

Two-Sites Are Better Than One: Revisiting the OER Mechanism on CoOOH by DFT with Electrode Polarization.

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Corresponding Author

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SUPPORTING INFORMATION

Selection of reaction steps

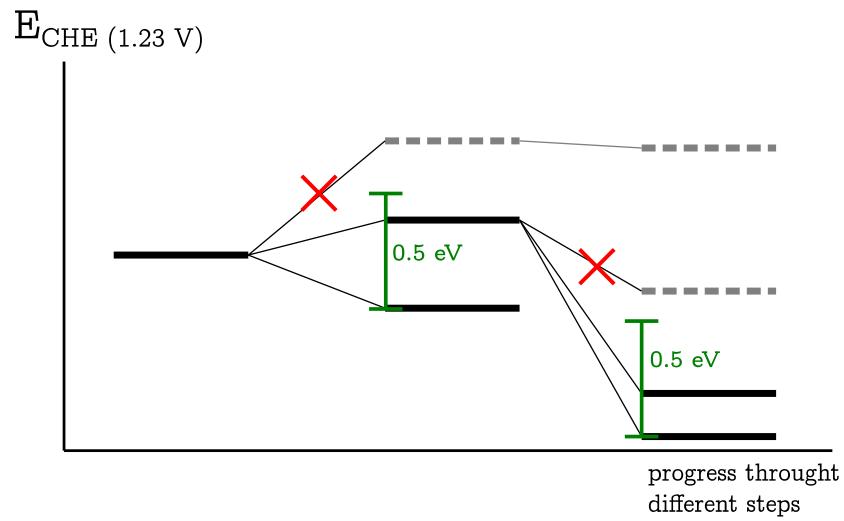


Figure S1: Illustration of mechanism selection criterion. 0.5~eV tolerance is represented by green segment.

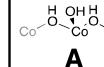
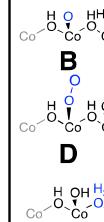
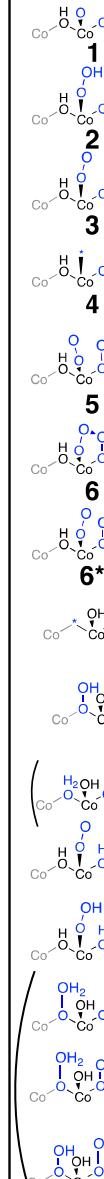
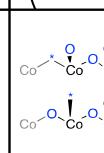
Reference	
1 site modification	
2 sites modification	
3 sites modification	

Table S1: All intermediates computed. (in brackets, structures that could not be converged in the represented geometry). Labels correspond to the ones used in the main article.

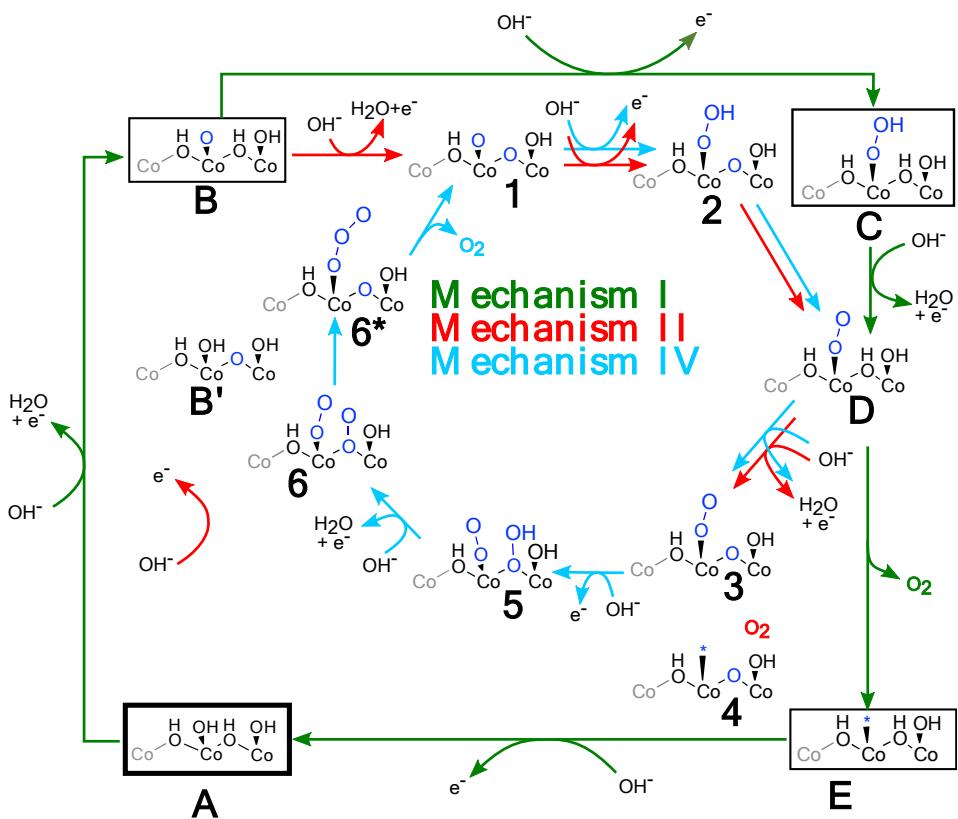


Figure S2: Best mechanisms after considering polarization effect and transition states.

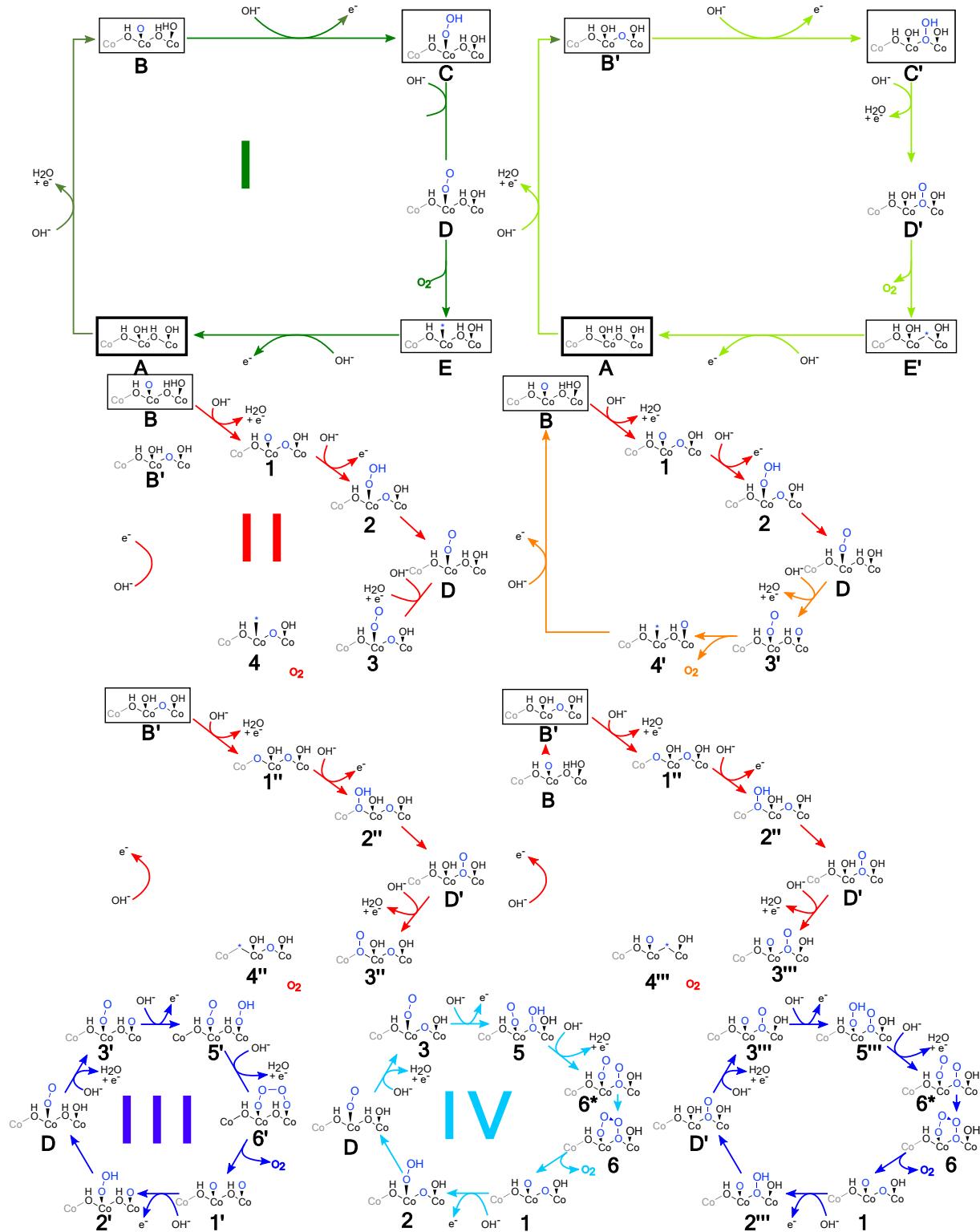


Figure S3: Comprehensive scheme of all reaction paths considered in the study. Best mechanisms are shown in Figure 2. The different shade of colours corresponds to the ones used in Figure S4.

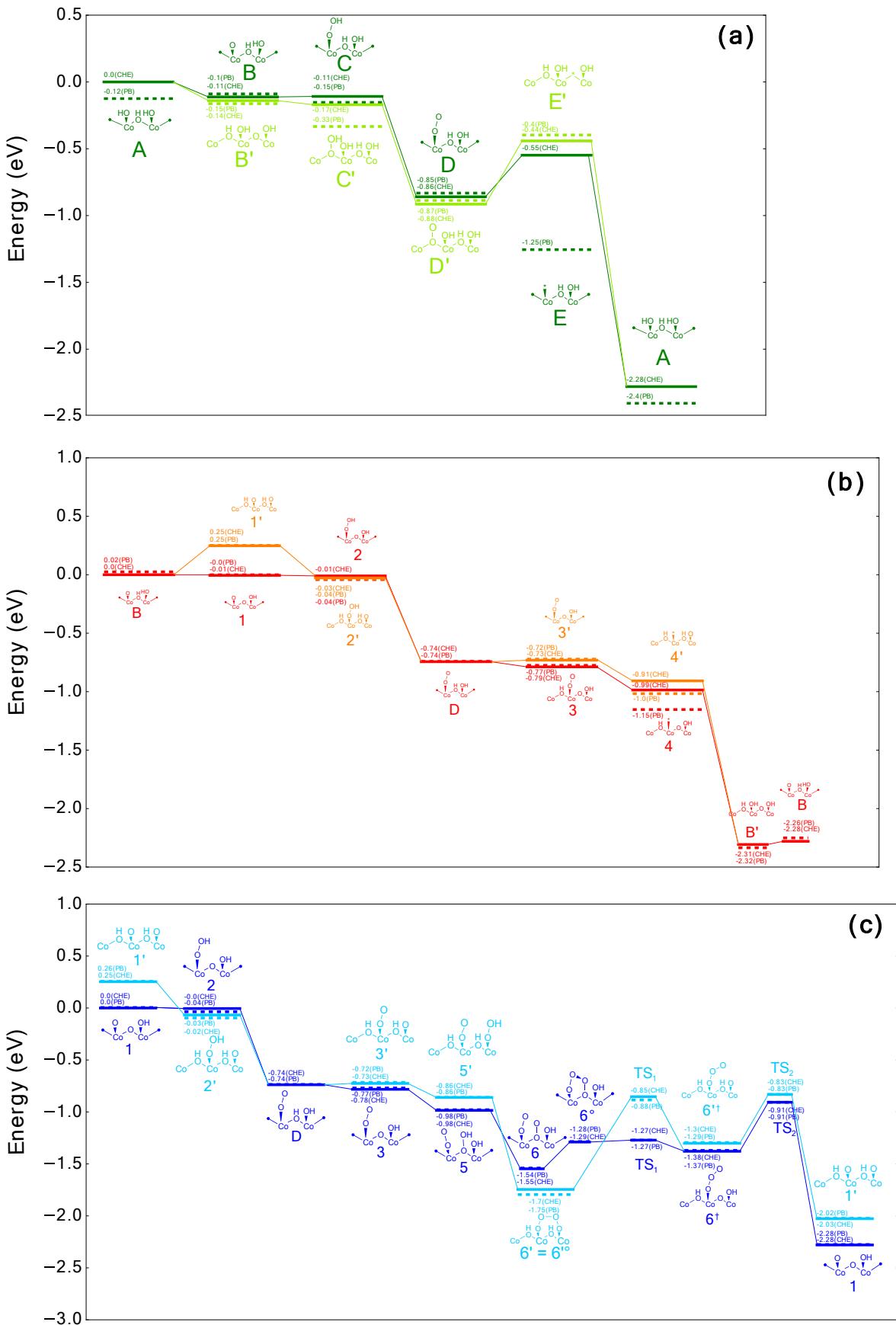


Figure S4: Detailed energy profiles and comparison between CHE (plain lines) and PB (dashed lines) approaches, for each mechanism, at 0.57V overpotential. (a), (b) and (c) refer to mechanism I, II and III respectively. Colors correspond to different configurations.

Transition States

Neglecting the activation barrier of desorption / adsorption reactions is a usual approximation in catalysis. In addition, the barrier of H dissociation and hopping steps have been shown to significantly decrease in water-assisted case¹. Most of the steps considered involve 1 site adsorption (OH^-) or 1 site desorption (H^+ , O_2) thus we assumed no activation barrier associated to these steps. Transition state study was operated only on the 2-sites O_2 desorption steps. Figure S5 illustrates the geometry of an obtained transition state. For transition states corresponding to 1-site O_2 desorption, thus corresponding to the escape of O_2 from the surface, no transition states were computing because it involves a two spin states (associated to an intersystem crossing of singlet oxygen to triplet oxygen) that are extremely difficult to model with a surface containing several Co atoms prone to change easily their spin and oxidations states.

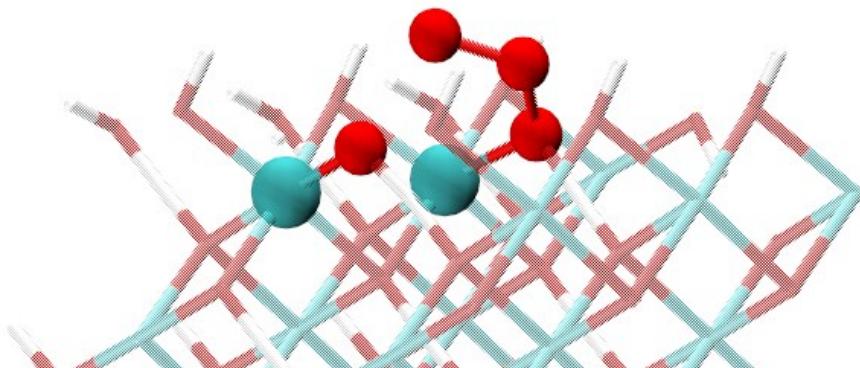
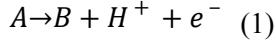


Figure S5: Computed transition state for the $6' \rightarrow 6''^\dagger$ step.

Free energy variation as a function of the potential

In the CHE model, the free energy of a surface does not depend on the applied potential (workfunction). And for an electrochemical step such as in (1), the Gibbs' free energy variation is given by (2). A pH 14 has been used on our modelling to get closer to real experimental conditions.



$$\Delta G = G_B + \left(\frac{1}{2} G_{H_2} - 0.059 pH \right) - U - G_A \quad (2)$$

Where the G_B and G_A Gibbs' free energies are computed at neutral charge, thus don't include any polarization of the surface induced by the applied electrochemical potential and the Gibbs' free energy of the step (ΔG) is linearly dependent to the potential (U).

In order to consider this potential, the total number of electrons in the surface was modified, along with a Poisson-Boltzmann distribution of counter charges for keeping electroneutrality (cf Computational Details). At oxidative potentials (region of interest) a quadratic dependence on the potential was observed (see Figure S6), which is in agreement with previous studies using this model on metal surfaces². When the surface charge is too high, this model loses its validity, therefore we limited the surface charge to 1 electron per cell in the parabolic fit.

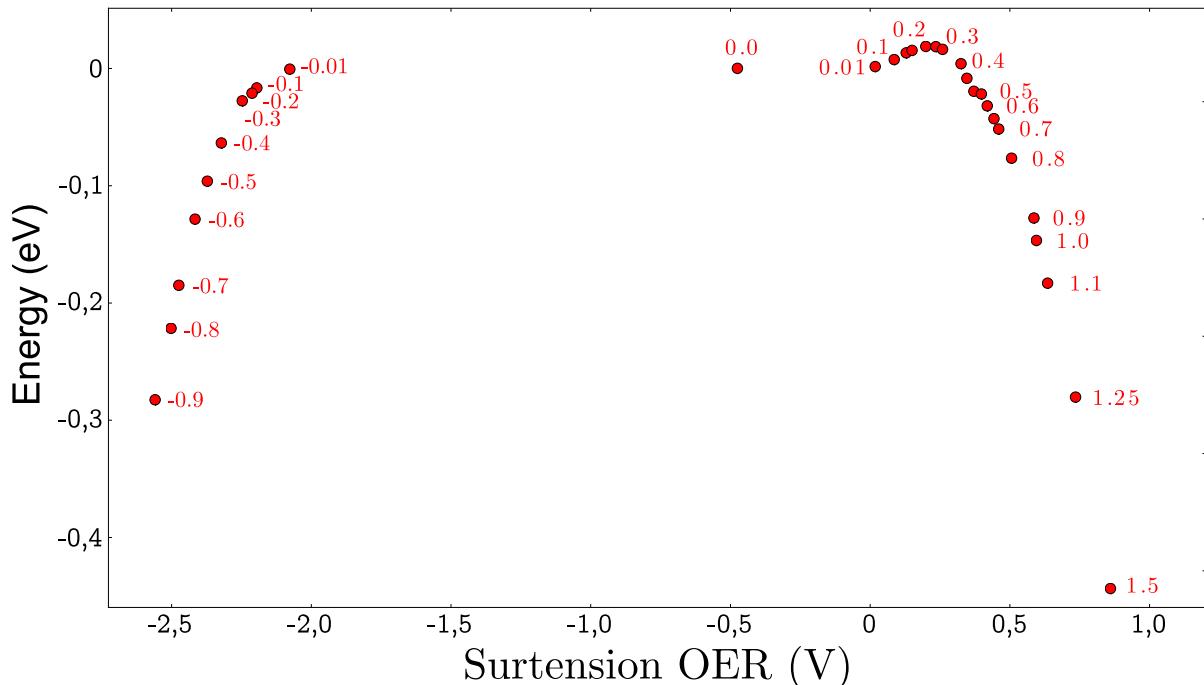


Figure S6: Free energy of A surface as a function of the overpotential. The potential versus SHE can be obtained by adding 1.23 V to the overpotential. The numbers given for each point correspond to the total charge of the slab used to obtain this potential.

Because in this approach, the Gibbs' free energy of each intermediate depends on the potential, the Gibbs' energy associated to a step is no longer linear with the potential (equation (3)).

$$\Delta G = G_B(U) + \left(\frac{1}{2} G_{H_2} - 0.059 pH \right) - U - G_A(U) \quad (3)$$

Readers interested by interested by this approach are invited to read to following reference where it is presented in more details.³

References

- 1 J. Fester, M. García-Melchor, A. S. Walton, M. Bajdich, Z. Li, L. Lammich, A. Vojvodic and J. V. Lauritsen, *Nat. Com.*, 2017, **8**, 6–13.
- 2 S. N. Steinmann and P. Sautet, *J. Phys. Chem. C*, 2016, **120**, 5619–5623.
- 3 Y. Hajar, L. Treps, C. Michel, E. Baranova and S. Steinmann, *Catal. Sci. Technol.*, 2019, 10.1039/c9cy01421g.

List of optimized structures for 0 charge systems. POSCAR format.

A

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Co H O

24 48 60

Selective dynamics

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Co H O

24 46 60

Selective dynamics

Direct

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Selective dynamics

Direct

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Selective dynamics

Direct

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 0.0833333129999971 0.6817300319999973 0.4673556090000019 F F F

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0.916666687000029	0.318269968000027	0.532644390999981	F	F	F
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0.7504082534892714	0.9525261848873875	0.5996251099303783	T	T	T
0.4182896221780107	0.9502811344002774	0.5992130300849418	T	T	T
0.7503612968072374	0.4534652605177412	0.6004868513218001	T	T	T
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24 48 62

Selective dynamics

Direct

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0.7488712965407984	0.7923891490651087	0.5732529098903427	T	T	T
0.0837476290364663	0.1155716105588240	0.6233871910678985	T	T	T
0.0856097473513344	0.6157582432743425	0.6230623355754830	T	T	T
0.4003468181976828	0.1130421172470264	0.6244994741243985	T	T	T
0.9145468871591476	0.9025993542511799	0.6388036352747761	T	T	T
0.7565202732873715	0.1169590897793782	0.6233653886228083	T	T	T
0.5809529905899780	0.9048359877930352	0.6388831226956526	T	T	T
0.9197065781072666	0.4025546073272466	0.6386912923540606	T	T	T
0.2475253992551956	0.8997593860490625	0.6385388720736316	T	T	T
0.4145842044624715	0.6182006286473509	0.6236494885019326	T	T	T
0.7637771885827647	0.6176282218681948	0.6237231813480122	T	T	T
0.2513682168244173	0.4127703243123690	0.6401225069238663	T	T	T
0.5842967356169382	0.4275943794273758	0.6405175394975871	T	T	T
0.5821845546196727	0.3101916392357680	0.6641724883694735	T	T	T

D

1.000000000000000		
8.508600234999994	0.000000000000000	0.000000000000000
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Co H O
24 46 62

Selective dynamics

Direct

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0.5810977051083245	0.0489870707886507	0.4008056567829412	T	T	T
0.5855040945741332	0.5512220761803769	0.4004351223470803	T	T	T
0.9143893301927947	0.0470908651315313	0.4002187897172034	T	T	T
0.9181645090549898	0.5505037953566683	0.4001732385113794	T	T	T
0.0833333129999971	0.1817300920000022	0.4673556090000019	F	F	F
0.0833333129999971	0.6817300319999973	0.4673556090000019	F	F	F
0.4166666870000029	0.1817300920000022	0.4673556090000019	F	F	F
0.4166666870000029	0.6817300319999973	0.4673556090000019	F	F	F
0.750000000000000	0.1817300920000022	0.4673556090000019	F	F	F
0.750000000000000	0.6817300319999973	0.4673556090000019	F	F	F
0.250000000000000	0.3182699680000027	0.5326443909999981	F	F	F
0.250000000000000	0.8182699079999978	0.5326443909999981	F	F	F
0.5833333129999971	0.3182699680000027	0.5326443909999981	F	F	F
0.5833333129999971	0.8182699079999978	0.5326443909999981	F	F	F
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0.9166666870000029	0.8182699079999978	0.5326443909999981	F	F	F
0.0818354909450102	0.449496204643317	0.5998267614886206	T	T	T
0.0856106698072053	0.9529091348684687	0.5997812102827965	T	T	T
0.4144959054258668	0.4487779238196231	0.5995648776529197	T	T	T
0.4189022948916755	0.9510129292113493	0.5991943432170588	T	T	T
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0.4193177861478724	0.5377654775121603	0.3364798680891531	T	T	T
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0.7442633891267144	0.0429545740747680	0.3349504248716692	T	T	T
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0.9822204043310124	0.3687628824171306	0.3534643796184933	T	T	T
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0.4141948834956867	0.0437580731759150	0.3345740298947079	T	T	T
0.4691608806133536	0.8713671935269253	0.3642527723798228	T	T	T
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0.8158319705811423	0.8683972522200315	0.3613889819384535	T	T	T

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D'

1.0000000000000000
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Co H O
24 46 62

Selective dynamics

Direct

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 0.2507208598825050 0.4806153271080033 0.5579467209359974 T T T
 0.2489622834383290 0.9799942961726390 0.5579889502777237 T T T
 0.5846383847952010 0.4805715800656767 0.5583634286864877 T T T
 0.5820687989357178 0.9802730551054768 0.5580310167669328 T T T
 0.9183531206612657 0.4803087110916742 0.5578472630783646 T T T
 0.9156559207245405 0.9805861473955932 0.5581193809778708 T T T
 0.0839553782460946 0.2913514029282858 0.5735309490528765 T T T
 0.0826020317136294 0.7912902808671859 0.5734072047839874 T T T
 0.4166245064908899 0.2919963799504066 0.5736963612675173 T T T
 0.4163707734855935 0.7910547747879543 0.5730719848556987 T T T
 0.750774332976567 0.2916454697136102 0.5734241836486916 T T T
 0.7494247645876088 0.7915647457582670 0.5732539131279716 T T T
 0.0916616580420225 0.1167847016279911 0.6234273166680846 T T T
 0.0825627028331850 0.6163128444889292 0.6231264095273190 T T T
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 0.9152439280592181 0.9031694271600682 0.6387175315553247 T T T
 0.7461602961000151 0.1158773593184187 0.6248757940275809 T T T
 0.5815327458224681 0.9005430456791540 0.6383836403514975 T T T
 0.9194599004876686 0.4013853963190748 0.6384226356739069 T T T
 0.2486295883596433 0.8995203201420169 0.6383511463987562 T T T
 0.4171590507491455 0.6171529137919995 0.6238602394677242 T T T
 0.7592936104272379 0.6161776635353527 0.6237605379076081 T T T
 0.2498419948818043 0.4149303976096134 0.6401769147174530 T T T
 0.5856748008965595 0.4104407225372170 0.6373119698456470 T T T
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E'

1.000000000000000
 8.508600234999994 0.000000000000000 0.000000000000000
 0.000000000000000 10.854810714699993 0.000000000000000
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Co H O
24 46 58

Selective dynamics

Direct

0.5823776894214771 0.5459562261277181 0.4015106171582076 T T T
 0.2374161848332393 0.5321784069628400 0.3966221722586921 T T T
 0.5862112112882818 0.0475086273339842 0.4000563746054877 T T T

0.2516282950183170	0.0491494735570643	0.3999251365822452	T	T	T
0.9193548158742346	0.0500747939749070	0.4007402953002808	T	T	T
0.9109855801775861	0.5496046945546991	0.4005778436590675	T	T	T
0.0833333129999971	0.1817300920000022	0.4673556090000019	F	F	F
0.0833333129999971	0.6817300319999973	0.4673556090000019	F	F	F
0.4166666870000029	0.1817300920000022	0.4673556090000019	F	F	F
0.4166666870000029	0.6817300319999973	0.4673556090000019	F	F	F
0.7500000000000000	0.1817300920000022	0.4673556090000019	F	F	F
0.7500000000000000	0.6817300319999973	0.4673556090000019	F	F	F
0.2500000000000000	0.3182699680000027	0.5326443909999981	F	F	F
0.2500000000000000	0.8182699079999978	0.5326443909999981	F	F	F
0.5833333129999971	0.3182699680000027	0.5326443909999981	F	F	F
0.5833333129999971	0.8182699079999978	0.5326443909999981	F	F	F
0.9166666870000029	0.3182699680000027	0.5326443909999981	F	F	F
0.9166666870000029	0.8182699079999978	0.5326443909999981	F	F	F
0.089350933584322	0.4503343205971219	0.5994293882620031	T	T	T
0.0806237254080269	0.9498756716935606	0.5992425600187440	T	T	T
0.7484373688048375	0.9508505320821991	0.6000605863436597	T	T	T
0.4137486813678551	0.9524296114147619	0.5999560820364690	T	T	T
0.7629749904221254	0.4676825396701361	0.6033841942468330	T	T	T
0.4179435729850404	0.4539626637852237	0.5985009465815769	T	T	T
0.7371182321750598	0.5448551779778558	0.3346419438045859	T	T	T
0.4661234889531677	0.3721905157241527	0.3647114734741495	T	T	T
0.7839623870503860	0.3731486223997377	0.3679063919891080	T	T	T
0.7558167460392136	0.0438187659797586	0.3347296143921076	T	T	T
0.0500686761783931	0.5335494355228986	0.3315600782018786	T	T	T
0.1899419985183475	0.3420092571565816	0.3476528128872058	T	T	T
0.0369096439543364	0.8740553896568317	0.3665765501229411	T	T	T
0.4217600666113325	0.0386905816044050	0.3348232138195069	T	T	T
0.3362289457538145	0.8719977312830001	0.3582626787570942	T	T	T
0.0871875352053634	0.0440939847682775	0.3355354059825066	T	T	T
0.7041156267359980	0.8718332155012052	0.3655123053862756	T	T	T
0.2583462873420483	0.2851037794141703	0.3995649389026212	T	T	T
0.2467308340655946	0.7896134725642654	0.4074862516502927	T	T	T
0.5835413636560909	0.2869886518100513	0.4045536098149657	T	T	T
0.5833984557634250	0.8057157183228060	0.4000242294773950	T	T	T
0.9151155778643649	0.3092458163569344	0.3987219911940142	T	T	T
0.9162596598542665	0.8043317595557062	0.4007347306216169	T	T	T
0.0833333129999971	0.4317300920000022	0.4673556090000019	F	F	F
0.0833333129999971	0.9317300920000022	0.4673556090000019	F	F	F
0.4166666870000029	0.4317300920000022	0.4673556090000019	F	F	F
0.4166666870000029	0.9317300920000022	0.4673556090000019	F	F	F
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0.2500000000000000	0.5682699079999978	0.5326443909999981	F	F	F
0.5833333129999971	0.0682699079999978	0.5326443909999981	F	F	F
0.5833333129999971	0.5682699079999978	0.5326443909999981	F	F	F
0.9166666870000029	0.0682699079999978	0.5326443909999981	F	F	F
0.9166666870000029	0.5682699079999978	0.5326443909999981	F	F	F
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0.4165461977189088	0.7131299261391276	0.5954381698168982	T	T	T
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0.7418842856084754	0.7144323899466621	0.6006812644504275	T	T	T
0.2949402202806071	0.1277977787667629	0.6343924377157717	T	T	T
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0.6647650061199813	0.1280699893352191	0.6420207852257602	T	T	T
0.5783248913420824	0.9611867429117278	0.6651829432454538	T	T	T
0.9633302726549720	0.1259294440957249	0.6334272287549748	T	T	T
0.8095787035260329	0.6586109538857429	0.6525156533209425	T	T	T
0.9505792224885631	0.4658961279954417	0.6685073234520439	T	T	T

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 0.9147446291914482 0.9801227333341370 0.5580609224345142 T T T
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 0.7600077341493537 0.1117818604289696 0.6248408130306737 T T T
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 0.4238089879086807 0.612125643332291 0.6251963782698732 T T T
 0.7312302282100210 0.6340262843608844 0.6305542178290042 T T T
 0.2625791126931244 0.4015270373111646 0.6391537477176843 T T T

E

1.000000000000000
8.508600234999994 0.000000000000000 0.000000000000000
0.000000000000000 10.854810714699993 0.000000000000000
0.000000000000000 0.000000000000000 30.000000000000000

Co H O

24 46 58

Selective dynamics

Direct

0.5870075998490364 0.5477212754644667 0.4002695932781212 T T T
0.2523182075927644 0.5502373378472646 0.3956049148013824 T T T
0.5805072572851265 0.0484053637051820 0.4007030769008710 T T T
0.2475154047531768 0.0479055339056059 0.3991716260719868 T T T
0.9142034849235025 0.0469487224219617 0.4000190694055440 T T T
0.9169015319952545 0.5476718604761519 0.3997220240235341 T T T
0.0833333129999971 0.1817300920000022 0.4673556090000019 F F F
0.0833333129999971 0.6817300319999973 0.4673556090000019 F F F
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0.2500000000000000 0.8182699079999978 0.5326443909999981 F F F
0.5833333129999971 0.3182699680000027 0.5326443909999981 F F F
0.5833333129999971 0.8182699079999978 0.5326443909999981 F F F
0.9166666870000029 0.3182699680000027 0.5326443909999981 F F F
0.9166666870000029 0.8182699079999978 0.5326443909999981 F F F
0.0830984680047453 0.4523281395238482 0.6002779759764658 T T T
0.0857965150764974 0.9530512775780385 0.5999809305944557 T T T
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0.0781466221567666 0.0417539502493851 0.3345858604311809 T T T
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0.7474424477787895	0.2045997241898388	0.5916142908179255	T	T	T
0.7496454157525780	0.7198017729946115	0.5942109535887025	T	T	T
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0.8594191760189729	0.1267766845026938	0.6353059868938200	T	T	T
0.0221593770029445	0.6329456523100025	0.6476254400942877	T	T	T
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0.2838336580823864	0.6258676498444141	0.6303133346468518	T	T	T
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0.5834370684612844	0.7079107491954374	0.4263259548994862	T	T	T
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0.9181646525983371	0.7075741695098333	0.4262385663529070	T	T	T
0.0826150289887234	0.0192840306344704	0.4415702560430424	T	T	T
0.0813504815431755	0.5185742536783317	0.4422011376838241	T	T	T
0.4133770571678602	0.0194531453475910	0.4417557143221164	T	T	T
0.4212340176366284	0.5179402234123178	0.4422440421684067	T	T	T
0.7485312454663439	0.0188741455856196	0.4419517712152749	T	T	T
0.7520071515767801	0.5204328826778140	0.4423066582299127	T	T	T
0.083333129999971	0.3437488080000008	0.4914442899999969	F	F	F
0.083333129999971	0.8437487779999984	0.4914442899999969	F	F	F
0.4166666870000029	0.3437488080000008	0.4914442899999969	F	F	F
0.4166666870000029	0.8437487779999984	0.4914442899999969	F	F	F
0.7500000000000000	0.3437488080000008	0.4914442899999969	F	F	F
0.7500000000000000	0.8437487779999984	0.4914442899999969	F	F	F
0.2500000000000000	0.1562512220000016	0.5085557100000031	F	F	F
0.2500000000000000	0.6562511919999992	0.5085557100000031	F	F	F
0.583333129999971	0.1562512220000016	0.5085557100000031	F	F	F
0.583333129999971	0.6562511919999992	0.5085557100000031	F	F	F
0.9166666870000029	0.1562512220000016	0.5085557100000031	F	F	F
0.9166666870000029	0.6562511919999992	0.5085557100000031	F	F	F
0.2479928484232199	0.4795671173221857	0.5576933417700872	T	T	T
0.2514687545336563	0.9811258544143804	0.5580482287847321	T	T	T
0.5787659823633718	0.4820597765876822	0.5577559578316006	T	T	T
0.5866229428321397	0.9805468546524090	0.5582442856778836	T	T	T
0.9186495184568245	0.4814257463216683	0.5577988623161758	T	T	T
0.9173849710112767	0.9807159693655297	0.5584297439569577	T	T	T
0.0818353474016628	0.2924258304901665	0.5737614336470928	T	T	T
0.0832942049336176	0.793157858744147	0.5734028421680363	T	T	T
0.4165629315387159	0.2920892508045626	0.5736740451005138	T	T	T
0.4178484416304932	0.7930389394487024	0.5730765704206380	T	T	T
0.7494991224032211	0.2846445893185163	0.5720506591442864	T	T	T
0.7503869329437891	0.7903085385358930	0.5741433061311081	T	T	T

0.0826555538580643	0.1160579949816218	0.6238672523400633	T	T	T
0.0938962128303056	0.6178276882789177	0.6229135228521552	T	T	T
0.4261445108544328	0.1175941174075247	0.6239306978346495	T	T	T
0.9196046485168832	0.9035756240846688	0.6395297327048474	T	T	T
0.7508337232321782	0.1107348387609487	0.6252895624990430	T	T	T
0.5853502418963163	0.9033107151162596	0.6392764441939502	T	T	T
0.9277419196575278	0.4113996218207990	0.6439596509058658	T	T	T
0.2526643592877618	0.9063144222555202	0.6389959154161428	T	T	T
0.4003032563911826	0.6170884752267739	0.6247076851657865	T	T	T
0.2483510340709294	0.4016157104882334	0.6389639203133258	T	T	T
0.5676688192563929	0.4199528812381547	0.6449746763289174	T	T	T

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8.508600234999994	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.854810714699993	0.0000000000000000
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Selective dynamics

Direct

0.5801534956689551	0.5503281227063778	0.3999493874448730	T	T	T
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0.5818751744068683	0.0506478449782914	0.4004780169262522	T	T	T
0.2485125196461912	0.0501054676520764	0.4002148269485969	T	T	T
0.9159416543969833	0.0509866370883631	0.4007646621032195	T	T	T
0.9159952953208137	0.5521165161694895	0.3997266818731265	T	T	T
0.0833333129999971	0.1817300920000022	0.4673556090000019	F	F	F
0.0833333129999971	0.6817300319999973	0.4673556090000019	F	F	F
0.4166666870000029	0.1817300920000022	0.4673556090000019	F	F	F
0.4166666870000029	0.6817300319999973	0.4673556090000019	F	F	F
0.7500000000000000	0.1817300920000022	0.4673556090000019	F	F	F
0.7500000000000000	0.6817300319999973	0.4673556090000019	F	F	F
0.2500000000000000	0.3182699680000027	0.5326443909999981	F	F	F
0.2500000000000000	0.8182699079999978	0.5326443909999981	F	F	F
0.5833333129999971	0.3182699680000027	0.5326443909999981	F	F	F
0.5833333129999971	0.8182699079999978	0.5326443909999981	F	F	F
0.9166666870000029	0.3182699680000027	0.5326443909999981	F	F	F
0.9166666870000029	0.8182699079999978	0.5326443909999981	F	F	F
0.0840047046791863	0.447883483305034	0.6002733181268735	T	T	T
0.0840583456030169	0.9490133629116371	0.5992353378967804	T	T	T
0.7514874803538089	0.9498945323479238	0.5997851730514030	T	T	T
0.4181248255931318	0.9493521550217087	0.5995219830737479	T	T	T
0.7475175789904192	0.4508902174545600	0.6000412188209731	T	T	T
0.4198465043310450	0.4496718772936292	0.6000506125551270	T	T	T
0.7450613698597007	0.5525627348003233	0.3346144338925792	T	T	T
0.7322570957221900	0.3848712141058943	0.3722620571115592	T	T	T
0.7459655700237966	0.0440482218388133	0.3354156033709065	T	T	T
0.0876140105666449	0.5490131307748033	0.3349187113752174	T	T	T
0.1164084454317559	0.3837732202085452	0.3713196945403373	T	T	T
0.1267638516742847	0.8761042469031040	0.3666635234016651	T	T	T
0.4134581969160058	0.0504692305640045	0.3339928650146899	T	T	T
0.4726354976777499	0.8735865096448511	0.3608790383570893	T	T	T
0.0806112363866838	0.0520998748209158	0.3344852278950687	T	T	T
0.8486135675154016	0.8668240432714359	0.3542468140802003	T	T	T
0.2499145460738624	0.2908212198173849	0.4053092353141607	T	T	T
0.2530190379981459	0.8124291458474618	0.3980737804553833	T	T	T
0.5880312659203377	0.3114241742900863	0.3998515964703877	T	T	T
0.5862543114991901	0.8118149034796270	0.3966125173471249	T	T	T
0.9174435770465775	0.3252861732580712	0.3959627560391061	T	T	T
0.9195512885075766	0.7997649684247560	0.4025840442154384	T	T	T
0.0833333129999971	0.4317300920000022	0.4673556090000019	F	F	F
0.0833333129999971	0.9317300920000022	0.4673556090000019	F	F	F

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 0.750000000000000 0.931730092000022 0.467355609000019 F F F
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 0.250000000000000 0.5682699079999978 0.5326443909999981 F F F
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 0.583333129999971 0.5682699079999978 0.5326443909999981 F F F
 0.916666687000029 0.0682699079999978 0.5326443909999981 F F F
 0.916666687000029 0.5682699079999978 0.5326443909999981 F F F
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 0.0827111264449181 0.1009487167535991 0.3618518146632936 T T T
 0.5775247886287824 0.8851206352802949 0.3740232379870578 T T T
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 0.9292494509515276 0.8835652558427158 0.3766126193513374 T T T
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 0.5824450233113044 0.7063346229642953 0.4266559748576113 T T T
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 0.9167478255740339 0.7112325668143892 0.4270357753123789 T T T
 0.0833598197396751 0.0201847267985061 0.4421123335196677 T T T
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 0.583333129999971 0.656251191999992 0.5085557100000031 F F F
 0.916666687000029 0.156251222000016 0.5085557100000031 F F F
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 0.0834926146793191 0.7919196169262819 0.5727471796602563 T T T
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 0.4175481051274017 0.7915093153603241 0.5732599633073826 T T T
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 0.7491240083845053 0.7914303630151751 0.5734388462197606 T T T
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 0.5814803589630843 0.4128204347964372 0.6354527471439788 T T T

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 0.0000000000000000 10.8548107146999993 0.0000000000000000
 0.0000000000000000 0.0000000000000000 30.0000000000000000

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Selective dynamics

Direct

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 0.2512796600224711 0.0493468295321563 0.4006439730278628 T T T
 0.9185194407923963 0.0515713911936376 0.4011281938970885 T T T
 0.9185259370277726 0.5527437786402237 0.4004405447207123 T T T
 0.083333129999971 0.181730092000022 0.4673556090000019 F F F
 0.083333129999971 0.6817300319999973 0.4673556090000019 F F F
 0.4166666870000029 0.181730092000022 0.4673556090000019 F F F
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 0.583333129999971 0.8182699079999978 0.5326443909999981 F F F
 0.9166666870000029 0.318269968000027 0.5326443909999981 F F F
 0.9166666870000029 0.8182699079999978 0.5326443909999981 F F F
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 0.0814805592076042 0.9484286088063631 0.5988718061029114 T T T
 0.7487203399775283 0.9506531704678437 0.5993560269721440 T T T
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 0.0350309508460115 0.874877709221880 0.3660857328972938 T T T

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0.3208792354195790	0.8686687892417855	0.3550701252846039	T	T	T
0.0861029506737521	0.0515850830613384	0.3353082560421119	T	T	T
0.7044567018337616	0.8746848852369001	0.3638229615332947	T	T	T
0.2629396917873181	0.3303996952968993	0.3918801989808654	T	T	T
0.2480399997300091	0.7959113014919451	0.4039240256091458	T	T	T
0.5786759502131545	0.3301616292904659	0.3976137749329121	T	T	T
0.5834216684368160	0.8102584240856666	0.3976031127445677	T	T	T
0.9138920266163819	0.3226646038434752	0.3946287450578517	T	T	T
0.9142752565934402	0.8104284250836699	0.3999637288426733	T	T	T
0.0833333129999971	0.4317300920000022	0.4673556090000019	F	F	F
0.0833333129999971	0.9317300920000022	0.4673556090000019	F	F	F
0.4166666870000029	0.4317300920000022	0.4673556090000019	F	F	F
0.4166666870000029	0.9317300920000022	0.4673556090000019	F	F	F
0.7500000000000000	0.4317300920000022	0.4673556090000019	F	F	F
0.7500000000000000	0.9317300920000022	0.4673556090000019	F	F	F
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0.2500000000000000	0.5682699079999978	0.5326443909999981	F	F	F
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0.5833333129999971	0.5682699079999978	0.5326443909999981	F	F	F
0.9166666870000029	0.0682699079999978	0.5326443909999981	F	F	F
0.9166666870000029	0.5682699079999978	0.5326443909999981	F	F	F
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0.4165783315631844	0.1897415759143335	0.6023968872554325	T	T	T
0.4213240497868451	0.6698383707095406	0.6023862250670883	T	T	T
0.7519600002699911	0.2040886985080545	0.5960759743908541	T	T	T
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0.2955432981662383	0.1253151147630998	0.6361770384667050	T	T	T
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0.4189663459224738	0.0942153954631577	0.3616922381829298	T	T	T
0.2384214160403575	0.8845671911036829	0.3769728198944194	T	T	T
0.0854411576688630	0.1011227472547914	0.3625338029837220	T	T	T
0.5955522130875310	0.8850728763401722	0.3746693510443005	T	T	T
0.9397610826124267	0.3933438196548081	0.3734700216241904	T	T	T
0.9232968133930362	0.8852343910592034	0.3758143100540796	T	T	T
0.2560447790760095	0.2060523579776789	0.4278131211143081	T	T	T
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0.5791070026691291	0.2063559638431063	0.4275909856709614	T	T	T
0.5821096496757348	0.7075726516644848	0.4263236727263677	T	T	T
0.9156891797687023	0.2087713763928816	0.4273077355615025	T	T	T
0.9145374617226324	0.7103786060574803	0.4273698216193972	T	T	T
0.0847841324424841	0.0201856387741320	0.4423611834745287	T	T	T
0.0837175479998015	0.5212938316367581	0.4420231951970452	T	T	T
0.4182313227754582	0.0189171012592471	0.4424670422047589	T	T	T
0.4164732727607908	0.5191868236384055	0.4420682425346491	T	T	T
0.7512880971788648	0.0191519341138457	0.4424926276183273	T	T	T
0.7499623367740811	0.5198628263072813	0.4418915086804887	T	T	T
0.0833333129999971	0.3437488080000008	0.4914442899999969	F	F	F

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Selective dynamics

Direct

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 0.9166666870000029 0.8182699079999978 0.5326443909999981 F F F

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0.4182698191860916	0.4496769603420114	0.5999710718892350	T	T	T
0.4759394544156290	0.3759459557712453	0.3607264885342368	T	T	T
0.8280441598064836	0.3754797302197386	0.3587338915757782	T	T	T
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0.2464411956246623	0.9537492832306412	0.6655299282702133	T	T	T
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0.7516859071626770	0.0969284663079745	0.3613840794513618	T	T	T
0.0816051228295135	0.6021413442557209	0.3614787571472115	T	T	T
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Selective dynamics

Direct

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 0.5833333129999971 0.8182699079999978 0.5326443909999981 F F F
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 0.0126768825249695 0.6314507847493160 0.6454269512479652 T T T
 0.9008148488391379 0.4606799312546668 0.6636186115066162 T T T
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 0.2495862639688387 0.4502237427705666 0.6654322713311274 T T T

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0.2551316209318130	0.3918965379410876	0.3797739479495558	T	T	T
0.5982912158543149	0.3873430300882216	0.3741108272877799	T	T	T
0.7475792882182684	0.0950959964242753	0.3613002757138328	T	T	T
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0.2406169739627545	0.8821666339363924	0.3757544504209632	T	T	T
0.0808618680994481	0.0952823455143743	0.3612393646211945	T	T	T
0.5805949304576954	0.8822711999536438	0.3758114546255713	T	T	T
0.9068547578066191	0.3851368918530006	0.3770385129212854	T	T	T
0.9190658544756859	0.8836989049103977	0.3766230612417690	T	T	T
0.2493899149040857	0.2055093497623463	0.4262497519527205	T	T	T
0.2506885095030900	0.7098980107283411	0.4271631225352648	T	T	T
0.5817272143247352	0.2073200626549163	0.4268579180203698	T	T	T
0.5836701307551823	0.7092734096410642	0.4269798068644769	T	T	T
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0.9148091585111611	0.4796694102017720	0.5583522791193436	T	T	T
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0.0833515626377947	0.7917474441889916	0.5735081539962354	T	T	T
0.4163298692448179	0.2907265903589358	0.5730201931355160	T	T	T
0.4182727856752649	0.7926799373450839	0.5731420819796300	T	T	T
0.7493114904969099	0.2901019892716588	0.5728368774647351	T	T	T
0.7506100850959141	0.7944906502376539	0.5737502480472793	T	T	T
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0.7593830260372455	0.1178333660636077	0.6242455495790369	T	T	T
0.5864231718914678	0.9061837751873946	0.6386848964850079	T	T	T
0.9115399495445796	0.4011818440746535	0.6391106128793578	T	T	T
0.2524207117817316	0.9049040035757246	0.6386997242861673	T	T	T
0.4017087841456853	0.6126569699117784	0.6258891727122202	T	T	T
0.7448683790681869	0.6081034620589124	0.6202260520504442	T	T	T
0.2493612744792991	0.3984926704861890	0.6387795739694538	T	T	T
0.5855402509245385	0.4064499037565774	0.6357325468460758	T	T	T
0.7899381904595449	0.6212999775286713	0.6663687406791711	T	T	T

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0.000000000000000 0.000000000000000 30.000000000000000

Co H O
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Selective dynamics

Direct

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0.0833333129999971 0.6817300319999973 0.4673556090000019 F F F
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0.2500000000000000 0.8182699079999978 0.5326443909999981 F F F
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0.5833333129999971 0.8182699079999978 0.5326443909999981 F F F
0.9166666870000029 0.3182699680000027 0.5326443909999981 F F F
0.9166666870000029 0.8182699079999978 0.5326443909999981 F F F
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0.0853062623073464 0.9502513243469503 0.5992732607757608 T T T
0.4167941954913504 0.4522261356443690 0.5993055603991526 T T T
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0.7478866521607626	0.7169399686220255	0.5954450423478713	T	T	T
0.1861265844077052	0.1293314484467585	0.6397786739303754	T	T	T
0.9222333156235544	0.9566296369842262	0.6651117867297819	T	T	T
0.5363799692563987	0.1252736195631179	0.6350745712263880	T	T	T
0.5846144807314456	0.9514026021660599	0.6654628515034198	T	T	T
0.8426491977918485	0.1312751788047191	0.6401341445264495	T	T	T
0.9550678253994347	0.6208571380498629	0.6312779106477704	T	T	T
0.9168070652080043	0.4460932907343104	0.6653568609860088	T	T	T
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0.2529691696411555	0.4705832589825584	0.6613278043087567	T	T	T
0.5895387114692769	0.4613065189115018	0.6626295378457697	T	T	T
0.5620476691459247	0.6317897542510963	0.6511633297559083	T	T	T
0.3263610679617701	0.3749109607907639	0.3347212031128826	T	T	T
0.4185449520447138	0.6005953190755461	0.3614297875936054	T	T	T
0.7486878277010403	0.5946602697253028	0.3612993612100602	T	T	T
0.2357559350164741	0.3920962184586914	0.3754041360269239	T	T	T
0.5803763877309766	0.3962627134455646	0.3767459191125833	T	T	T
0.7481565818334246	0.0976453621650203	0.3616885794455740	T	T	T
0.0828119862703723	0.6042803408934442	0.3616658548256336	T	T	T
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0.2542815157867707	0.8834850832577997	0.3766922859224552	T	T	T
0.0818015115662036	0.0957910876707114	0.3613340241078983	T	T	T
0.5745308005846377	0.8848186377827945	0.3746902057801403	T	T	T
0.9290135389574469	0.3878188391932392	0.3748252233757487	T	T	T
0.9145820249210362	0.8834048843988027	0.3754062208307315	T	T	T
0.2503001596102650	0.2078958906184149	0.4260917430163147	T	T	T
0.2508513511019332	0.7110058188125832	0.4271224196893902	T	T	T
0.5833768527351786	0.2084592609296300	0.4270886737502700	T	T	T
0.5849598763026214	0.7071062073056653	0.4262205183903867	T	T	T
0.9158381035530213	0.2079784670949324	0.4268152800512497	T	T	T
0.9163291126636274	0.7090104214620645	0.4269335327676822	T	T	T
0.0826833644961439	0.0194153359944625	0.4420340284037756	T	T	T
0.0844066130524015	0.5201067596225938	0.4416783505566546	T	T	T
0.4149387332278279	0.0197077536551863	0.4421593112848893	T	T	T
0.4168770653558846	0.5200908559275840	0.4415770161300653	T	T	T
0.7486349579115915	0.0194272467910465	0.4422033661630998	T	T	T
0.7498259121594995	0.5191396546933602	0.4418447061151096	T	T	T
0.0833333129999971	0.3437488080000008	0.4914442899999969	F	F	F
0.0833333129999971	0.8437487779999984	0.4914442899999969	F	F	F
0.4166666870000029	0.3437488080000008	0.4914442899999969	F	F	F
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0.7500000000000000	0.3437488080000008	0.4914442899999969	F	F	F
0.7500000000000000	0.8437487779999984	0.4914442899999969	F	F	F
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0.9166666870000029	0.1562512220000016	0.5085557100000031	F	F	F
0.9166666870000029	0.6562511919999992	0.5085557100000031	F	F	F
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0.2513650420884077	0.9805727532089543	0.5577966338368999	T	T	T
0.5831229346441166	0.4799091440724168	0.5584229838699335	T	T	T
0.5850612667721715	0.9802922463448142	0.5578406887151111	T	T	T
0.9155933869475980	0.4798932403774059	0.5583216494433449	T	T	T
0.9173166355038566	0.9805846640055379	0.5579659715962246	T	T	T
0.0836708873363717	0.2909895785379358	0.5730664672323170	T	T	T
0.0841618964469777	0.7920215329050676	0.5731847199487494	T	T	T
0.4150401236973800	0.2928937926943352	0.5737794816096133	T	T	T

0.4166231472648212 0.7915407390703708 0.5729113262497302 T T T
 0.7491486488980655 0.2889941811874172 0.5728775803106104 T T T
 0.7496998403897349 0.7921041093815849 0.5739082569836854 T T T
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 0.0000000000000000 0.0000000000000000 30.0000000000000000

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Selective dynamics

Direct

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 0.0833333129999971 0.1817300920000022 0.4673556090000019 F F F
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 0.2500000000000000 0.8182699079999978 0.5326443909999981 F F F
 0.5833333129999971 0.3182699680000027 0.5326443909999981 F F F
 0.5833333129999971 0.8182699079999978 0.5326443909999981 F F F
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Selective dynamics

Direct

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Selective dynamics

Direct

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0.5833333129999971	0.8182699079999978	0.5326443909999981	F	F	F
0.9166666870000029	0.3182699680000027	0.5326443909999981	F	F	F
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Selective dynamics

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Selective dynamics

Direct

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Selective dynamics

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Selective dynamics

Direct

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Selective dynamics

Direct

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0.9187201178646917	0.0480956678342138	0.4007321831068122	T	T	T
0.9158963112654565	0.5458364859791064	0.4004112880013213	T	T	T
0.0833333129999971	0.1817300920000022	0.4673556090000019	F	F	F
0.0833333129999971	0.6817300319999973	0.4673556090000019	F	F	F
0.4166666870000029	0.1817300920000022	0.4673556090000019	F	F	F
0.4166666870000029	0.6817300319999973	0.4673556090000019	F	F	F
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0.2500000000000000	0.3182699680000027	0.5326443909999981	F	F	F
0.2500000000000000	0.8182699079999978	0.5326443909999981	F	F	F
0.5833333129999971	0.3182699680000027	0.5326443909999981	F	F	F
0.5833333129999971	0.8182699079999978	0.5326443909999981	F	F	F
0.9166666870000029	0.3182699680000027	0.5326443909999981	F	F	F
0.9166666870000029	0.8182699079999978	0.5326443909999981	F	F	F
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0.7555721328679808	0.0346566356720946	0.3362571056395091	T	T	T
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 0.5877243339083499 0.4142371747190963 0.6417839743244012 T T T

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Co H O
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Selective dynamics

Direct

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0.5559774863854869	0.6262034415128497	0.6345079009173133	T	T	T
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0.7511132155757849	0.0200897711820005	0.4420769232891999	T	T	T
0.7548306044619437	0.5198389650187849	0.4444392553615515	T	T	T
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0.0833333129999971	0.8437487779999984	0.4914442899999969	F	F	F
0.4166666870000029	0.3437488080000008	0.4914442899999969	F	F	F
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0.2500000000000000	0.6562511919999992	0.5085557100000031	F	F	F
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0.4173878150133632	0.2912395165057902	0.5736371373117493	T	T	T
0.4166126005340374	0.7906366355835885	0.5732662106325179	T	T	T
0.7503698529584995	0.2925298605463595	0.5738226672817177	T	T	T
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0.4107213387199380	0.1159178848030962	0.6236816034269310	T	T	T

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Co H O

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Selective dynamics

Direct

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 0.5833333129999971 0.8182699079999978 0.5326443909999981 F F F
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0.5833333129999971	0.5682699079999978	0.5326443909999981	F F F
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0.0833333129999971	0.8437487779999984	0.491444289999969	F F F
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0.2500000000000000	0.6562511919999992	0.5085557100000031	F F F
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0.5833333129999971	0.6562511919999992	0.5085557100000031	F F F
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0.916666687000029	0.6562511919999992	0.5085557100000031	F F F
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0.5794392464401784	0.4820453839069968	0.5597643465097354	T T T
0.5853086917334057	0.9803859661770519	0.5580840701882070	T T T
0.9262639973499899	0.4800191895211458	0.5563967050728565	T T T

0.9167862150036307	0.9797442645790478	0.5579751761548603	T	T	T
0.0831789158744803	0.2886898690441612	0.5729708694637276	T	T	T
0.0834370864499539	0.7916402406570382	0.5727886110598706	T	T	T
0.4175794866596534	0.2928564646661748	0.5738746728310635	T	T	T
0.4178576902577290	0.7917618725986808	0.5733124069101727	T	T	T
0.7467961741119722	0.2941373287424464	0.5740391608851635	T	T	T
0.7488776090885120	0.7910115128356232	0.5738067581000568	T	T	T
0.0726159374949751	0.1156231751361606	0.6233899017581278	T	T	T
0.0858099024698850	0.6050634344426499	0.6271858460425482	T	T	T
0.4215796936508234	0.1159599006910029	0.6253495645430170	T	T	T
0.9176061845150868	0.8996699251186692	0.6384712837910982	T	T	T
0.7617256603861761	0.1152545906769158	0.6246672242851137	T	T	T
0.5853471140550603	0.9034475145565242	0.6388353228682783	T	T	T
0.9148954711597667	0.3995642527248869	0.6389724583323653	T	T	T
0.2516798787409814	0.9031576400057605	0.6385701972407662	T	T	T
0.3912547685719830	0.6121522358523075	0.6244764635686284	T	T	T
0.7607958974490303	0.6088628813116181	0.6237504497427726	T	T	T
0.2510907545080652	0.3982789422858378	0.6392690613948832	T	T	T

5

1.000000000000000			
8.508600234999994	0.000000000000000	0.000000000000000	
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0.000000000000000	0.000000000000000	30.000000000000000	

Co H O

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Selective dynamics

Direct

0.5843216568011212	0.5517151340699648	0.4002310812075721	T	T	T
0.2500858638969380	0.5524805900345888	0.3994775498573146	T	T	T
0.5850872587867169	0.0491193573516488	0.4008217992896692	T	T	T
0.2519229282146084	0.0446801506345315	0.3998817733331391	T	T	T
0.9179699672900065	0.0470716566243333	0.4002047668571450	T	T	T
0.9167957817601682	0.5504397155496898	0.4000579711634133	T	T	T
0.0833333129999971	0.181730092000022	0.4673556090000019	F	F	F
0.0833333129999971	0.6817300319999973	0.4673556090000019	F	F	F
0.416666687000029	0.181730092000022	0.4673556090000019	F	F	F
0.416666687000029	0.6817300319999973	0.4673556090000019	F	F	F
0.750000000000000	0.181730092000022	0.4673556090000019	F	F	F
0.750000000000000	0.6817300319999973	0.4673556090000019	F	F	F
0.250000000000000	0.3182699680000027	0.5326443909999981	F	F	F
0.250000000000000	0.8182699079999978	0.5326443909999981	F	F	F
0.5833333129999971	0.3182699680000027	0.5326443909999981	F	F	F
0.5833333129999971	0.8182699079999978	0.5326443909999981	F	F	F
0.916666687000029	0.3182699680000027	0.5326443909999981	F	F	F
0.916666687000029	0.8182699079999978	0.5326443909999981	F	F	F
0.0832042182398319	0.4495602844503173	0.5999420288365868	T	T	T
0.0820300327099936	0.9529283433756668	0.5997952331428550	T	T	T
0.7480770717853914	0.9553198493654684	0.6001182266668609	T	T	T
0.4149127412132830	0.9508806426483511	0.5991782007103379	T	T	T
0.7499141361030619	0.4475194099654113	0.6005224501426855	T	T	T
0.4156783431988715	0.4482848659300283	0.5997689187924279	T	T	T
0.3562007659744962	0.4920864904013455	0.3174069779739327	T	T	T
0.7481229141444041	0.5519672424823521	0.3346222656636524	T	T	T
0.7116012437854771	0.3787479443845696	0.3692275443606093	T	T	T
0.7521985367969081	0.0457311256118492	0.3347374738249433	T	T	T
0.0882610140924124	0.5484983644046343	0.3344744522719899	T	T	T
0.9748637641923187	0.3690056363744383	0.3521183227957639	T	T	T
0.0149597335365700	0.8687854516905427	0.3611137257029914	T	T	T
0.4222478960762842	0.0430004053634813	0.3346098646125067	T	T	T
0.3585612738690954	0.8690498643107145	0.3629108152429784	T	T	T
0.0863201424772215	0.0430446259477213	0.3340615134563008	T	T	T
0.6952860161245376	0.8709648843431655	0.3637773165540541	T	T	T

0.2500935951586784 0.2763251242746109 0.4045986331311023 T T T
 0.2480964389387521 0.8012435274663162 0.4017513525029073 T T T
 0.5767101788278004 0.3161063632229090 0.3971163311560210 T T T
 0.5817229419014504 0.8059425853225128 0.4003636576240813 T T T
 0.9155736064870437 0.2902565465316003 0.4039151755474078 T T T
 0.9141538919223010 0.7977501053304679 0.4026613551961075 T T T
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 0.0833333129999971 0.9317300920000022 0.4673556090000019 F F F
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 0.4166666870000029 0.9317300920000022 0.4673556090000019 F F F
 0.7500000000000000 0.4317300920000022 0.4673556090000019 F F F
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 0.2500000000000000 0.5682699079999978 0.5326443909999981 F F F
 0.5833333129999971 0.0682699079999978 0.5326443909999981 F F F
 0.5833333129999971 0.5682699079999978 0.5326443909999981 F F F
 0.9166666870000029 0.0682699079999978 0.5326443909999981 F F F
 0.9166666870000029 0.5682699079999978 0.5326443909999981 F F F
 0.0858461080776989 0.2022498946695320 0.5973386448038924 T T T
 0.0844263935129563 0.7097434534683997 0.5960848244525920 T T T
 0.4182770580985496 0.1940574146774871 0.5996363423759189 T T T
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 0.4190813621250736 0.6094499656735358 0.3627904381614377 T T T
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 0.5951314567786713 0.3882453118483229 0.3746179306653401 T T T
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 0.5820199752810008 0.2076374892040546 0.4269300303693872 T T T
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 0.9165019371221077 0.7089784315364963 0.4267764150238041 T T T
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 0.0833333129999971 0.8437487779999984 0.4914442899999969 F F F

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 0.2500000000000000 0.6562511919999992 0.508555710000031 F F F
 0.583333312999971 0.156251222000016 0.508555710000031 F F F
 0.583333312999971 0.6562511919999992 0.508555710000031 F F F
 0.916666687000029 0.156251222000016 0.508555710000031 F F F
 0.916666687000029 0.6562511919999992 0.508555710000031 F F F
 0.2491795761008705 0.4798358896114993 0.5580458359763903 T T T
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 0.5838593546382213 0.4801981144121624 0.5586491616957725 T T T
 0.5826026747682975 0.9811392264807403 0.5579095248259245 T T T
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 0.9153920461163496 0.9812596891058035 0.5580216283788479 T T T
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 0.0825423519305814 0.7923493867315026 0.5736342205975662 T T T
 0.4173943524039424 0.2905118274068343 0.5728985219197842 T T T
 0.4179800247189991 0.7923625107959454 0.5730699696306129 T T T
 0.7507705990064687 0.2897502304263857 0.5729572577548188 T T T
 0.7501351895915512 0.7952128064116953 0.5739378287606502 T T T
 0.0852105939649933 0.1176116568038325 0.6233507246831616 T T T
 0.0956200680039647 0.6150244864424484 0.6228936330401319 T T T
 0.4118419264467895 0.1171263980047327 0.6241443090459282 T T T
 0.9149661544439562 0.9070810663296377 0.6388213588750727 T T T
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 0.5820879597277286 0.9061243992529744 0.6385357510410455 T T T
 0.9167607831143182 0.3994668207547251 0.6388500794634926 T T T
 0.2482781167429275 0.9033109412577802 0.6383972319219160 T T T
 0.4048685432213288 0.6117546881516769 0.6253820693346600 T T T
 0.7503612941499364 0.6042824710323429 0.6233771783947498 T T T
 0.2494574063024503 0.3977320452240897 0.6383558710025580 T T T
 0.5809186378749266 0.3905500343264642 0.6372095618385623 T T T
 0.7622932718858784 0.6165121239146342 0.6676048161757856 T T T
 0.5773359885886786 0.4302440374133594 0.6832463796043918 T T T

5'

1.0000000000000000
 8.508600234999994 0.0000000000000000 0.0000000000000000
 0.0000000000000000 10.854810714699993 0.0000000000000000
 0.0000000000000000 0.0000000000000000 30.0000000000000000

Co H O

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Selective dynamics

Direct

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 0.2520073537516794 0.5535272477311395 0.3995532851590156 T T T
 0.5813284699387467 0.0446187296029379 0.3998264331020991 T T T
 0.2476694591893747 0.0451576266988454 0.3999131304558716 T T T
 0.9143954677842814 0.0484901394904398 0.4007823937931789 T T T
 0.9186968427890676 0.5517405913013107 0.4005135566587512 T T T
 0.083333312999971 0.181730092000022 0.4673556090000019 F F F
 0.083333312999971 0.681730031999973 0.4673556090000019 F F F
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 0.2500000000000000 0.818269907999978 0.532644390999981 F F F
 0.583333312999971 0.3182699680000027 0.532644390999981 F F F
 0.583333312999971 0.818269907999978 0.532644390999981 F F F
 0.916666687000029 0.3182699680000027 0.532644390999981 F F F

0.916666687000029	0.8182699079999978	0.5326443909999981	F	F	F
0.0813031572109253	0.4482594086986893	0.5994864433412488	T	T	T
0.0856045322157186	0.9515098605095602	0.5992176062068282	T	T	T
0.7523305408106324	0.9548423733011546	0.6000868695441284	T	T	T
0.4186715300612533	0.9553812703970621	0.6001735668979009	T	T	T
0.7479926462483206	0.4464727522688534	0.6004467148409844	T	T	T
0.4149918997738453	0.4477075917438924	0.6001872705160167	T	T	T
0.3878679674637624	0.3611439315191021	0.3271849111594491	T	T	T
0.4201183943923397	0.5509364180525509	0.3350894610094599	T	T	T
0.7491727303572517	0.5348817798311032	0.3370545276511976	T	T	T
0.7478419642349650	0.0450755063478283	0.3343959393254536	T	T	T
0.0852231646417394	0.5553677330506090	0.3341865408013831	T	T	T
0.0482988705070824	0.3796210594374472	0.3715676798113208	T	T	T
0.1442395286669012	0.8683025988209749	0.3621557529102262	T	T	T
0.4123190249270081	0.0430616021913366	0.3338763716398745	T	T	T
0.4825635217320041	0.8677164755986198	0.3615390456097103	T	T	T
0.0773046301963234	0.0446007819238048	0.3345439322203703	T	T	T
0.8044213761508416	0.8711532025346642	0.3636372506773924	T	T	T
0.2543985194538863	0.2786682754386263	0.4035168688133552	T	T	T
0.2518498860689320	0.8005791434398120	0.4021314909531313	T	T	T
0.5825705545217872	0.2772823255691037	0.4046080657987545	T	T	T
0.5859394328867111	0.7964865119515423	0.4033587214400143	T	T	T
0.9100054929985149	0.3152277238609003	0.3973835746355192	T	T	T
0.9182599448992335	0.8060767272566309	0.4000782962874254	T	T	T
0.0833333129999971	0.431730092000022	0.4673556090000019	F	F	F
0.0833333129999971	0.931730092000022	0.4673556090000019	F	F	F
0.416666687000029	0.431730092000022	0.4673556090000019	F	F	F
0.416666687000029	0.931730092000022	0.4673556090000019	F	F	F
0.7500000000000000	0.431730092000022	0.4673556090000019	F	F	F
0.7500000000000000	0.931730092000022	0.4673556090000019	F	F	F
0.2500000000000000	0.0682699079999978	0.5326443909999981	F	F	F
0.2500000000000000	0.5682699079999978	0.5326443909999981	F	F	F
0.5833333129999971	0.0682699079999978	0.5326443909999981	F	F	F
0.5833333129999971	0.5682699079999978	0.5326443909999981	F	F	F
0.916666687000029	0.0682699079999978	0.5326443909999981	F	F	F
0.916666687000029	0.5682699079999978	0.5326443909999981	F	F	F
0.0817400551007665	0.1939232727433691	0.5999217037125675	T	T	T
0.0899945070014851	0.6847722761390997	0.6026164253644808	T	T	T
0.4140605671132889	0.2035134880484506	0.5966412785599857	T	T	T
0.4174294454782128	0.7227176744309034	0.5953919342012455	T	T	T
0.7481501139310680	0.1994208565601880	0.5978685090468687	T	T	T
0.7456014805461137	0.7213317245613737	0.5964831311866448	T	T	T
0.1955786238491584	0.1288467974653358	0.6363627493226076	T	T	T
0.9226953698036766	0.9553992180761952	0.6654560677796297	T	T	T
0.5174364782679959	0.1322835244013802	0.6384609543902897	T	T	T
0.5876809750729919	0.9569383978086634	0.6661236283601255	T	T	T
0.8557604713330988	0.1316974011790251	0.6378442470897738	T	T	T
0.9517011294929176	0.6203789405625528	0.6284323201886792	T	T	T
0.9147768353582606	0.4446322669493981	0.6658134591986169	T	T	T
0.2521580357650350	0.9549244936521717	0.6656040606745464	T	T	T
0.2508272696427554	0.4651182201688897	0.6629454723488024	T	T	T
0.5798816056076603	0.4490635819474491	0.6649105389905401	T	T	T
0.6121320325362376	0.6388560684808979	0.6728150888405509	T	T	T
0.5782440492902836	0.3861760442380273	0.3325337623870439	T	T	T
0.2719954524200858	0.3810481646869022	0.3284775505273103	T	T	T
0.4192562750938080	0.6041876057168807	0.3615198630819094	T	T	T
0.7520441438560752	0.5968394637929677	0.3609121291232213	T	T	T
0.2441673678002019	0.3911989152603041	0.3760553426859659	T	T	T
0.5813635411165876	0.3954899722948326	0.3771586897577208	T	T	T
0.7476006976258134	0.0945532174044459	0.3616212464362150	T	T	T
0.0844627615107356	0.6040560073421517	0.3616193734816093	T	T	T
0.4146400889411197	0.0921838184750143	0.3611738691901252	T	T	T
0.2473903298656523	0.8817685526176362	0.3762017215480284	T	T	T

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 0.9314704434097791 0.3879214776792281 0.3751567501602864 T T T
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Selective dynamics

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Selective dynamics

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Co H O

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Selective dynamics

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Co H O

24 44 64

Selective dynamics

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0.583333312999971	0.818269907999978	0.532644390999981	F F F
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0.083333312999971	0.931730092000022	0.4673556090000019	F F F
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 Selective dynamics
 Direct

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0.9185983358692127	0.5500330778975808	0.4003915518930157	T	T	T
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0.4166666870000029	0.1817300920000022	0.4673556090000019	F	F	F
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0.5833333129999971	0.8182699079999978	0.5326443909999981	F	F	F
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0.4188146664817296	0.9556218715277964	0.6001542351486577	T	T	T
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0.1443780022181116	0.8681785795641090	0.3620467454419938	T	T	T
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Selective dynamics

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Selective dynamics

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