215150286946070	0.2776837765427231	T	T	T
0.2107953561141684	0.9215155736531599	0.2776804544956164	T	T	T
0.2116159710454326	0.4215199957950233	0.2776954550322586	T	T	T
0.7896553748812352	0.5790660814174018	0.2997504066136258	T	T	T
0.2895438800245103	0.5790162413583104	0.2998042725770702	T	T	T
0.7896629663511803	0.0790858182236676	0.2995811516672262	T	T	T
0.2889910895261778	0.0787135976378366	0.2999524812613075	T	T	T
0.8685299240598425	0.7371376451289038	0.3213525140455076	T	T	T
0.3686817507150479	0.7371142623556182	0.3213301386587375	T	T	T
0.3691216556936325	0.2366355826104822	0.3209817265360755	T	T	T
0.8665166098762072	0.2364610307176278	0.3222831425413517	T	T	T
0.4486888392887352	0.8970738122284345	0.3416041798863176	T	T	T
0.9490629929645920	0.3970905069397261	0.3411426932461907	T	T	T
0.4480040972451960	0.3963022391171123	0.3419765310536178	T	T	T
0.9485442427627788	0.8971169046691259	0.3416087168243251	T	T	T
0.5280317172179139	0.5552757592895219	0.3638850839243446	T	T	T
0.5289262538958539	0.0560240887107710	0.3636997293554813	T	T	T
0.0264883588263203	0.0559243801388973	0.3639311759723896	T	T	T
0.0277940657100686	0.5557165641959330	0.3640433054656853	T	T	T
0.5985739563005836	0.2114527414954992	0.3881990604328109	T	T	T
0.1108163998588410	0.2125622436541406	0.3859937170238155	T	T	T
0.6057160417483729	0.7114154179811507	0.3859465148332717	T	T	T
0.1058163285357807	0.7112933002864992	0.3859528777653551	T	T	T
0.1833828627558276	0.8667125115966670	0.4034113591309776	T	T	T
0.6837793513614585	0.8671298724175927	0.4034234767233116	T	T	T
0.6886602843532472	0.3686836577276509	0.4034301299227252	T	T	T
0.1809069701356236	0.3682437729976016	0.4033664331818585	T	T	T
0.2620012144904322	0.5217461806351267	0.4266443128410486	T	T	T
0.7606377445295394	0.0216554978043746	0.4264095017183536	T	T	T
0.2608450592695490	0.0203358457649401	0.4256414720305060	T	T	T
0.7603266589902518	0.5220437399360165	0.4268380119624879	T	T	T
0.8487954614546922	0.6975457377382810	0.4502399582369350	T	T	T
0.3489032637625513	0.6973710403938824	0.4502530675565950	T	T	T
0.8538648973095491	0.1990960341186963	0.4490674149931095	T	T	T
0.3254928722194208	0.1876773637636546	0.4541556122571677	T	T	T
0.4263031330590223	0.8518292914792340	0.4687905877026139	T	T	T
0.9258516929130778	0.8520514052211965	0.4688365303594892	T	T	T
0.9270185952496561	0.3533641625297648	0.4701759147513798	T	T	T
0.4245476761510929	0.3487907512763471	0.4671207313058687	T	T	T
0.4018878928673928	0.1787475817780901	0.4868556346874513	T	T	T
0.5107176802420099	0.1895667269476959	0.5128224159626456	T	T	T

C. MS

 MS-(110)

110-MS

1.0000000000000000	0.0000000000000000	0.0000000000000000
11.000311999999992	15.556789000000002	0.0000000000000000
0.0000000000000000		

0.0000000000000000	0.0000000000000000	30.556788999999984			
Ce	O	H			
64	128	2			
Selective dynamics					
Direct					
0.1250000000000000	0.0000000000000000	0.0690346698404696	F	F	F
0.1250000000000000	0.5000000000000000	0.0690346698404696	F	F	F
0.6250000000000000	0.0000000000000000	0.0690346698404696	F	F	F
0.6250000000000000	0.5000000000000000	0.0690346698404696	F	F	F
0.3736505025973518	0.1234761128288039	0.5035586791396760	T	T	T
0.3714116210054467	0.6307238404248864	0.5039437819675604	T	T	T
0.8732427461236123	0.1248592644008317	0.5035037072200774	T	T	T
0.8760833303456008	0.6249991910536000	0.5033643332949403	T	T	T
0.1237660021662506	0.2493068841705212	0.4486261275682471	T	T	T
0.1232192174211402	0.7508783362591548	0.4483341819619643	T	T	T
0.6237119391218094	0.2500974181270599	0.4489855579741186	T	T	T
0.6245250997642448	0.7500259290918391	0.4487080959795027	T	T	T
0.1233179988172431	0.0000364085487972	0.4485058869773288	T	T	T
0.1269954525567879	0.4996253017122878	0.4492182768699536	T	T	T
0.6239573712028123	-0.0000879916229254	0.4485027647988996	T	T	T
0.6282448748031543	0.5003028944337898	0.4480243659793279	T	T	T
0.3748524989774562	0.3752014791661851	0.3817710111051575	T	T	T
0.3745014067195954	0.8750633080658398	0.3803806550666451	T	T	T
0.8755204491604276	0.3747848377488163	0.3805076440080898	T	T	T
0.8742210488678458	0.8750911259873850	0.3803378059982997	T	T	T
0.3743328925200971	0.1248882368556744	0.3805962958004171	T	T	T
0.3749768964769211	0.6250651101175668	0.3808317023321020	T	T	T
0.8741299568947059	0.1250482000901219	0.3803952153409165	T	T	T
0.8756288270644236	0.6249612219502396	0.3803668496908474	T	T	T
0.1253418200449661	0.2500617958143765	0.3189769439943877	T	T	T
0.1251486284736481	0.7500331347702861	0.3188519386202899	T	T	T
0.6248132607993173	0.2504405634750351	0.3190933399005713	T	T	T
0.6249408544753327	0.7497745705041403	0.3189700678369303	T	T	T
0.1247382237397413	0.0000951663262555	0.3188879617034889	T	T	T
0.1252472707511808	0.4997679669690842	0.3190953078713439	T	T	T
0.6246486116310056	0.0000584092797277	0.3188931003493396	T	T	T
0.6247208783074478	0.4997853018819638	0.3189165870613554	T	T	T
0.3750000000000000	0.1250000003213998	0.2536646301415999	F	F	F
0.3750000000000000	0.6250000003213998	0.2536646301415999	F	F	F
0.8750000000000000	0.1250000003213998	0.2536646301415999	F	F	F
0.8750000000000000	0.6250000003213998	0.2536646301415999	F	F	F
0.1250000000000000	0.2500000000000000	0.1920963901017245	F	F	F
0.1250000000000000	0.7500000000000000	0.1920963901017245	F	F	F
0.6250000000000000	0.2500000000000000	0.1920963901017245	F	F	F
0.6250000000000000	0.7500000000000000	0.1920963901017245	F	F	F
0.1250000000000000	0.0000000000000000	0.1920963901017245	F	F	F
0.1250000000000000	0.5000000000000000	0.1920963901017245	F	F	F
0.6250000000000000	0.0000000000000000	0.1920963901017245	F	F	F
0.6250000000000000	0.5000000000000000	0.1920963901017245	F	F	F
0.3750000000000000	0.3749999996786002	0.2536646301415999	F	F	F
0.3750000000000000	0.8750000003213998	0.2536646301415999	F	F	F
0.8750000000000000	0.3749999996786002	0.2536646301415999	F	F	F
0.8750000000000000	0.8750000003213998	0.2536646301415999	F	F	F
0.3706549982902938	0.3681702670866610	0.5067966575743394	T	T	T
0.3733773310725316	0.8765259070342628	0.5034330061973187	T	T	T
0.8753087503501890	0.3744161823139132	0.5034559037948036	T	T	T
0.8734018753157898	0.8751989064184637	0.5034950323119068	T	T	T
0.1250000000000000	0.2500000000000000	0.0690346698404696	F	F	F
0.1250000000000000	0.7500000000000000	0.0690346698404696	F	F	F
0.6250000000000000	0.2500000000000000	0.0690346698404696	F	F	F
0.6250000000000000	0.7500000000000000	0.0690346698404696	F	F	F
0.3750000000000000	0.1250000003213998	0.1237068799997303	F	F	F
0.3750000000000000	0.6250000003213998	0.1237068799997303	F	F	F
0.8750000000000000	0.1250000003213998	0.1237068799997303	F	F	F
0.8750000000000000	0.6250000003213998	0.1237068799997303	F	F	F
0.3750000000000000	0.3749999996786002	0.1237068799997303	F	F	F
0.3750000000000000	0.8750000003213998	0.1237068799997303	F	F	F
0.8750000000000000	0.3749999996786002	0.1237068799997303	F	F	F
0.8750000000000000	0.8750000003213998	0.1237068799997303	F	F	F
0.2546290742326954	0.9994204890774409	0.5083036979459761	T	T	T
0.2654190739593187	0.5011332724384839	0.5061010735418914	T	T	T
0.7551563035074746	0.9997882203341810	0.5082192066901352	T	T	T

0.7599836953025157	0.4987188265464896	0.5070524929450333	T	T	T
0.9916984681636847	0.9997727630230430	0.5082262202125264	T	T	T
0.9964322595334292	0.5005402389339069	0.5086609435794428	T	T	T
0.4922357480064272	0.9992977032154036	0.5084808702602281	T	T	T
0.5093865224545975	0.5147391451194268	0.5151346803250457	T	T	T
0.2476922645252628	0.3719425896580780	0.4457833159078607	T	T	T
0.2489332910068333	0.8753168220500241	0.4449863860723484	T	T	T
0.7498489880054410	0.3744917012185056	0.4448763686379342	T	T	T
0.7490576092898679	0.8747690706166791	0.4452156876366386	T	T	T
0.9990732988615599	0.3752197624346920	0.4453857361690249	T	T	T
0.9981418454476377	0.8752416489357452	0.4452388202092911	T	T	T
0.4993000203007041	0.3793995336571186	0.4488541561820894	T	T	T
0.4987768905836408	0.8753162739683699	0.4451076872410399	T	T	T
0.2433605601368427	0.1250000003213998	0.0641464598914467	F	F	F
0.2433605601368427	0.6250000003213998	0.0641464598914467	F	F	F
0.7433605601368427	0.1250000003213998	0.0641464598914467	F	F	F
0.7433605601368427	0.6250000003213998	0.0641464598914467	F	F	F
0.2495424637397008	0.0000846128471836	0.3818854394176383	T	T	T
0.2511877526123578	0.5000178095892976	0.3830279087469941	T	T	T
0.7494983684964579	-0.0000186880974713	0.3819889532256733	T	T	T
0.7505387614752091	0.5001568641291440	0.3823152609196264	T	T	T
0.2487783052129833	0.1245234654912548	0.4451458537998137	T	T	T
0.2485369020007788	0.6279658806545119	0.4453162915197783	T	T	T
0.7488413772960570	0.1250903412780106	0.4452922315080898	T	T	T
0.7499344860164255	0.6253112304300371	0.4452056864574387	T	T	T
0.998055558494165	0.1246158259676118	0.4452937365981388	T	T	T
0.9993532460404614	0.6247683813576326	0.4451942505842709	T	T	T
0.4985897059087579	0.1232364805421698	0.4447024566825240	T	T	T
0.4980392032725494	0.6234243415556175	0.4461756115598557	T	T	T
0.9918058397722552	0.2498204733047659	0.5081627310985452	T	T	T
0.9920802769703435	0.7497873018378634	0.5080788612452365	T	T	T
0.4911856787751586	0.2449906720418775	0.5072132687788599	T	T	T
0.4912206607195581	0.7515168261432844	0.5081066049642199	T	T	T
0.0066394298634407	0.3749999996786002	0.0641464598914467	F	F	F
0.0066394298634407	0.8750000003213998	0.0641464598914467	F	F	F
0.5066394398631573	0.3749999996786002	0.0641464598914467	F	F	F
0.5066394398631573	0.8750000003213998	0.0641464598914467	F	F	F
0.2503362996601264	0.2494133894866033	0.3818320433749267	T	T	T
0.2501407039198938	0.7504331915638477	0.3816391391744992	T	T	T
0.7500861430512528	0.2497628274472740	0.3817555688809707	T	T	T
0.7500959089164988	0.7499406198851636	0.3819467811151599	T	T	T
0.9997735273916140	0.2499451151663286	0.3820901909694440	T	T	T
0.9997397587333142	0.7501385324469372	0.3820158656944651	T	T	T
0.4998089617299998	0.2520271100083907	0.3833377351632494	T	T	T
0.4999904056677270	0.7493044941993049	0.3824544143919912	T	T	T
0.2433605601368427	0.3749999996786002	0.0641464598914467	F	F	F
0.2433605601368427	0.8750000003213998	0.0641464598914467	F	F	F
0.7433605601368427	0.3749999996786002	0.0641464598914467	F	F	F
0.7433605601368427	0.8750000003213998	0.0641464598914467	F	F	F
0.0066394298634407	0.1250000003213998	0.0641464598914467	F	F	F
0.0066394298634407	0.6250000003213998	0.0641464598914467	F	F	F
0.5066394398631573	0.1250000003213998	0.0641464598914467	F	F	F
0.5066394398631573	0.6250000003213998	0.0641464598914467	F	F	F
0.2498003202090970	0.2500000000000000	0.1271687800704484	F	F	F
0.2498003202090970	0.7500000000000000	0.1271687800704484	F	F	F
0.7498003002096638	0.2500000000000000	0.1271687800704484	F	F	F
0.7498003002096638	0.7500000000000000	0.1271687800704484	F	F	F
0.0001319391544191	0.3748580282793691	0.3179576268949382	T	T	T
0.9996793532761705	0.8749181671810513	0.3179838286679008	T	T	T
0.4997286956804626	0.3749586499488001	0.3183047289196106	T	T	T
0.4998021607149780	0.8744452176998981	0.3179852740003163	T	T	T
0.0001536701868119	0.1250000003213998	0.1905233400014623	F	F	F
0.0001536701868119	0.6250000003213998	0.1905233400014623	F	F	F
0.5001536601870953	0.1250000003213998	0.1905233400014623	F	F	F
0.5001536601870953	0.6250000003213998	0.1905233400014623	F	F	F
0.2498463198134715	0.1250000003213998	0.1905233400014623	F	F	F
0.2498463198134715	0.6250000003213998	0.1905233400014623	F	F	F
0.7498463398129047	0.1250000003213998	0.1905233400014623	F	F	F
0.7498463398129047	0.6250000003213998	0.1905233400014623	F	F	F
0.0001996797909030	0.2500000000000000	0.1271687800704484	F	F	F
0.0001996797909030	0.7500000000000000	0.1271687800704484	F	F	F
0.5001996997903362	0.2500000000000000	0.1271687800704484	F	F	F

0.5001996997903362	0.7500000000000000	0.1271687800704484	F	F	F
0.0001536701868119	0.3749999996786002	0.1905233400014623	F	F	F
0.0001536701868119	0.8750000003213998	0.1905233400014623	F	F	F
0.5001536601870953	0.3749999996786002	0.1905233400014623	F	F	F
0.5001536601870953	0.8750000003213998	0.1905233400014623	F	F	F
0.2498463198134715	0.3749999996786002	0.1905233400014623	F	F	F
0.2498463198134715	0.8750000003213998	0.1905233400014623	F	F	F
0.7498463398129047	0.3749999996786002	0.1905233400014623	F	F	F
0.7498463398129047	0.8750000003213998	0.1905233400014623	F	F	F
0.0000256401818390	0.0000000000000000	0.2546287700582681	F	F	F
0.0000256401818390	0.5000000000000000	0.2546287700582681	F	F	F
0.5000256601812723	0.0000000000000000	0.2546287700582681	F	F	F
0.5000256601812723	0.5000000000000000	0.2546287700582681	F	F	F
0.9991384125918242	0.9999533632023379	0.3819288406994890	T	T	T
0.0005114553278748	0.4998508889418193	0.3818474926860576	T	T	T
0.4992360785724931	0.9995615020856535	0.3815252896225143	T	T	T
0.5012245770307632	0.4996203775020533	0.3823916401726953	T	T	T
0.2499743498184444	0.0000000000000000	0.2546287700582681	F	F	F
0.2499743498184444	0.5000000000000000	0.2546287700582681	F	F	F
0.7499743398187277	0.0000000000000000	0.2546287700582681	F	F	F
0.7499743398187277	0.5000000000000000	0.2546287700582681	F	F	F
0.2499743498184444	0.2500000000000000	0.2546287700582681	F	F	F
0.2499743498184444	0.7500000000000000	0.2546287700582681	F	F	F
0.7499743398187277	0.2500000000000000	0.2546287700582681	F	F	F
0.7499743398187277	0.7500000000000000	0.2546287700582681	F	F	F
0.2533059043831815	0.2468964434667599	0.5095671940564690	T	T	T
0.2536286423953442	0.7525334477916384	0.5090165202684526	T	T	T
0.7555387530532663	0.2499208097291520	0.5080803380399151	T	T	T
0.7555261529534485	0.7499877836798081	0.5081233809501049	T	T	T
0.2498003202090970	0.0000000000000000	0.1271687800704484	F	F	F
0.2498003202090970	0.5000000000000000	0.1271687800704484	F	F	F
0.7498003002096638	0.0000000000000000	0.1271687800704484	F	F	F
0.7498003002096638	0.5000000000000000	0.1271687800704484	F	F	F
0.9996987053380993	0.1251221217042231	0.3180317363480834	T	T	T
0.0001471339497795	0.6250586018696513	0.3179865304915197	T	T	T
0.4997523416247301	0.1259418253250620	0.3183533673261197	T	T	T
0.4998364855484202	0.6248184407735917	0.3181769199819188	T	T	T
0.2497830213986826	0.1248743368068021	0.3178321444148157	T	T	T
0.2501309101722926	0.6245153953070823	0.3182437284789222	T	T	T
0.7495009400839868	0.1249111267527140	0.3179055586528388	T	T	T
0.7500019974293957	0.6247670328783902	0.3180214974154990	T	T	T
0.0001996797909030	0.0000000000000000	0.1271687800704484	F	F	F
0.0001996797909030	0.5000000000000000	0.1271687800704484	F	F	F
0.5001996997903362	0.0000000000000000	0.1271687800704484	F	F	F
0.5001996997903362	0.5000000000000000	0.1271687800704484	F	F	F
0.0000256401818390	0.2500000000000000	0.2546287700582681	F	F	F
0.0000256401818390	0.7500000000000000	0.2546287700582681	F	F	F
0.5000256601812723	0.2500000000000000	0.2546287700582681	F	F	F
0.5000256601812723	0.7500000000000000	0.2546287700582681	F	F	F
0.2503331065818930	0.3754430718464816	0.3185468956478670	T	T	T
0.2497307838585218	0.8751311810618740	0.3178347453097736	T	T	T
0.7499540112308556	0.3752635468948206	0.3180652237592072	T	T	T
0.7496094322163742	0.8750166272711335	0.3179484982031425	T	T	T
0.4586131542209743	0.4090055705991109	0.5693594023587055	T	T	T
0.5087230985094674	0.4782350846776947	0.5436638591230520	T	T	T

MS-(111)

111-MS

1.0000000000000000

11.6532959999999992

5.8266479999999996

0.0000000000000000

0.0000000000000000

10.0920520000000007

0.0000040000000000

0.0000000000000000

0.0000000000000000

26.0000000000000000

Ce O H

36 72 2

Selective dynamics

Direct

0.333333100000004

0.333333100000004

0.0000000000000000

0.3333333400000029

0.2309503299999989

0.2309503299999989

F F F

F F F

0.3333333100000004	0.6666666899999996	0.2309503299999989	F	F	F
0.6666666300000017	0.0000000000000000	0.2309503299999989	F	F	F
0.6666666300000017	0.3333333400000029	0.2309503299999989	F	F	F
0.6666666300000017	0.6666666899999996	0.2309503299999989	F	F	F
0.0000000000000000	0.0000000000000000	0.2309503299999989	F	F	F
0.0000000000000000	0.3333333400000029	0.2309503299999989	F	F	F
0.0000000000000000	0.6666666899999996	0.2309503299999989	F	F	F
0.2223104165261773	0.2224566369149272	0.3535673381279167	F	F	F
0.2228333783660617	0.5553011586146752	0.3535057698149799	F	F	F
0.222307684403617	0.8887350916148051	0.3535668584828855	F	F	F
0.5555883309738476	0.2233738945501642	0.3543867267911267	F	F	F
0.5555207268409816	0.5546435900741145	0.3543668106976270	F	F	F
0.5562961467005181	0.8886356980318197	0.3537480154036459	F	F	F
0.8891009304131643	0.2221883783690117	0.3536279298074518	F	F	F
0.8889514833223515	0.5558847266303957	0.3531179766712427	F	F	F
0.8889326160493027	0.8886326863415448	0.3531263805592104	F	F	F
0.11111110800000006	0.1111111600000001	0.1094482800000023	F	F	F
0.11111110800000006	0.4444444800000014	0.1094482800000023	F	F	F
0.11111110800000006	0.7777778499999997	0.1094482800000023	F	F	F
0.4444444200000035	0.1111111600000001	0.1094482800000023	F	F	F
0.4444444200000035	0.4444444800000014	0.1094482800000023	F	F	F
0.4444444200000035	0.7777778499999997	0.1094482800000023	F	F	F
0.7777777299999968	0.1111111600000001	0.1094482800000023	F	F	F
0.7777777299999968	0.4444444800000014	0.1094482800000023	F	F	F
0.7777777299999968	0.7777778499999997	0.1094482800000023	F	F	F
0.1119442900139802	0.1108341378937894	0.4745378985095954	F	F	F
0.1109881324030795	0.4445305486960791	0.4749223565946181	F	F	F
0.1108558318735717	0.7780836903423776	0.4749483203115119	F	F	F
0.4446295409222216	0.1114439718652704	0.4752332332003846	F	F	F
0.4361670879087427	0.4488560854578125	0.4775107949348865	T	T	T
0.4444722283958669	0.7777719843998199	0.4751984814541856	F	F	F
0.7828024455735942	0.1048643116339107	0.4749416122634571	T	T	T
0.7827566009766400	0.4462646597562596	0.4749079045733851	T	T	T
0.7783239713126662	0.7777131251963851	0.4752189318244788	F	F	F
0.3345291032961057	0.9995330649464620	0.3235662696291683	F	F	F
0.3336745679681599	0.3328103876483155	0.3229854835695889	F	F	F
0.3336297122490919	0.6670038956423738	0.3229814195853962	F	F	F
0.6662325876264887	0.0002439258729723	0.3230226543401997	F	F	F
0.6666790344393405	0.3334212952904636	0.3235280055130190	F	F	F
0.6662091672167989	0.6670123780905683	0.3230362844215122	F	F	F
0.0001727042172419	0.9998141508268361	0.3228566053740067	F	F	F
0.0001922491646340	0.3334207342648412	0.3228639045508785	F	F	F
0.0000409559354893	0.6666804725606355	0.3227913897737622	F	F	F
0.2222221899999965	0.2222227000000032	0.0793340600000008	F	F	F
0.2222221899999965	0.5555558000000036	0.0793340600000008	F	F	F
0.2222221899999965	0.8888889500000019	0.0793340600000008	F	F	F
0.5555551999999986	0.2222227000000032	0.0793340600000008	F	F	F
0.5555551999999986	0.5555558000000036	0.0793340600000008	F	F	F
0.5555551999999986	0.8888889500000019	0.0793340600000008	F	F	F
0.8888888399999999	0.2222227000000032	0.0793340600000008	F	F	F
0.8888888399999999	0.5555558000000036	0.0793340600000008	F	F	F
0.8888888399999999	0.8888889500000019	0.0793340600000008	F	F	F
0.2218714327297704	0.2204113192297967	0.4435346670513525	F	F	F
0.2209496748613802	0.5563278419017195	0.4448613443346261	F	F	F
0.2217499533876506	0.8913102439115903	0.4435473621765880	F	F	F
0.5592553618242917	0.2265729597778972	0.4467663814421243	T	T	T
0.5590834971874514	0.5481240337069337	0.4467085103635213	T	T	T
0.5551386349414429	0.8892502773485376	0.4442127157547517	F	F	F
0.8883554209466951	0.2226258461595592	0.4436842098150109	T	T	T
0.8902246416937558	0.5562795080743825	0.4436849911909135	F	F	F
0.8901362046954091	0.8872756231241041	0.4437259160481304	F	F	F
0.2222221600000012	0.2222227000000032	0.2615932499999971	F	F	F
0.2222221600000012	0.5555558000000036	0.2615932499999971	F	F	F
0.2222221600000012	0.8888889500000019	0.2615932499999971	F	F	F
0.5555551999999986	0.2222227000000032	0.2615932499999971	F	F	F
0.5555551999999986	0.5555558000000036	0.2615932499999971	F	F	F
0.5555551999999986	0.8888889500000019	0.2615932499999971	F	F	F
0.8888888399999999	0.2222227000000032	0.2615932499999971	F	F	F
0.8888888399999999	0.5555558000000036	0.2615932499999971	F	F	F
0.8888888399999999	0.8888889500000019	0.2615932499999971	F	F	F
0.3333333400000029	0.0000000000000000	0.1403399000000007	F	F	F
0.3333333400000029	0.3333333400000029	0.1403399000000007	F	F	F

0.3333333400000029	0.6666666899999996	0.1403399000000007	F	F	F
0.6666666899999996	0.0000000000000000	0.1403399000000007	F	F	F
0.6666666899999996	0.3333333400000029	0.1403399000000007	F	F	F
0.6666666899999996	0.6666666899999996	0.1403399000000007	F	F	F
0.0000000000000000	0.0000000000000000	0.1403399000000007	F	F	F
0.0000000000000000	0.3333333400000029	0.1403399000000007	F	F	F
0.0000000000000000	0.6666666899999996	0.1403399000000007	F	F	F
0.3338699724315788	0.9998369981652004	0.5050814597141482	F	F	F
0.3289663484819840	0.3314072372554833	0.5039267263137432	T	T	T
0.3288947982117634	0.6732578985343380	0.5039428502360437	T	T	T
0.6688767643349962	0.9983788788564425	0.5047869838357428	F	F	F
0.6957399541351563	0.3193738898962692	0.5151440080276473	T	T	T
0.6689596791666546	0.6664853001220408	0.5047568354705376	F	F	F
0.0007273098354545	0.9984719467353642	0.5047449125899703	F	F	F
0.0008300880401109	0.3344866496870509	0.5046858891254402	F	F	F
0.9988822742026926	0.6674147382440339	0.5053791545938111	F	F	F
0.1111111049999981	0.1111111600000001	0.1997374099999973	F	F	F
0.1111111049999981	0.4444444800000014	0.1997374099999973	F	F	F
0.1111111049999981	0.7777778499999997	0.1997374099999973	F	F	F
0.4444443900000010	0.1111111600000001	0.1997374099999973	F	F	F
0.4444443900000010	0.4444444800000014	0.1997374099999973	F	F	F
0.4444443900000010	0.7777778499999997	0.1997374099999973	F	F	F
0.7777777299999968	0.1111111600000001	0.1997374099999973	F	F	F
0.7777777299999968	0.4444444800000014	0.1997374099999973	F	F	F
0.7777777299999968	0.7777778499999997	0.1997374099999973	F	F	F
0.1104483980599156	0.1115074465461632	0.3843323844413717	F	F	F
0.1117577689028408	0.4443028067395218	0.3845816304542851	F	F	F
0.1116794121630917	0.7774465751816422	0.3845866961321676	F	F	F
0.4462216957729481	0.1127031889704213	0.3857620221248084	F	F	F
0.4425174214858529	0.4455184256687019	0.3844651333763593	F	F	F
0.4460483472789321	0.7748479090481055	0.3857270454728621	F	F	F
0.7782934452487069	0.1096302276873260	0.3847425473641195	F	F	F
0.7782714987685537	0.4456385010416710	0.3847288421935957	F	F	F
0.7775666091966400	0.7780120292462414	0.3846118561763774	F	F	F
0.6133384192139602	0.3604463625411398	0.5434378061888978	T	T	T
0.5027034891180477	0.4154144775876674	0.5598191249477154	T	T	T

MS-(221)

221-MS

1.0000000000000000

15.5567890000000002

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0.0000000000000000

-3.8891979999999999

11.6675919999999991

0.0000000000000000

0.0000000000000000

0.0000000000000000

29.1170809999999989

Ce O H

52 104 2

Selective dynamics

Direct

0.1766254202158919	0.2065023699834541	0.0961653298969054	F	F	F
0.6766254298579781	0.2065023699834541	0.0961653298969054	F	F	F
0.4266254002888985	0.2065023699834541	0.0961653298969054	F	F	F
0.9266254298579781	0.2065023699834541	0.0961653298969054	F	F	F
0.2346029498078082	0.9384064501055605	0.1251644400755723	F	F	F
0.7346029600927082	0.9384064501055605	0.1251644400755723	F	F	F
0.4846029600927082	0.9384064501055605	0.1251644400755723	F	F	F
0.9846029600927082	0.9384064501055605	0.1251644400755723	F	F	F
0.2922178798754160	0.6688738396063201	0.1555735799890101	F	F	F
0.7922178798754160	0.6688738396063201	0.1555735799890101	F	F	F
0.0422178901603161	0.6688738396063201	0.1555735799890101	F	F	F
0.5422178798754160	0.6688738396063201	0.1555735799890101	F	F	F
0.0986668701218960	0.3946651802702732	0.1800825398672359	F	F	F
0.5986668797639894	0.3946651802702732	0.1800825398672359	F	F	F
0.3486668501949097	0.3946651802702732	0.1800825398672359	F	F	F
0.8486668199830163	0.3946651802702732	0.1800825398672359	F	F	F
0.4029684001360181	0.1118754803904665	0.2183137698452668	F	F	F
0.9029684303479115	0.1118754803904665	0.2183137698452668	F	F	F
0.1529683802090318	0.1118754803904665	0.2183137698452668	F	F	F
0.6529683699241318	0.1118754803904665	0.2183137698452668	F	F	F
0.4578611801550281	0.8314441900265308	0.2509747099992623	F	F	F

0.9578611801550281	0.8314441900265308	0.2509747099992623	F	F	F
0.2078611698701280	0.8314441900265308	0.2509747099992623	F	F	F
0.7078611801550281	0.8314441900265308	0.2509747099992623	F	F	F
0.0138888899483263	0.5555555799345768	0.2801990800520144	F	F	F
0.5138889002332263	0.5555555799345768	0.2801990800520144	F	F	F
0.2638889002332263	0.5555555799345768	0.2801990800520144	F	F	F
0.7638889002332263	0.5555555799345768	0.2801990800520144	F	F	F
0.0700242701208167	0.2800475554782269	0.3093438369555869	T	T	T
0.5699767820186183	0.2795435744424399	0.3094123195108703	T	T	T
0.3200334770563326	0.2801473513552308	0.3093167311123221	T	T	T
0.8198378029186885	0.2798712002931509	0.3093387549326294	T	T	T
0.1251201747023424	0.0002938381280439	0.3420580143122774	T	T	T
0.6248883593996407	0.9988472876746776	0.3430638329359814	T	T	T
0.3748463027322002	0.0001091508980626	0.3422015765294067	T	T	T
0.8750764548325444	-0.0002567492984784	0.3422484701125397	T	T	T
0.1792659131804356	0.7180134448624292	0.3800041110824538	T	T	T
0.6790474084419148	0.7152924318597120	0.3791303189244108	T	T	T
0.4297191653666556	0.7188324137542346	0.3805580895838515	T	T	T
0.9295521184341002	0.7179314390218883	0.3802276795579633	T	T	T
0.2362276082562236	0.4448042715627721	0.4046769527626772	T	T	T
0.7359248313794335	0.4426873408330030	0.4049047794577604	T	T	T
0.4855784552867696	0.4437636854807457	0.4046814372469210	T	T	T
0.9856993220811704	0.4435706304835484	0.4048189717505110	T	T	T
0.0447162310208444	0.1761159872145785	0.4350535666971411	T	T	T
0.5433324715574219	0.1748513462113908	0.4352534970762802	T	T	T
0.2938220044202039	0.1753838053229701	0.4350490742897482	T	T	T
0.7931040521264822	0.1727301987675154	0.4351027749409688	T	T	T
0.3501530004474247	0.9067533338378150	0.4643517053383063	T	T	T
0.8584807737678856	0.9099037019336549	0.4650793343625407	T	T	T
0.1036181989020095	0.9072531924026523	0.4643953301829288	T	T	T
0.5954914029670910	0.9083279319764015	0.4677296165812854	T	T	T
0.0234363103996174	0.0937380703747621	0.0769361300330900	F	F	F
0.5234363103996174	0.0937380703747621	0.0769361300330900	F	F	F
0.2734363103996174	0.0937380703747621	0.0769361300330900	F	F	F
0.7734363103996174	0.0937380703747621	0.0769361300330900	F	F	F
0.0784225797357294	0.3136766901002375	0.1040784799135608	F	F	F
0.5784225598087431	0.3136766901002375	0.1040784799135608	F	F	F
0.3284225900206295	0.3136766901002375	0.1040784799135608	F	F	F
0.8284225598087431	0.3136766901002375	0.1040784799135608	F	F	F
0.3327759300076707	0.8311121103651899	0.1087520098597778	F	F	F
0.8327759300076707	0.8311121103651899	0.1087520098597778	F	F	F
0.0827759100806773	0.8311121103651899	0.1087520098597778	F	F	F
0.5827759300076707	0.8311121103651899	0.1087520098597778	F	F	F
0.1382287901406798	0.0529157198846164	0.1411541799124691	F	F	F
0.6382288100676732	0.0529157198846164	0.1411541799124691	F	F	F
0.3882288100676732	0.0529157198846164	0.1411541799124691	F	F	F
0.8882288100676732	0.0529157198846164	0.1411541799124691	F	F	F
0.3914908601835094	0.5659549596866285	0.1386544200636024	F	F	F
0.8914908801104957	0.5659549596866285	0.1386544200636024	F	F	F
0.1414908601835094	0.5659549596866285	0.1386544200636024	F	F	F
0.6414908897525891	0.5659549596866285	0.1386544200636024	F	F	F
0.1942389101827544	0.2769545498334196	0.1681039201697416	F	F	F
0.6942389198248478	0.2769545498334196	0.1681039201697416	F	F	F
0.4442388902557610	0.2769545498334196	0.1681039201697416	F	F	F
0.9442388600438676	0.2769545498334196	0.1681039201697416	F	F	F
0.1950204497033852	0.7800809695779591	0.1728901599030479	F	F	F
0.6950204297763918	0.7800809695779591	0.1728901599030479	F	F	F
0.4450204599882852	0.7800809695779591	0.1728901599030479	F	F	F
0.9450204902001715	0.7800809695779591	0.1728901599030479	F	F	F
0.2498572200825677	0.9994266203343400	0.2024984599246054	F	F	F
0.7498572200825677	0.9994266203343400	0.2024984599246054	F	F	F
0.9997305300349453	0.4989176901283514	0.1994941398830434	F	F	F
0.4997305300349453	0.4989176901283514	0.1994941398830434	F	F	F
0.2497305403198453	0.4989176901283514	0.1994941398830434	F	F	F
0.7497305300349453	0.4989176901283514	0.1994941398830434	F	F	F
0.9998572200825677	0.9994266203343400	0.2024984599246054	F	F	F
0.4998572200825677	0.9994266203343400	0.2024984599246054	F	F	F
0.0559230502172525	0.2236992903077208	0.2314988401481557	F	F	F
0.5559230302902591	0.2236992903077208	0.2314988401481557	F	F	F
0.0550411900627665	0.7201729997072235	0.2335694700990132	F	F	F
0.5550411797778665	0.7201729997072235	0.2335694700990132	F	F	F
0.3059230598593459	0.2236992903077208	0.2314988401481557	F	F	F

0.8059230900712322	0.2236992903077208	0.2314988401481557	F	F	F
0.3050411797778665	0.7201729997072235	0.2335694700990132	F	F	F
0.8050411797778665	0.7201729997072235	0.2335694700990132	F	F	F
0.1114771396974064	0.4458940996565559	0.2627358999344764	F	F	F
0.6114771499823064	0.4458940996565559	0.2627358999344764	F	F	F
0.3614771197704130	0.4458940996565559	0.2627358999344764	F	F	F
0.8614770902013333	0.4458940996565559	0.2627358999344764	F	F	F
0.3608369999896937	0.9433489403811848	0.2652951499499565	F	F	F
0.8608369697778002	0.9433489403811848	0.2652951499499565	F	F	F
0.1108369999896937	0.9433489403811848	0.2652951499499565	F	F	F
0.6108369697778002	0.9433489403811848	0.2652951499499565	F	F	F
0.1662259430593507	0.6654024561748638	0.2976944012653829	T	T	T
0.6665112257578577	0.6650433529123957	0.2977433984267172	T	T	T
0.4162785019341214	0.6656487437274524	0.2973783844649783	T	T	T
0.9163558650052205	0.6656559967909004	0.2976103043666801	T	T	T
0.1669407897633235	0.1677621200672803	0.2951030101540724	F	F	F
0.6669408199752169	0.1677621200672803	0.2951030101540724	F	F	F
0.4169407601942439	0.1677621200672803	0.2951030101540724	F	F	F
0.9169407601942439	0.1677621200672803	0.2951030101540724	F	F	F
0.2228787760009869	0.3917002989623322	0.3267559167949789	T	T	T
0.7230310894875289	0.3915216733341101	0.3268745677158757	T	T	T
0.4728849868829525	0.3914607117261776	0.3268093138490366	T	T	T
0.9726757468709220	0.3914593756166484	0.3268338001859947	T	T	T
0.2216143728115116	0.8885779262268835	0.3285416444473974	T	T	T
0.7216020574437200	0.8868926465213224	0.3288392351858956	T	T	T
0.4731804672733083	0.8868666868354430	0.3298953872285610	T	T	T
0.9712941109142417	0.8875406732572620	0.3292785385328574	T	T	T
0.0287985656696647	0.1131167940773122	0.3575767365589351	T	T	T
0.5276451844257897	0.1120918357670811	0.3576751853953255	T	T	T
0.2782846315837092	0.1130107615371380	0.3578762134492964	T	T	T
0.7777736312484717	0.1110789682295225	0.3583232485767568	T	T	T
0.0278277348318830	0.6136130128503609	0.3608041842831941	T	T	T
0.5283308569418141	0.6139822160260122	0.3604020494501898	T	T	T
0.2786788521063477	0.6139211165744263	0.3608332601086819	T	T	T
0.7788143598895829	0.6137344115057650	0.3607528096583295	T	T	T
0.0842962067190021	0.8359735990087676	0.3922299200692078	T	T	T
0.5876520044355766	0.8337670344260100	0.3953204252708716	T	T	T
0.0833226793241971	0.3329989354078327	0.3873615843241458	T	T	T
0.5830014260209242	0.3316691971357492	0.3873848846924070	T	T	T
0.3329728137620792	0.3329462674995750	0.3872848838823241	T	T	T
0.8328194232900172	0.3314183551120297	0.3874055834396031	T	T	T
0.3319028751384968	0.8364280831322821	0.3916619268421833	T	T	T
0.8325761047223071	0.8368684614572092	0.3934320435694106	T	T	T
0.1365201190532202	0.5470524300677185	0.4214877514702804	T	T	T
0.6358327015375882	0.5454079435684048	0.4207093105798653	T	T	T
0.1402570327339980	0.0606524455948801	0.4191580752132893	T	T	T
0.6382049740267709	0.0618581143579001	0.4196773924268766	T	T	T
0.3869278065295432	0.5473519574326754	0.4214480570771095	T	T	T
0.8866140815484899	0.5467858210793300	0.4216205252500803	T	T	T
0.3897736809825304	0.0605239713370326	0.4192174915545324	T	T	T
0.8931259535033315	0.0615794744747611	0.4190552314353423	T	T	T
0.1958901575604446	0.2828799216920925	0.4515607979225098	T	T	T
0.6959742652522785	0.2824510408806297	0.4517934855920853	T	T	T
0.4451752837008371	0.8015557821801275	0.4549032825658665	T	T	T
0.9517141643665532	0.8008765694811205	0.4563744778445572	T	T	T
0.1990128327560570	0.7991773325911888	0.4566240878864913	T	T	T
0.7068595790434710	0.7792441290415097	0.4606511287670038	T	T	T
0.4449597363471052	0.2824657186489832	0.4514562265083943	T	T	T
0.9456029282545768	0.2821195350864334	0.4515881926895459	T	T	T
0.2542007856822998	0.0197646397808693	0.4834863359279031	T	T	T
0.7558421849080929	0.0137254514960431	0.4809230497560527	T	T	T
0.0063770467324210	0.0207749789718892	0.4842478996665742	T	T	T
0.5032399777513706	0.0208619198661645	0.4846302866027773	T	T	T
0.6664260412184924	0.7541301658421798	0.4893578367927091	T	T	T
0.6015386308712870	0.7830098359754951	0.5208814128119514	T	T	T

 MS-(331)

331-MS

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Selective dynamics

Direct

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0.7069911099281967	0.4139822900530987	0.0802282099838578	F	F	F
0.7069911099281967	0.9139822900530987	0.0802282099838578	F	F	F
0.2069911394972763	0.9139822900530987	0.0802282099838578	F	F	F
0.3682377197941804	0.7364754297565810	0.1193459000875450	F	F	F
0.8682377493632600	0.7364754297565810	0.1193459000875450	F	F	F
0.3682377195372268	0.2364754498124739	0.1193459000875450	F	F	F
0.8682377503919270	0.2364754498124739	0.1193459000875450	F	F	F
0.0273628300986104	0.5547256300206129	0.1557375799851783	F	F	F
0.5273628403835104	0.5547256300206129	0.1557375799851783	F	F	F
0.0273628298416639	0.0547256500765059	0.1557375799851783	F	F	F
0.5273628401265640	0.0547256500765059	0.1557375799851783	F	F	F
0.6848900306063328	0.8697800599553318	0.2046350700172681	F	F	F
0.1848900100365398	0.8697800599553318	0.2046350700172681	F	F	F
0.6848900297061462	0.3697800298714924	0.2046350700172681	F	F	F
0.1848900104219595	0.3697800298714924	0.2046350700172681	F	F	F
0.8412300703288835	0.6824601300565902	0.2462408598710937	F	F	F
0.3412300600439835	0.6824601300565902	0.2462408598710937	F	F	F
0.8412300601724638	0.1824601200286438	0.2462408598710937	F	F	F
0.3412300601724638	0.1824601200286438	0.2462408598710937	F	F	F
0.0005916156964210	0.5019194228272298	0.2880959653427280	T	T	T
0.5010920108975033	0.5020614087608961	0.2880743581920585	T	T	T
0.0003119680854762	0.0019207778956117	0.2880101890452947	T	T	T
0.5016985612131051	0.0019186962825405	0.2880118481116440	T	T	T
0.6575126319148830	0.8150158301611223	0.3298047854560739	T	T	T
0.6567490134143733	0.3147959128777428	0.3306959610544810	T	T	T
0.1576610746695722	0.8151196846790819	0.3298063299127795	T	T	T
0.1576864732666147	0.3150789042578815	0.3300441345817305	T	T	T
0.3155460820324282	0.6307520127478201	0.3786635610821270	T	T	T
0.3143761508667033	0.1288617291407753	0.3771450914136004	T	T	T
0.8149512988954204	0.6309282348810823	0.3786745206728695	T	T	T
0.8154714742397204	0.1314039020332874	0.3789503959710241	T	T	T
0.9742843832588411	0.9489436481084826	0.4150049866790947	T	T	T
0.4742811653227533	0.4488753775167630	0.4147470524995015	T	T	T
0.4752899158173849	0.9489317922527828	0.4149842461216033	T	T	T
0.9740542550221859	0.4503798667875192	0.4147535389038371	T	T	T
0.6358491193959641	0.7717722052879418	0.4543484743000503	T	T	T
0.1360083526513846	0.7716846620973975	0.4542513153165169	T	T	T
0.1286154922157436	0.2747554583023336	0.4549486509325865	T	T	T
0.6444261989915149	0.2739366140062013	0.4575291201475706	T	T	T
0.4170010295437478	0.3340020598585909	0.0655032800553457	F	F	F
0.9170010295437478	0.8340020598585909	0.0655032800553457	F	F	F
0.4170010295437478	0.8340020598585909	0.0655032800553457	F	F	F
0.9170010295437478	0.3340020598585909	0.0655032800553457	F	F	F
0.4942802306857885	0.4885604602710387	0.0841822598979007	F	F	F
0.9942802306857885	0.4885604602710387	0.0841822598979007	F	F	F
0.4942802306857885	0.9885604602710387	0.0841822598979007	F	F	F
0.9942802306857885	0.9885604602710387	0.0841822598979007	F	F	F
0.5822149300609212	0.6644298698372282	0.1077273498789495	F	F	F
0.0822149300609212	0.6644298698372282	0.1077273498789495	F	F	F
0.5822149300609212	0.1644298698372282	0.1077273498789495	F	F	F
0.0822149300609212	0.1644298698372282	0.1077273498789495	F	F	F
0.6592633198417985	0.8185266501579136	0.1309383199820644	F	F	F
0.1592633198417985	0.8185266501579136	0.1309383199820644	F	F	F
0.6592633198417985	0.3185266501579136	0.1309383199820644	F	F	F
0.1592633198417985	0.3185266501579136	0.1309383199820644	F	F	F
0.7370480597433584	0.9740961202457186	0.1485278501003080	F	F	F
0.2370480803131514	0.9740961202457186	0.1485278501003080	F	F	F
0.7370480603486058	0.4740961497396867	0.1485278501003080	F	F	F
0.2370480796327925	0.4740961497396867	0.1485278501003080	F	F	F
0.8149496602444728	0.1298993500709642	0.1703081098582615	F	F	F
0.3149496602444728	0.1298993500709642	0.1703081098582615	F	F	F
0.3149496606298925	0.6298993199871177	0.1703081098582615	F	F	F
0.8149496606298925	0.6298993199871177	0.1703081098582615	F	F	F

0.3940778297765704	0.2881556302211692	0.1928188500296599	F	F	F
0.8940778002074836	0.2881556302211692	0.1928188500296599	F	F	F
0.8940777995271247	0.7881556597151373	0.1928188500296599	F	F	F
0.3940778303818178	0.7881556597151373	0.1928188500296599	F	F	F
0.9739475699162554	0.9478951902419794	0.2131436001604143	F	F	F
0.4739475994853350	0.9478951902419794	0.2131436001604143	F	F	F
0.9739475703016751	0.4478951601581329	0.2131436001604143	F	F	F
0.4739475998707547	0.4478951601581329	0.2131436001604143	F	F	F
0.5528264995671677	0.6056530601169641	0.2345971901601871	F	F	F
0.0528265201369678	0.6056530601169641	0.2345971901601871	F	F	F
0.5528264998241141	0.1056530400610640	0.2345971901601871	F	F	F
0.0528265203939142	0.1056530400610640	0.2345971901601871	F	F	F
0.6314923196156457	0.7629846902720629	0.2567009699963734	F	F	F
0.1314923504703387	0.7629846902720629	0.2567009699963734	F	F	F
0.6314923196156457	0.2629846902720629	0.2567009699963734	F	F	F
0.1314923504703387	0.2629846902720629	0.2567009699963734	F	F	F
0.7094555342303113	0.4212936923447502	0.2778996806279129	T	T	T
0.7107883904599787	0.9214297717405311	0.2776647002324134	T	T	T
0.2108196040421269	0.9215035599341979	0.2776634711203173	T	T	T
0.2114417887832468	0.4214217108004620	0.2777597965344993	T	T	T
0.7893756749802567	0.5790283500561428	0.2997275378157891	T	T	T
0.2893125691753933	0.5789480797233096	0.2997854931442694	T	T	T
0.7898171349750364	0.0790495896613370	0.2994664253384030	T	T	T
0.2890877937260335	0.0785672325654156	0.2999522586224585	T	T	T
0.8684633278334041	0.7371016164629605	0.3213440348158773	T	T	T
0.3685842469018029	0.7370611264249612	0.3213126165700145	T	T	T
0.3691179016879431	0.2363728941903531	0.3207818202220430	T	T	T
0.8668230108077831	0.2361879892874177	0.3226950591934687	T	T	T
0.4487233141980855	0.8968979234676298	0.3415710239704193	T	T	T
0.9479915490683846	0.3969639449062860	0.3410704129418582	T	T	T
0.4476592585290309	0.3959696880211594	0.3420785804237203	T	T	T
0.9485436818909574	0.8970879590571006	0.3415924658910259	T	T	T
0.5276009415312176	0.5551322866003409	0.3638189332342370	T	T	T
0.5294681494777989	0.0557332117632226	0.3635343920770505	T	T	T
0.0265845175392760	0.0559469476334702	0.3638301091692104	T	T	T
0.0272819989763193	0.5556831806821794	0.3640005438504857	T	T	T
0.5963567203996260	0.2108155296087702	0.3885102189310232	T	T	T
0.1145722974109087	0.2127952844411408	0.3864999921996705	T	T	T
0.6055087291318296	0.7113214358913175	0.3859401245607192	T	T	T
0.1056050017849356	0.7112457982869631	0.3859345778910520	T	T	T
0.1834793790179140	0.8667053844532039	0.4033938886344190	T	T	T
0.6839049117406510	0.8670560582643940	0.4034113261671168	T	T	T
0.6881866694092458	0.3685506751837578	0.4037394410315669	T	T	T
0.1790802655478009	0.3685462211532126	0.4031466824945296	T	T	T
0.2616180250507108	0.5218458563397971	0.4266068844468027	T	T	T
0.7609060486130479	0.0216388834398661	0.4263631421071933	T	T	T
0.2614069546234228	0.0203888270802210	0.4255037211292882	T	T	T
0.7595560152938128	0.5221117120408931	0.4268315003850760	T	T	T
0.8486460123042889	0.6975377749188806	0.4502307219972354	T	T	T
0.3487148889482677	0.6973426754214090	0.4502396831096229	T	T	T
0.8560712846182431	0.1994843952790247	0.4486640907945769	T	T	T
0.3238579702879843	0.1852830132863754	0.4554656614079062	T	T	T
0.4264415775180009	0.8517670303913021	0.4687406605453070	T	T	T
0.9260161240750786	0.8520465591646755	0.4687759393786041	T	T	T
0.9284466621440685	0.3540255734287383	0.4705222282037364	T	T	T
0.4201413148851889	0.3484646614313169	0.4668145173007860	T	T	T
0.3808436846495105	0.1701060474201429	0.4846500418106009	T	T	T
0.5402759503831548	0.1961652404675027	0.5150327073834954	T	T	T

D. (H⁺,H⁻)

 (H⁺,H⁻)-(100)-Ce

100-Ce-product

1.0000000000000000

11.0003119999999992

0.0000000000000000

0.0000000000000000

11.0003119999999992

0.0000000000000000

0.0000000000000000

0.0000000000000000	0.0000000000000000	41.1257400000000004			
Ce	O	H			
72	144	2			
Selective dynamics					
Direct					
0.2500000000000000	0.0000000000000000	0.04312184999999986	F	F	F
0.2500000000000000	0.5000000000000000	0.04312184999999986	F	F	F
0.7500000000000000	0.0000000000000000	0.04312184999999986	F	F	F
0.7500000000000000	0.5000000000000000	0.04312184999999986	F	F	F
0.9998758151466589	0.2498707676490355	0.5687510498149138	T	T	T
0.9985730507600437	0.7504661626082836	0.5686365890035603	T	T	T
0.5032560524682026	0.2467591935406475	0.5685021467962699	T	T	T
0.5002718979291672	0.7484200565796328	0.5688280072488539	T	T	T
0.2504040390546791	0.9988487049552219	0.5686844207046207	T	T	T
0.2476131899534906	0.5050397942848264	0.5679941892694416	T	T	T
0.7504816897683213	0.9990514756189768	0.5686985738778318	T	T	T
0.7482215293486121	0.4996919542312597	0.5689602595545438	T	T	T
0.2500814133150087	0.2500346200590897	0.5020362452320910	T	T	T
0.2497957953204519	0.7508925479220565	0.5014015698680367	T	T	T
0.7506015878482515	0.2498453544848900	0.5016155127642108	T	T	T
0.7496828820365877	0.7497108007068647	0.5016556349480865	T	T	T
0.0001285129188204	0.0002008292853546	0.5016242044565900	T	T	T
0.9989289051984827	0.5000259678923342	0.5016074703015931	T	T	T
0.5001288632978955	0.9992266864483881	0.5015831689509795	T	T	T
0.5000049880938349	0.4996441745556766	0.5018099464450216	T	T	T
0.0002182263621862	0.2500721534731483	0.4347261326217904	T	T	T
0.9998105229275609	0.7500769480308378	0.4346476963752366	T	T	T
0.5001018344667827	0.2497809930507842	0.4348269766123707	T	T	T
0.4999022440421612	0.7497202425221730	0.4346419087989375	T	T	T
0.2500646738029531	0.0003741066995957	0.4346719779687476	T	T	T
0.2497697912904897	0.5001617041433732	0.4348249896780843	T	T	T
0.7500633599502464	0.9998427202081004	0.4346758352358719	T	T	T
0.7497130492287738	0.4998657974858887	0.4346667210958444	T	T	T
0.2500265505935957	0.2500569624078750	0.3677813137084556	T	T	T
0.2499631478800666	0.7500158717199170	0.3677514379879199	T	T	T
0.7500066794025813	0.2499675042084135	0.3677647486385851	T	T	T
0.7499716680998958	0.7499906992998220	0.3677255564623394	T	T	T
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0.9999661542619620	0.5000237724138259	0.3677590930090204	T	T	T
0.5000221891479271	0.9999664018517080	0.3677541183135133	T	T	T
0.4999288130041677	0.4999485154920151	0.3677708915608804	T	T	T
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0.9991546979769055	0.5005687967222556	0.6256010544194694	T	T	T
0.5007442649157454	0.9978584044226579	0.6255780977202932	T	T	T
0.5045103652660714	0.5056745885285139	0.6281549161297733	T	T	T
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0.0000000000000000	0.7500000000000000	0.3008260100000015	F	F	F
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0.5000000000000000	0.7500000000000000	0.3008260100000015	F	F	F
0.2500000000000000	0.0000000000000000	0.3008259200000012	F	F	F
0.2500000000000000	0.5000000000000000	0.3008259200000012	F	F	F
0.7500000000000000	0.0000000000000000	0.3008259200000012	F	F	F
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0.2500000000000000	0.7500000000000000	0.2337953799999966	F	F	F
0.7500000000000000	0.2500000000000000	0.2337953799999966	F	F	F
0.7500000000000000	0.7500000000000000	0.2337953799999966	F	F	F
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0.5000000000000000	0.5000000000000000	0.0997988199999966	F	F	F
0.0000000000000000	0.2500000000000000	0.1667670499999971	F	F	F
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0.5000000000000000	0.2500000000000000	0.1667670499999971	F	F	F
0.5000000000000000	0.7500000000000000	0.1667670499999971	F	F	F
0.2500000000000000	0.0000000000000000	0.1668236300000032	F	F	F
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0.2500000000000000	0.7500000000000000	0.0997936999999993	F	F	F
0.7500000000000000	0.2500000000000000	0.0997936999999993	F	F	F
0.7500000000000000	0.7500000000000000	0.0997936999999993	F	F	F
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0.6251622622239665	0.1246905260241959	0.4682971198264099	T	T	T
0.6246305953361144	0.6245813639192406	0.4683817596445863	T	T	T
0.3750355781828745	0.1251032091010558	0.4682236167944680	T	T	T
0.3749281293575635	0.6247880360293721	0.4679640876472533	T	T	T
0.8754270308739933	0.1248619924162568	0.4681213995771927	T	T	T
0.8746750269576111	0.6248267859850998	0.4681664729246862	T	T	T
0.1249574542257434	0.3751479839108143	0.4683603094491815	T	T	T
0.1248597648795524	0.8755879622206351	0.4680437232703980	T	T	T
0.6247582898068131	0.3748899477277092	0.4680520702099145	T	T	T
0.6248798563228917	0.8746610807511317	0.4680917813992309	T	T	T
0.3747764806620495	0.3748088161949497	0.4691733437972303	T	T	T
0.3749778604836109	0.8750992629452128	0.4681769923082726	T	T	T
0.8749198867073744	0.3749477439378026	0.4682224744272929	T	T	T
0.8749065180589852	0.8748752980227081	0.4682452825464267	T	T	T
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0.6295997699999987	0.3796014699999972	0.0666311900000025	F	F	F
0.6295997699999987	0.8796014699999972	0.0666311900000025	F	F	F
0.3704001999999988	0.1203985399999965	0.0666311900000025	F	F	F
0.3704001999999988	0.6203985300000028	0.0666311900000025	F	F	F
0.8704001700000035	0.1203985399999965	0.0666311900000025	F	F	F
0.8704001700000035	0.6203985300000028	0.0666311900000025	F	F	F
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0.6255364012271301	0.1240292039452342	0.5352567958478005	T	T	T
0.6238996475337188	0.6235474000455454	0.5353756670876706	T	T	T
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0.3759663818613319	0.3761280164606404	0.5374632293216095	T	T	T
0.3749652647778632	0.8751128474209651	0.5351785874820649	T	T	T
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0.8748309860910553	0.8749063157299446	0.5351017048668751	T	T	T
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0.6226528487137415	0.6225975100561669	0.6024425781309262	T	T	T
0.3802968398777509	0.1190282661950945	0.6015218045721724	T	T	T
0.3808846299117477	0.6142263511868151	0.6003992548570380	T	T	T
0.8807683003960491	0.1201104786082325	0.6015051316720204	T	T	T
0.8796604434813915	0.6199233179500041	0.6016723239001891	T	T	T
0.1230962963468656	0.3786792390919871	0.6025922014571350	T	T	T
0.1201606285676604	0.8799708490711566	0.6014570721870172	T	T	T
0.6129355123303810	0.3811107863259622	0.6006484117074820	T	T	T
0.6204497146454884	0.8793895629587567	0.6013426564493329	T	T	T
0.3664225759283752	0.3661499600951998	0.6072564309920665	T	T	T
0.3799242522787836	0.8779645545463666	0.6019313624566678	T	T	T
0.8801301759695903	0.3796941402293825	0.6017373547160361	T	T	T
0.8798097288525355	0.8797251110277458	0.6018695543294470	T	T	T
0.3756893581038554	0.1253255553547845	0.5349598855388820	T	T	T
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0.8755241871457571	0.1250479975948622	0.5350430844588132	T	T	T
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0.1250870042546666	0.3760619882258780	0.5353176862202105	T	T	T
0.1248823511628743	0.8753103111230658	0.5349425660218330	T	T	T
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0.8750092458748355	0.3749648034937820	0.4013131262559355	T	T	T
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0.1250439564980752	0.3750548959391082	0.4013178713921945	T	T	T
0.1249642363358632	0.8751076071715076	0.4012309248513546	T	T	T
0.6248709082675035	0.3748415845322128	0.4012313028105154	T	T	T
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0.3750000000000000	0.3749996499999995	0.3343499599999973	F	F	F
0.3750000000000000	0.8749996499999995	0.3343499599999973	F	F	F
0.8750000000000000	0.3749996499999995	0.3343499599999973	F	F	F
0.8750000000000000	0.8749996499999995	0.3343499599999973	F	F	F
0.1249694099999985	0.1250320299999998	0.1333152999999996	F	F	F
0.1249694099999985	0.6250320299999998	0.1333152999999996	F	F	F
0.6249694300000002	0.1250320299999998	0.1333152999999996	F	F	F
0.6249694300000002	0.6250320299999998	0.1333152999999996	F	F	F
0.1250791830964602	0.1251542633669231	0.4013507682450239	T	T	T
0.1249407982141406	0.6249610136821886	0.4013161315302298	T	T	T
0.6249489325155295	0.1249533365074882	0.4013549430981698	T	T	T
0.6248589092951633	0.6248351628813609	0.4013262026112372	T	T	T
0.3750422584478414	0.1251112924805682	0.4012711624172880	T	T	T
0.3748393587385905	0.6248769472329769	0.4011976276676634	T	T	T
0.8750749124177091	0.1249848759875434	0.4012618821146177	T	T	T
0.8748589932747564	0.6249776583929858	0.4012546580482379	T	T	T
0.1250082800000030	0.1249915799999997	0.2002911699999999	F	F	F
0.1250082800000030	0.6249915799999997	0.2002911699999999	F	F	F
0.6250082999999975	0.1249915799999997	0.2002911699999999	F	F	F

0.6250082999999975	0.6249915799999997	0.2002911699999999	F	F	F
0.3750000000000000	0.1250003600000014	0.3343499599999973	F	F	F
0.3750000000000000	0.6250003500000005	0.3343499599999973	F	F	F
0.8750000000000000	0.1250003600000014	0.3343499599999973	F	F	F
0.8750000000000000	0.6250003500000005	0.3343499599999973	F	F	F
0.5190159781398904	0.5229795616373067	0.6817943629655332	T	T	T
0.2929857654648771	0.3184841224002142	0.6134149493875043	T	T	T

 (H⁺,H⁻)-(100)-O-(a)

100-o-a-product

1.0000000000000000		
11.000311999999992	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.000311999999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	41.1257400000000004

Ce O H
72 144 2

Selective dynamics

Direct

0.1250000000000000	0.1250000000000000	0.3343499599999973	F	F	F
0.1250000000000000	0.6250000000000000	0.3343499599999973	F	F	F
0.6250000000000000	0.1250000000000000	0.3343499599999973	F	F	F
0.6250000000000000	0.6250000000000000	0.3343499599999973	F	F	F
0.124937353989628	0.3748885098641566	0.4012975965997256	T	T	T
0.1250742016307527	0.8749878523588706	0.4012874271793052	T	T	T
0.6248871858934706	0.3751863700873201	0.4014263858640916	T	T	T
0.6250899891972992	0.8750422989709037	0.4014289082029237	T	T	T
0.3750000000000000	0.3750000000000000	0.3343499599999973	F	F	F
0.3750000000000000	0.8750000000000000	0.3343499599999973	F	F	F
0.8750000000000000	0.3750000000000000	0.3343499599999973	F	F	F
0.8750000000000000	0.8750000000000000	0.3343499599999973	F	F	F
0.1246211581307648	0.1244013198736411	0.4683702162778758	T	T	T
0.1258004742220820	0.6248907325438395	0.4680915427593177	T	T	T
0.6249050129384344	0.1256953815017496	0.4684144515057866	T	T	T
0.6255634770704290	0.6253733830967576	0.4687388237250616	T	T	T
0.1250000000000000	0.3750000000000000	0.2673391499999980	F	F	F
0.1250000000000000	0.8750000000000000	0.2673391499999980	F	F	F
0.6250000000000000	0.3750000000000000	0.2673391499999980	F	F	F
0.6250000000000000	0.8750000000000000	0.2673391499999980	F	F	F
0.3750000000000000	0.1250000000000000	0.2673391499999980	F	F	F
0.3750000000000000	0.6250000000000000	0.2673391499999980	F	F	F
0.8750000000000000	0.1250000000000000	0.2673391499999980	F	F	F
0.8750000000000000	0.6250000000000000	0.2673391499999980	F	F	F
0.3747456096773121	0.3751397626363229	0.4684332185966085	T	T	T
0.3751769848843125	0.8749426330147543	0.4683930246244401	T	T	T
0.8742123353415892	0.3747860291426051	0.4683599115721719	T	T	T
0.8754321123425726	0.8750750522249575	0.4684172012885526	T	T	T
0.3750000000000000	0.3750000000000000	0.2003054999999989	F	F	F
0.3750000000000000	0.8750000000000000	0.2003054999999989	F	F	F
0.8750000000000000	0.3750000000000000	0.2003054999999989	F	F	F
0.8750000000000000	0.8750000000000000	0.2003054999999989	F	F	F
0.3749349690851460	0.1250020880009046	0.4013665659953674	T	T	T
0.3752461109247562	0.6249708903814977	0.4013695033786036	T	T	T
0.8749393289420411	0.1249902469598538	0.4013387476000148	T	T	T
0.8750101299469861	0.6250169985199534	0.4013683490762574	T	T	T
0.3743309216347797	0.1255590044582391	0.5355215382929899	T	T	T
0.3753100215995389	0.6239162902003557	0.5358959306811002	T	T	T
0.8741762924647034	0.1256529024437611	0.5355513923428248	T	T	T
0.8782791006026471	0.6236542438777448	0.5354871518331024	T	T	T
0.1243464585342906	0.3757882003910069	0.5350036883823250	T	T	T
0.1269161060382729	0.8725533636799270	0.5356759555958561	T	T	T
0.6229916793767387	0.3765697523897771	0.5362983409282407	T	T	T
0.6248936036892587	0.8767576084427091	0.5353507395503101	T	T	T
0.1250000000000000	0.1250000000000000	0.2003054999999989	F	F	F
0.1250000000000000	0.6250000000000000	0.2003054999999989	F	F	F
0.6250000000000000	0.1250000000000000	0.2003054999999989	F	F	F
0.6250000000000000	0.6250000000000000	0.2003054999999989	F	F	F
0.3750000000000000	0.3750000000000000	0.0652280199999993	F	F	F
0.3750000000000000	0.8750000000000000	0.0652280199999993	F	F	F

0.8750000000000000	0.3750000000000000	0.0652280199999999	F	F	F
0.8750000000000000	0.8750000000000000	0.0652280199999999	F	F	F
0.3750000000000000	0.1250000000000000	0.1330989599999981	F	F	F
0.3750000000000000	0.6250000000000000	0.1330989599999981	F	F	F
0.8750000000000000	0.1250000000000000	0.1330989599999981	F	F	F
0.8750000000000000	0.6250000000000000	0.1330989599999981	F	F	F
0.3603299208221316	0.3704915171692704	0.6033949983951814	T	T	T
0.3757606990511562	0.8773790715678231	0.6034878757282911	T	T	T
0.8740447825788920	0.3748421496509309	0.6035141563309594	T	T	T
0.8783704867110913	0.8751988867458635	0.6025003444258772	T	T	T
0.1217212605678242	0.1204716007882283	0.6028078622991373	T	T	T
0.1309906484463639	0.6199876384015965	0.6049686835590222	T	T	T
0.6240126395041656	0.1265760080250260	0.6032507326112508	T	T	T
0.6338280671888299	0.6330553485686394	0.6018103875966503	T	T	T
0.1250000000000000	0.3750000000000000	0.1330989599999981	F	F	F
0.1250000000000000	0.8750000000000000	0.1330989599999981	F	F	F
0.6250000000000000	0.3750000000000000	0.1330989599999981	F	F	F
0.6250000000000000	0.8750000000000000	0.1330989599999981	F	F	F
0.1250000000000000	0.1250000000000000	0.0652280199999999	F	F	F
0.1250000000000000	0.6250000000000000	0.0652280199999999	F	F	F
0.1250000000000000	0.1250000000000000	0.0652280199999999	F	F	F
0.6250000000000000	0.6250000000000000	0.0652280199999999	F	F	F
0.9971618013587644	0.9976971239418830	0.6290018989975863	T	T	T
0.9889877695362870	0.5040333487653328	0.6284953674709115	T	T	T
0.5022399256527308	0.0011353076771741	0.6288325640452541	T	T	T
0.5119252144447657	0.4947673665677641	0.6334989431005980	T	T	T
0.0000259506452380	0.9999045219442735	0.4337467770529315	T	T	T
0.9999367298698800	0.4998755456840343	0.4336215055996604	T	T	T
0.5000082491146713	0.0001358140898091	0.4337413574495272	T	T	T
0.5001655639770846	0.5002051528850799	0.4343625328587706	T	T	T
0.2499705662922054	0.9998333261680514	0.4359435177488180	T	T	T
0.2502530890654171	0.4998402723105286	0.4355407585116424	T	T	T
0.7500622148398364	0.0001877120674862	0.4360318538050478	T	T	T
0.7498104564515700	0.5002059418629869	0.4360810441636715	T	T	T
0.9997032192772650	0.2498233194819761	0.4359295347166281	T	T	T
0.0001700357289067	0.7501105439434781	0.4358941484801733	T	T	T
0.4998740848330669	0.2502042606668766	0.4360036836466747	T	T	T
0.5003620069275314	0.7499623362494603	0.4360889630014242	T	T	T
0.2498933990131604	0.2499313998623975	0.4338077647104797	T	T	T
0.2503431983588342	0.7499915473794445	0.4336893617836282	T	T	T
0.7497425329900835	0.2501752907272632	0.4337634152629946	T	T	T
0.7501172094245447	0.7499847051719541	0.4338993250997447	T	T	T
0.9996422878158171	0.9980095815446290	0.5643675604684546	T	T	T
0.9996254308065176	0.4967376876963741	0.5640627301597618	T	T	T
0.5004196264926577	0.0021623174662722	0.5641304959902982	T	T	T
0.5020768606118438	0.5041880242033017	0.5673795913260875	T	T	T
0.2501897826536563	0.9994821273686156	0.5044462374483771	T	T	T
0.2503636928511312	0.4999273685660270	0.5034617892409798	T	T	T
0.7499179742588922	0.0007099939552049	0.5045133633729364	T	T	T
0.7498650151786421	0.5002513826139179	0.5047420644952538	T	T	T
0.9989057504270775	0.2495843052969988	0.5043505875442449	T	T	T
0.0011506101648919	0.7495012019354306	0.5044395046289907	T	T	T
0.4994962965787195	0.2507044601616926	0.5047149784309397	T	T	T
0.5008507386194623	0.7503490158277657	0.5046750582263471	T	T	T
0.2463532712849315	0.2493691348374369	0.5645859279494374	T	T	T
0.2541573743486438	0.7494920786554076	0.5643451809781084	T	T	T
0.7473340742179388	0.2503959513813143	0.5643053249810350	T	T	T
0.7526151223532480	0.7508615895746260	0.5644835617186175	T	T	T
0.9973008923570603	0.2474438375818053	0.5755306479705027	T	T	T
0.0030979516415570	0.7481754380387144	0.5754677198489233	T	T	T
0.4960123361890183	0.2517497208068917	0.5754842322784413	T	T	T
0.5038889361665326	0.7534654407307073	0.5754629880340190	T	T	T
0.2498374542919350	0.2495791886362611	0.4995422006360144	T	T	T
0.2506265827553094	0.7495260785784623	0.4994834190738402	T	T	T
0.749253772838336	0.2505052300748360	0.4996092936778638	T	T	T
0.7507049027719077	0.7505614346882368	0.4996932813100159	T	T	T
0.2495661766063293	0.9993061288334104	0.5747321589478531	T	T	T
0.2493706306508656	0.4980296694048860	0.5721398748190225	T	T	T
0.7505086361245148	0.0004253113465964	0.5753236013826637	T	T	T
0.7511387085275203	0.5016315014683599	0.5748546420160352	T	T	T
0.9999380662189097	0.9997537910562997	0.4996096308699620	T	T	T
0.0000214895638351	0.5001784658391557	0.4992191617436319	T	T	T

0.5001432784905759	0.0003486229016190	0.4994523082422404	T	T	T
0.5000655888479102	0.4999114775007314	0.5007974115965723	T	T	T
0.2500037007062446	0.2499338843721901	0.3675216666306440	T	T	T
0.2501264134363979	0.7499734655755077	0.3675258116866758	T	T	T
0.7498826833167485	0.2500921634705762	0.3675676894085811	T	T	T
0.7500025176822831	0.7500063646507300	0.3675690081176839	T	T	T
0.0000000000000000	0.0000000000000000	0.0400122400000029	F	F	F
0.0000000000000000	0.5000000000000000	0.0400122400000029	F	F	F
0.5000000000000000	0.0000000000000000	0.0400122400000029	F	F	F
0.5000000000000000	0.5000000000000000	0.0400122400000029	F	F	F
0.2499997679903530	0.0000005535462222	0.3681350218893868	T	T	T
0.2501288331113329	0.4999928509145590	0.3680208042505981	T	T	T
0.7500058697068113	0.9999986594618306	0.3681668682558410	T	T	T
0.7498981339883315	0.5000204251024982	0.3681938680883832	T	T	T
0.2500000000000000	0.2500000000000000	0.0400122400000029	F	F	F
0.2500000000000000	0.7500000000000000	0.0400122400000029	F	F	F
0.7500000000000000	0.0000000000000000	0.0400122400000029	F	F	F
0.7500000000000000	0.7500000000000000	0.0400122400000029	F	F	F
0.0000000000000000	0.0000000000000000	0.1044344100000032	F	F	F
0.0000000000000000	0.5000000000000000	0.1044344100000032	F	F	F
0.5000000000000000	0.0000000000000000	0.1044344100000032	F	F	F
0.5000000000000000	0.5000000000000000	0.1044344100000032	F	F	F
0.2500000000000000	0.0000000000000000	0.0931025300000030	F	F	F
0.2500000000000000	0.5000000000000000	0.0931025300000030	F	F	F
0.7500000000000000	0.0000000000000000	0.0931025300000030	F	F	F
0.7500000000000000	0.5000000000000000	0.0931025300000030	F	F	F
0.0000000000000000	0.2500000000000000	0.0931025300000030	F	F	F
0.0000000000000000	0.7500000000000000	0.0931025300000030	F	F	F
0.5000000000000000	0.2500000000000000	0.0931025300000030	F	F	F
0.5000000000000000	0.7500000000000000	0.0931025300000030	F	F	F
0.2500000000000000	0.2500000000000000	0.1044344100000032	F	F	F
0.2500000000000000	0.7500000000000000	0.1044344100000032	F	F	F
0.7500000000000000	0.2500000000000000	0.1044344100000032	F	F	F
0.7500000000000000	0.7500000000000000	0.1044344100000032	F	F	F
0.0000000000000000	0.0000000000000000	0.1692585199999996	F	F	F
0.0000000000000000	0.5000000000000000	0.1692585199999996	F	F	F
0.5000000000000000	0.0000000000000000	0.1692585199999996	F	F	F
0.5000000000000000	0.5000000000000000	0.1692585199999996	F	F	F
0.2500000000000000	0.0000000000000000	0.1640114400000030	F	F	F
0.2500000000000000	0.5000000000000000	0.1640114400000030	F	F	F
0.7500000000000000	0.0000000000000000	0.1640114400000030	F	F	F
0.7500000000000000	0.5000000000000000	0.1640114400000030	F	F	F
0.0000000000000000	0.2500000000000000	0.1640114400000030	F	F	F
0.0000000000000000	0.7500000000000000	0.1640114400000030	F	F	F
0.5000000000000000	0.2500000000000000	0.1692585199999996	F	F	F
0.5000000000000000	0.7500000000000000	0.1692585199999996	F	F	F
0.2500000000000000	0.2500000000000000	0.1692585199999996	F	F	F
0.2500000000000000	0.7500000000000000	0.1692585199999996	F	F	F
0.0000000000000000	0.0000000000000000	0.2349782499999975	F	F	F
0.0000000000000000	0.5000000000000000	0.2349782499999975	F	F	F
0.5000000000000000	0.0000000000000000	0.2349782499999975	F	F	F
0.5000000000000000	0.5000000000000000	0.2349782499999975	F	F	F
0.2500000000000000	0.0000000000000000	0.2326338900000025	F	F	F
0.2500000000000000	0.5000000000000000	0.2326338900000025	F	F	F
0.7500000000000000	0.0000000000000000	0.2326338900000025	F	F	F
0.7500000000000000	0.5000000000000000	0.2326338900000025	F	F	F
0.0000000000000000	0.2500000000000000	0.2326338900000025	F	F	F
0.0000000000000000	0.7500000000000000	0.2326338900000025	F	F	F
0.5000000000000000	0.2500000000000000	0.2326338900000025	F	F	F
0.5000000000000000	0.7500000000000000	0.2326338900000025	F	F	F
0.2500000000000000	0.2500000000000000	0.2349782499999975	F	F	F
0.2500000000000000	0.7500000000000000	0.2349782499999975	F	F	F
0.7500000000000000	0.2500000000000000	0.2349782499999975	F	F	F
0.7500000000000000	0.7500000000000000	0.2349782499999975	F	F	F
0.0000000000000000	0.0000000000000000	0.3011801099999971	F	F	F
0.0000000000000000	0.5000000000000000	0.3011801099999971	F	F	F
0.5000000000000000	0.0000000000000000	0.3011801099999971	F	F	F
0.5000000000000000	0.5000000000000000	0.3011801099999971	F	F	F
0.2500000000000000	0.0000000000000000	0.3004992500000014	F	F	F
0.2500000000000000	0.5000000000000000	0.3004992500000014	F	F	F

0.7500000000000000	0.0000000000000000	0.3004992500000014	F	F	F
0.7500000000000000	0.5000000000000000	0.3004992500000014	F	F	F
0.0000000000000000	0.2500000000000000	0.3004992500000014	F	F	F
0.0000000000000000	0.7500000000000000	0.3004992500000014	F	F	F
0.5000000000000000	0.2500000000000000	0.3004992500000014	F	F	F
0.5000000000000000	0.7500000000000000	0.3004992500000014	F	F	F
0.2500000000000000	0.2500000000000000	0.3011801099999971	F	F	F
0.2500000000000000	0.7500000000000000	0.3011801099999971	F	F	F
0.7500000000000000	0.2500000000000000	0.3011801099999971	F	F	F
0.7500000000000000	0.7500000000000000	0.3011801099999971	F	F	F
0.9999901502200501	0.9999834686014211	0.3675255451642272	T	T	T
0.9999350592980321	0.4999874029560516	0.3674757456131204	T	T	T
0.5000177275871138	0.0000088204859665	0.3675343713677890	T	T	T
0.5000814447004700	0.5000159746602080	0.3677415056392732	T	T	T
0.9999126038144084	0.2499006273189792	0.3681114336043265	T	T	T
0.0000077950464004	0.7500049241088718	0.3681326390171122	T	T	T
0.4999886956067030	0.2501135367545189	0.3681802477796197	T	T	T
0.5001118997837040	0.7499846186902630	0.3681783763492916	T	T	T
0.2508799662312171	0.2360020109360121	0.6288334248789553	T	T	T
0.2498611342098158	0.7595883006103392	0.6287317462584667	T	T	T
0.7480391378228148	0.2503389975868018	0.6288911005548883	T	T	T
0.7486678616700146	0.7505965693916608	0.6289389062922481	T	T	T
0.2510843061445200	0.4959574868984689	0.6326613194732715	T	T	T
0.5037708587676164	0.4999263951855966	0.6574195448321092	T	T	T

 (H⁺,H⁻)-(100)-O-(b)

100-o-b-product

1.0000000000000000		
11.0003119999999992	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.0003119999999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	41.1257400000000004

Ce O H
72 144 2

Selective dynamics

Direct

0.1246898997046628	0.1252015697372926	0.3340906998877102	F	F	F
0.1246858498195351	0.6252062996031356	0.3340898799632512	F	F	F
0.6246841598674635	0.1252012897452346	0.3340938101053013	F	F	F
0.6246813999457501	0.6252035196819890	0.3340928399099923	F	F	F
0.1251460858676836	0.3748255409644798	0.4010897055663136	T	T	T
0.1251682354522217	0.8747441768436701	0.4011274559186546	T	T	T
0.6251701654482105	0.3746381645239723	0.4009371925239833	T	T	T
0.6250555986226161	0.8747206791302560	0.4010137086016528	T	T	T
0.3746887997358641	0.3746385202528799	0.3340905199517366	F	F	F
0.3746829299023489	0.8746401102077854	0.3340909999431005	F	F	F
0.8746888097355807	0.3746399702117529	0.3340933301139373	F	F	F
0.8746837798782465	0.8746405301958688	0.3340923100715045	F	F	F
0.1260868625561358	0.1256349730446971	0.4681232356237999	T	T	T
0.1249540662872448	0.6259686320996281	0.4682163727836866	T	T	T
0.6259795570192210	0.1252990601861086	0.4679090857100547	T	T	T
0.6250694423218590	0.6252323123606587	0.4677074175508125	T	T	T
0.1244827501256296	0.3752981497252108	0.2671191001061644	F	F	F
0.1244812801673234	0.8752964997720056	0.2671158500734592	F	F	F
0.6244815601593814	0.3752960197856225	0.2671210200716132	F	F	F
0.6244788002376680	0.8752976297399542	0.2671192498906976	F	F	F
0.3744837000986863	0.1246078102148402	0.2671173999543868	F	F	F
0.3744793102232009	0.6246112301178357	0.2671165000313707	F	F	F
0.8744818701505892	0.1246109501257777	0.2671220700223245	F	F	F
0.8744801401996583	0.6246148800143132	0.2671188700799050	F	F	F
0.3757717962388512	0.3729143719757531	0.4678788906482225	T	T	T
0.3754784652817662	0.8730317560492793	0.4682390118021829	T	T	T
0.8758711112524011	0.3718713094939403	0.4679427606377615	T	T	T
0.8758681622580156	0.8718465476943251	0.4679200505507595	T	T	T
0.3739253195727557	0.3732039900322803	0.2001611100493292	F	F	F
0.3739255395665140	0.8732018100941161	0.2001570700004436	F	F	F
0.8739224496541524	0.3732001701406276	0.2001653699118862	F	F	F
0.8739196697330058	0.8731960302580504	0.2001606799050890	F	F	F
0.3752343644896285	0.1241974776900179	0.4010770221637756	T	T	T

0.3749104497005789	0.6243379527821631	0.4010608611032183	T	T	T
0.8752449412941274	0.1240190725408539	0.4010255713781490	T	T	T
0.8751047808911352	0.6240075450358660	0.4010042516084766	T	T	T
0.3768980060843461	0.1225553630241194	0.5353079691477518	T	T	T
0.3758934320228065	0.6195084989384796	0.5349512365074105	T	T	T
0.8775883721248903	0.1181631732162955	0.5350427814560277	T	T	T
0.8732706560617984	0.6179323071507028	0.5351108798172390	T	T	T
0.1265370786864679	0.3776449476355594	0.5351309720256765	T	T	T
0.1256791411645892	0.8785237430707866	0.5355420301420608	T	T	T
0.6259846273726168	0.3770364331293266	0.5347885340075322	T	T	T
0.6265992489386676	0.8765010705290734	0.5345927671278190	T	T	T
0.1239225996499016	0.1267160104186118	0.2001628298967972	F	F	F
0.1239199697244970	0.6267117496303740	0.2001587300313616	F	F	F
0.6239278604097791	0.1267219302507030	0.2001635399144206	F	F	F
0.6239216396771283	0.6267245601761147	0.2001600100083323	F	F	F
0.3860662497572775	0.3538793599672445	0.0667625100484486	F	F	F
0.3860989997374631	0.8539165398217818	0.0667542098938512	F	F	F
0.8861009796813022	0.3538839198379122	0.0667634899700289	F	F	F
0.8861345296387952	0.8538787299851123	0.0667570200560519	F	F	F
0.3730373402136209	0.1203232999209476	0.1330688199166730	F	F	F
0.3730421000786137	0.6203245598852121	0.1330658200922343	F	F	F
0.8730232297047564	0.1203135001989040	0.1330687399181159	F	F	F
0.8730332803287766	0.6203053604297750	0.1330628900537718	F	F	F
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0.8863767369614735	0.3512039652559977	0.6013520181703740	T	T	T
0.8854848160694857	0.8502648295755790	0.6009363865171196	T	T	T
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0.6298746508065562	0.6415213486377525	0.6021062357819602	T	T	T
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0.1230339103109088	0.8795975195976240	0.1330663200224507	F	F	F
0.6230308503976971	0.3796219898126552	0.1330679999922211	F	F	F
0.6230404501254156	0.8796336503910069	0.1330615799253678	F	F	F
0.1361103003260240	0.1459789704146601	0.0667656000840324	F	F	F
0.1361495501218499	0.6460345097484534	0.0667587999632318	F	F	F
0.6360554400638847	0.1460594999487270	0.0667598900348025	F	F	F
0.6360967698007087	0.6461079103938161	0.0667579199790680	F	F	F
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0.5000531041941585	0.7491964726912954	0.4342832751523460	T	T	T
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0.7503084431115639	0.7492988704811765	0.4340725915855614	T	T	T
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0.5030097390332386	0.9959908152735153	0.5707699680518346	T	T	T
0.5028156512286941	0.4937915429371529	0.5687407834170273	T	T	T
0.2510268004631868	0.9987809074109322	0.5028919459367316	T	T	T
0.2501992695305333	0.4983210700553329	0.5025173987059688	T	T	T
0.7514729419408255	0.9970885226742610	0.5020509575830019	T	T	T
0.7502674293564766	0.4972046469767619	0.5021974502375244	T	T	T
0.0017770558886454	0.2494995575763710	0.5009361865293442	T	T	T
0.0006819902409347	0.7499435985601295	0.5007217398907073	T	T	T
0.5010043417282617	0.2501428085119599	0.5008117857486170	T	T	T
0.5008060721717911	0.7499777760897572	0.5007920535420212	T	T	T
0.2543997075646800	0.2590738564533055	0.5661601590612548	T	T	T
0.2501639821035226	0.7559562422359321	0.5673591975365255	T	T	T
0.7532914962212445	0.2532234071401689	0.5651093021154026	T	T	T
0.7497834285122948	0.7528443308819988	0.5653715726435564	T	T	T
0.0035151946106211	0.2415113692727218	0.5658361779913790	T	T	T

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0.5047375698404437	0.2422488463032408	0.5660332433590796	T	T	T
0.4984581891456656	0.7433069638197054	0.5658632772820695	T	T	T
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0.2507083039202342	0.7484548996464611	0.5014763267064524	T	T	T
0.7520195244589019	0.2464895195779562	0.5003958560496287	T	T	T
0.7505381447346551	0.7469247488244193	0.5004645017270448	T	T	T
0.2541480758629007	0.0048265429461622	0.5725878231151853	T	T	T
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0.7531627666540004	0.9986269293806274	0.5707402213021382	T	T	T
0.7509784551597392	0.5008279580234358	0.5723246090965972	T	T	T
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0.0003728450682061	0.4991320392874528	0.5022671841682254	T	T	T
0.5010140396205713	0.0001407314239685	0.5021440706571028	T	T	T
0.5000070318213332	0.5001727292085008	0.5012613032017725	T	T	T
0.2499325732943163	0.2496469994795234	0.3675349062818682	T	T	T
0.2498260393851126	0.7497132000812030	0.3676082853878100	T	T	T
0.7500017141703665	0.2495544036821116	0.3674288080086612	T	T	T
0.7498888165253845	0.7495936219918491	0.3674621891990952	T	T	T
0.2498858081246880	0.9996765400549350	0.3677393264988780	T	T	T
0.2497697083226242	0.4997332274900259	0.3676884657736395	T	T	T
0.7498809066989125	0.9996449089217379	0.3675969145598117	T	T	T
0.7498893256178008	0.4996305813963033	0.3676008771096093	T	T	T
0.0532281602558200	0.3046782400353720	0.0426641599640547	F	F	F
0.0533040299220602	0.8048595503473024	0.0426661399892154	F	F	F
0.5531611203391336	0.3048182497005527	0.0426631800424744	F	F	F
0.5532578703222271	0.8050041798814433	0.0426705900003270	F	F	F
0.3032756098190674	0.1950254001886478	0.0426785798869531	F	F	F
0.3033534803376483	0.6949410398541431	0.0426840599099236	F	F	F
0.8030963803572106	0.1952831601503675	0.0426421900250276	F	F	F
0.8032114298212605	0.6951369397522527	0.0426544699256510	F	F	F
0.9982576103295955	0.9954272596995466	0.0967859501129951	F	F	F
0.9982530995484495	0.4954189099363759	0.0967887999097385	F	F	F
0.4982546104146834	0.9955085101222565	0.0967891400859884	F	F	F
0.4982617602118893	0.4954857898575966	0.0968016201045856	F	F	F
0.2482561303715727	0.0044396904378701	0.0967929800168932	F	F	F
0.2482395999313454	0.5044797902095866	0.0968010199938050	F	F	F
0.7482787397302886	0.0044690596048582	0.0967749000990636	F	F	F
0.7482632701690619	0.5045029895515682	0.0967742700800045	F	F	F
0.9988718201811011	0.2427698296193768	0.1024386700397386	F	F	F
0.9989150498640385	0.7427596199089592	0.1024268300096267	F	F	F
0.4988703902216614	0.2428275598001193	0.1024348400782600	F	F	F
0.4989006802716176	0.7428516800250762	0.1024295001135513	F	F	F
0.2488725501603923	0.2571189198997246	0.1024369698879610	F	F	F
0.2489089300376222	0.7571551997797883	0.1024271400344432	F	F	F
0.7488755400755878	0.2571227197919512	0.1024366498937184	F	F	F
0.7489135099077160	0.7571420801519082	0.1024312600818860	F	F	F
0.9982823896267661	0.0014245595943123	0.1659372300656443	F	F	F
0.9982643901373009	0.5014227096467820	0.1659431499591264	F	F	F
0.4982911002887889	0.0014431699755448	0.1659380200818248	F	F	F
0.4982733098843042	0.5014404900515572	0.1659510999680478	F	F	F
0.2482878003823856	0.9984840502705765	0.1659420800695628	F	F	F
0.2482738298695537	0.4984857802215075	0.1659395300850548	F	F	F
0.7482799896948364	0.9984906800825257	0.1659395899016047	F	F	F
0.7482739698655791	0.4984914800598403	0.1659335999789917	F	F	F
0.9989954703102981	0.2515531895822605	0.1673610899159499	F	F	F
0.9989739100127366	0.7515501596681986	0.1673518801120650	F	F	F
0.4990059300136238	0.2515663201189184	0.1673530900598976	F	F	F
0.4989905104509731	0.7515775697998350	0.1673473999495201	F	F	F
0.2490026601063704	0.2483542203166635	0.1673561599134743	F	F	F
0.2489813898005835	0.7483511204045854	0.1673469999567203	F	F	F
0.7489990102098929	0.2483605801362714	0.1673599599666744	F	F	F
0.7489802898317777	0.7483606601340043	0.1673517799315007	F	F	F
0.9992446096074374	0.9995716803305186	0.2333607699217097	F	F	F
0.9992515503196628	0.4995741602601811	0.2333658900727400	F	F	F
0.4992499303656146	0.9995638496435362	0.2333615300296117	F	F	F
0.4992542902419501	0.4995644296270854	0.2333733501208712	F	F	F
0.2492496403738400	0.0003477101376745	0.2333652500842547	F	F	F
0.2492479904206348	0.5003565698863781	0.2333601000249459	F	F	F
0.7492457595748192	0.0003537499663651	0.2333658100741758	F	F	F
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0.4992509803358303	0.2496376002789731	0.2339018400641564	F	F	F
0.4992392997580453	0.7496414201706258	0.2338973000850544	F	F	F
0.2492479804209182	0.2502810602099288	0.2339020499084015	F	F	F
0.2492422996729573	0.7502793202592812	0.2338964500091691	F	F	F
0.7492507203432055	0.2502772003194096	0.2339107500558057	F	F	F
0.7492419596825997	0.7502796002513392	0.2339044501083762	F	F	F
0.9996949295619970	0.0000126696406397	0.3005636000713920	F	F	F
0.9996950695580296	0.5000160904527107	0.3005672199454636	F	F	F
0.4996949595611468	0.0000099197186429	0.3005663701127332	F	F	F
0.4996942595809983	0.5000121596551068	0.3005711999346374	F	F	F
0.2497006003102484	0.9998811797338121	0.3005650201066317	F	F	F
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0.7496976503939194	0.9998794397831645	0.3005668700429496	F	F	F
0.7497015802824478	0.4998824896966525	0.3005617199836408	F	F	F
0.9997278704458594	0.2499863303877206	0.3006414700379878	F	F	F
0.9997164298612589	0.7499880903378013	0.3006381300372922	F	F	F
0.4997293604035988	0.2499784997007382	0.3006358399873150	F	F	F
0.4997182598093559	0.7499838695484300	0.3006371999628428	F	F	F
0.2497225196885324	0.2499082098762315	0.3006379000110400	F	F	F
0.2497132999500380	0.7499135997233566	0.3006355601139319	F	F	F
0.7497224696899494	0.2499056499488361	0.3006474499911747	F	F	F
0.7497118599908816	0.7499121397647599	0.3006418398793542	F	F	F
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0.0498987855364419	0.7863847468739280	0.6259298230595434	T	T	T
0.5626603059523063	0.2899458771609389	0.6264187993677268	T	T	T
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0.0000320600119039	0.9995948597834001	0.3676560359839982	T	T	T
0.9999497361195324	0.4996162614327133	0.3676354636042660	T	T	T
0.4998656138119557	0.9997012760535426	0.3676114845615501	T	T	T
0.4998104664849663	0.4997499019759744	0.3674879261509005	T	T	T
0.9999430597766334	0.2497156667445495	0.3675441074553376	T	T	T
0.9999123032062585	0.7497186866020442	0.3675118728647249	T	T	T
0.4998312776385916	0.2496675111267379	0.3675179237444155	T	T	T
0.4997291614325334	0.7497821972795862	0.3675232517243359	T	T	T
0.3048571929511681	0.2017093774365506	0.6269518481296217	T	T	T
0.3027245456274201	0.6930138336779592	0.6300944609236652	T	T	T
0.8140650901929263	0.1858636264086115	0.6241127589880975	T	T	T
0.7929464054780340	0.7027497540675185	0.6264213183500829	T	T	T
0.4721811740588251	0.5355402774572013	0.6315138997685636	T	T	T
0.3715492750442877	0.6346027572474284	0.6354773113992280	T	T	T

 (H⁺, H)-(110)

110-product

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11.0003119999999992	0.0000000000000000	0.0000000000000000
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64 128 2

selective dynamics

Direct

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0.8738164349633806	0.1252074637292324	0.5035645098020396	T	T	T
0.8744889332447627	0.6252688847189347	0.5034283472583425	T	T	T
0.1249325040924063	0.2498154037465525	0.4489053914768348	T	T	T
0.1232454798759051	0.7508882693282217	0.4486057461344330	T	T	T
0.6231961114060880	0.2504437660292922	0.4489402623229495	T	T	T
0.6243838346495068	0.7495624373020036	0.4485851291389906	T	T	T
0.1236944686636647	0.0002175168516132	0.4486024700208802	T	T	T
0.1274137670954261	0.4998676409989216	0.4491347758952671	T	T	T
0.6239251895234403	0.9999184940908208	0.4486277901981808	T	T	T
0.6272360518487190	0.4993424137747056	0.4457816561354804	T	T	T

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0.8742676522227200	0.8751987360095228	0.3804242804295228	T	T	T
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0.3744449231588405	0.6253400949034003	0.3808383267723343	T	T	T
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0.8762174938088734	0.6251765570217103	0.3803174012759527	T	T	T
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0.1251706195742557	0.7502084567763987	0.3188357313054198	T	T	T
0.6247065592983461	0.2504940884425721	0.3191234560509884	T	T	T
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0.3750000000000000	0.6250000000000000	0.2536646300000029	F	F	F
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0.8750000000000000	0.6250000000000000	0.2536646300000029	F	F	F
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0.3750000000000000	0.8750000000000000	0.2536646300000029	F	F	F
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0.3750000000000000	0.3750000000000000	0.1237068800000003	F	F	F
0.3750000000000000	0.8750000000000000	0.1237068800000003	F	F	F
0.8750000000000000	0.3750000000000000	0.1237068800000003	F	F	F
0.8750000000000000	0.8750000000000000	0.1237068800000003	F	F	F
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0.7554348695417801	0.9997141366317379	0.5082362484530876	T	T	T
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0.9917560861127797	0.5003081701180179	0.5081763721593191	T	T	T
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0.2489915975830712	0.8751522133135055	0.4450535034148757	T	T	T
0.7511642234761950	0.3759006749184906	0.4449863459996308	T	T	T
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0.9980943179378627	0.8753586318613671	0.4453185527138572	T	T	T
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0.2433605599999993	0.6250000000000000	0.0641464600000035	F	F	F
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0.7433605599999993	0.6250000000000000	0.0641464600000035	F	F	F
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0.7495786588944000	0.9999852190011111	0.3821406714275994	T	T	T
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0.2491262042178377	0.6288555334690074	0.4451179961815583	T	T	T
0.7491182039786466	0.1253480108764649	0.4455069150051898	T	T	T
0.7503128733461608	0.6239793383275938	0.4449165870898355	T	T	T
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0.4989652978213002	0.1233609121734105	0.4447191472013685	T	T	T
0.4984565944320778	0.6217106602332692	0.4466332407131333	T	T	T
0.9915583406383774	0.2501998675985746	0.5083639630483034	T	T	T
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0.4927569623313701	0.2452051125795975	0.5071794906395013	T	T	T
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0.0066394299999999	0.8750000000000000	0.0641464600000035	F	F	F
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0.2501547351885023	0.7506635640938555	0.3814942559097929	T	T	T
0.7500979970478028	0.2501864344776905	0.3819424883273044	T	T	T
0.7500601123569481	0.7497637504795023	0.3820526709013876	T	T	T
0.9998248278075224	0.2500087630421035	0.3819627311102138	T	T	T
0.9997185150507235	0.7501900291650756	0.3820482991320944	T	T	T
0.4996329553612213	0.2516736696778494	0.3832271792253934	T	T	T
0.5000475275112777	0.7486689410051497	0.3827128483285307	T	T	T
0.2433605599999993	0.3750000000000000	0.0641464600000035	F	F	F
0.2433605599999993	0.8750000000000000	0.0641464600000035	F	F	F
0.7433605599999993	0.3750000000000000	0.0641464600000035	F	F	F
0.7433605599999993	0.8750000000000000	0.0641464600000035	F	F	F
0.0066394299999999	0.1250000000000000	0.0641464600000035	F	F	F
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0.5066394400000007	0.6250000000000000	0.0641464600000035	F	F	F
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0.9996369091568127	0.8749822029381562	0.3180266672214884	T	T	T
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0.0001996800000015	0.2500000000000000	0.1271687799999981	F	F	F
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0.5001997000000031	0.2500000000000000	0.1271687799999981	F	F	F
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0.5001536600000023	0.3750000000000000	0.1905233399999986	F	F	F
0.5001536600000023	0.8750000000000000	0.1905233399999986	F	F	F
0.2498463200000032	0.3750000000000000	0.1905233399999986	F	F	F
0.2498463200000032	0.8750000000000000	0.1905233399999986	F	F	F
0.7498463399999977	0.3750000000000000	0.1905233399999986	F	F	F
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0.4993159191059959	0.9993893387433417	0.3816399902806751	T	T	T
0.5011244621449364	0.4999753142873828	0.3820385602536405	T	T	T
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0.7499743400000014	0.5000000000000000	0.2546287699999965	F	F	F

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0.7499743400000014	0.2500000000000000	0.2546287699999965	F	F	F
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0.2539997702793215	0.2449724178755446	0.5084862287583434	T	T	T
0.2538498010501300	0.7522851743113819	0.5092059139293568	T	T	T
0.7557742595769454	0.2512465349606501	0.5081122891866485	T	T	T
0.7547487193051694	0.7487711534398187	0.5080303701618405	T	T	T
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0.9997520009358425	0.1251069217920175	0.3180425455939542	T	T	T
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0.4998534398248538	0.1257538998998768	0.3183352266987853	T	T	T
0.4998720159372567	0.6249581579938095	0.3180676918791363	T	T	T
0.2498320238821279	0.1250642244751461	0.3179635211385943	T	T	T
0.2502016687666853	0.6245039740666414	0.3182688287756221	T	T	T
0.7495722346139146	0.1249821756394880	0.3180464175308799	T	T	T
0.7502197375623041	0.6248641506391976	0.3179850598234921	T	T	T
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0.5000256599999986	0.2500000000000000	0.2546287699999965	F	F	F
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0.2503601629066736	0.3754599082944878	0.3186475115581970	T	T	T
0.2497844976381742	0.8751543337639873	0.3177498280980728	T	T	T
0.7502465029587597	0.3750970820552766	0.3179562833178906	T	T	T
0.7496265551706145	0.8749791992242848	0.3180300433676138	T	T	T
0.3838875826675121	0.3672819356275312	0.5786145331838242	T	T	T
0.5902668863239455	0.5039658661342870	0.5316705390382737	T	T	T

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221-product

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Ce O H
52 104 2

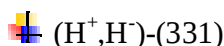
Selective dynamics

Direct

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0.7346029599999966	0.9384064500000022	0.1251644399999989	F	F	F
0.4846029599999966	0.9384064500000022	0.1251644399999989	F	F	F
0.9846029599999966	0.9384064500000022	0.1251644399999989	F	F	F
0.2922178800000026	0.6688738400000034	0.1555735800000022	F	F	F
0.7922178800000026	0.6688738400000034	0.1555735800000022	F	F	F
0.0422178900000034	0.6688738400000034	0.1555735800000022	F	F	F
0.5422178800000026	0.6688738400000034	0.1555735800000022	F	F	F
0.0986668700000024	0.3946651799999970	0.1800825400000008	F	F	F
0.5986668800000032	0.3946651799999970	0.1800825400000008	F	F	F
0.3486668500000007	0.3946651799999970	0.1800825400000008	F	F	F
0.8486668199999983	0.3946651799999970	0.1800825400000008	F	F	F
0.4029683999999989	0.1118754800000019	0.2183137700000017	F	F	F
0.9029684300000014	0.1118754800000019	0.2183137700000017	F	F	F
0.1529683799999972	0.1118754800000019	0.2183137700000017	F	F	F
0.6529683699999964	0.1118754800000019	0.2183137700000017	F	F	F
0.4578611800000019	0.8314441899999991	0.2509747100000013	F	F	F
0.9578611800000019	0.8314441899999991	0.2509747100000013	F	F	F
0.2078611700000010	0.8314441899999991	0.2509747100000013	F	F	F

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0.0138888899999969	0.5555558000000036	0.2801990800000027	F	F	F
0.5138888999999978	0.5555558000000036	0.2801990800000027	F	F	F
0.2638888999999978	0.5555558000000036	0.2801990800000027	F	F	F
0.7638888999999978	0.5555558000000036	0.2801990800000027	F	F	F
0.0701485586248936	0.2801065259824327	0.3093266339564238	T	T	T
0.5701090985296204	0.2797465209803747	0.3094648496662131	T	T	T
0.3201585856288816	0.2802100722052216	0.3093584314962783	T	T	T
0.8197484556916663	0.2798992419546522	0.3093403104618346	T	T	T
0.1251910193242836	0.0003977302538374	0.3420834852066150	T	T	T
0.6246493061772327	0.9986671971773333	0.3435829957717331	T	T	T
0.3747452755632921	0.0002353955275396	0.3422470488601022	T	T	T
0.8753616486914098	0.9999727399948810	0.3422787026784562	T	T	T
0.1793433092338788	0.7182213695060682	0.3801243788687430	T	T	T
0.6787303765450474	0.7168701751663633	0.3777659982142936	T	T	T
0.4300468082183855	0.7193810129632396	0.3806307920261958	T	T	T
0.9292870357033394	0.7180127107691305	0.3802250656847121	T	T	T
0.2364894892299674	0.4449683368580040	0.4046903580260661	T	T	T
0.7360342198842318	0.4430706893262411	0.4050730332550074	T	T	T
0.4859281018648076	0.4440997626058731	0.4049122851501821	T	T	T
0.9857774947338811	0.4435485863038764	0.4047835684963772	T	T	T
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0.2940767103266566	0.1754837541709904	0.4350598752223291	T	T	T
0.7932867948140228	0.1722022620322150	0.4349307285569921	T	T	T
0.3509972950309432	0.9071106011566954	0.4644664955023927	T	T	T
0.8589588875887912	0.9103541649097906	0.4654400931021812	T	T	T
0.1041613271760440	0.9075208919015481	0.4644699044827618	T	T	T
0.5948650274750023	0.9064932680923476	0.4695828715929409	T	T	T
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0.7780759500714112	0.6135313280144743	0.3605711357335792	T	T	T
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0.3333527316825950	0.3332188204568709	0.3873557056666357	T	T	T
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0.3318546018019290	0.8366121491763749	0.3915718149472340	T	T	T
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331-product

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40	80	2			
Selective dynamics					
Direct					
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0.1577875962135096	0.3155643263424608	0.3301092379950745	T	T	T
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0.7898504298803388	0.0791261887673826	0.2995449207989864	T	T	T
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0.6874899562237786	0.3683641648967182	0.4043375286275008	T	T	T
0.1787126154906815	0.3687597906612581	0.4028647454808905	T	T	T
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