

Supporting Information for

Interactions of Water with the (111) and (100) Surfaces of Ceria

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- 1. Structural Parameters for Monomeric Adsorption Structures**
- 2. Top View on Water Oligomers on $p(4\times4)$ Surface Cells**
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- 5. Optimized Structures (Alphabetical Order)**

1. Structural Parameters for Monomeric Adsorption Structures

Table S1 compiles structural parameters for monomeric water adsorption structures discussed in section 4.1. This includes Ce–O distances for all Ce ions coordinated by the water O atom. For H bonds, the distance between the H-bonded O atoms is given along with the O–H··O angle.

Table S1. Adsorption energies E_a in kJ/mol as well as structural parameters in pm for monomeric water adsorption structures obtained with PBE+U. Selected structures have been optimized using dispersion corrections. This is indicated by an asterisk.

	E_a	$r_{\text{Ce-O}}$	$r_{\text{O-O}}$	$\angle \text{O-H}\cdots\text{O}$
P₁₁₁1m	-51	259	259	143°
P₁₁₁1d	-57	222	256	152°
P₁₁₁1d*	-70	222	256	152°

2. Top View on Water Oligomers on p(4×4) Surface Cells

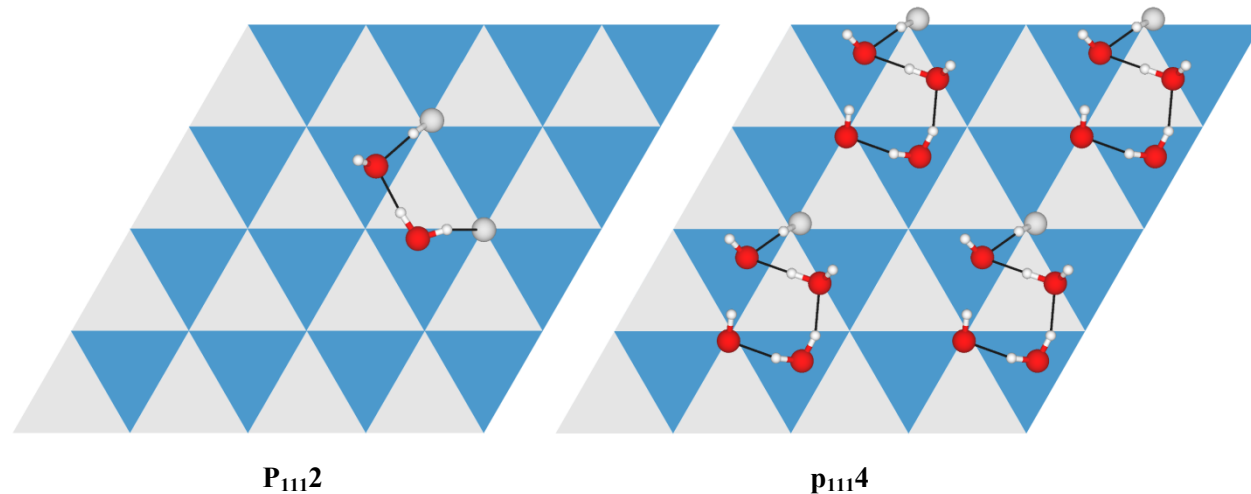


Figure S1. Top views on water oligomers **P₁₁₁2** and **p₁₁₁4** at the pristine ceria (111) surface. H bonds are indicated by black lines. Ce ions are represented by blue polygons; each vertex represents a surface O ion (surface ions participating in H bonds are shown explicitly).

3. Top View on Molecularly Adsorbed Water on a $p(1\times 1)$ Surface Cell

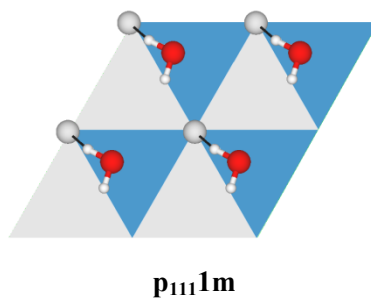


Figure S2. Top views on a water monomer at a $p(1\times 1)$ surface cell of ceria (111). H bonds are indicated by black lines. Ce ions are represented by blue polygons; each vertex represents a surface O ion (surface ions participating in H bonds are shown explicitly).

4. Table of Total Energies

The following table compiles the total energies of all structures discussed in this work.

Table S3. Total energies obtained using PBE+U.

	PBE+U [eV]		PBE+U [eV]
H ₂ O	-14.240	P₁₀₀23	-1304.301
P₁₀₀0	-956.945	P₁₀₀24	-1319.088
P₁₀₀1d	-972.838	P₁₁₁0	-1162.215
P₁₀₀1m	-972.126	P₁₁₁1d	-1177.046
P₁₀₀2	-987.133	P₁₁₁1m	-1176.983
P₁₀₀2d	-988.495	P₁₁₁2	-1192.051
P₁₀₀7	-1066.289	P₁₁₁2d	-1191.788
P₁₀₀8d	-1081.667	p₁₁₁4	-349.696
P₁₀₀15	-1185.771	p₁₁₁6	-379.463
P₁₀₀16	-1200.844	p₁₁₁7	-394.224

6. Optimized Structures (Alphabetical Order)

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1.0

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Ce O

40 80

Selective dynamics

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Selective dynamics

Direct

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0.6882554740556870	0.9383641431937804	0.2241865425215579	T	T	T
0.9379370163403422	0.1888452855073481	0.2239317460318446	T	T	T
0.9383518167428022	0.4389984738993036	0.2246360561964451	T	T	T
0.9379476083202007	0.6887287413399434	0.2242496726720731	T	T	T
0.9382944251119341	0.9387068050616278	0.2244230040754260	T	T	T
0.1885738105400563	0.1897460964034394	0.3290396095511383	T	T	T
0.1868257933417397	0.4397724340662847	0.3298899199837066	T	T	T
0.1886740675242677	0.6895727071589093	0.3297725387535806	T	T	T
0.1867298621097717	0.9395522186365781	0.3296093663400939	T	T	T
0.4385049793985445	0.1878694354317716	0.3288159065173559	T	T	T
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0.4386975208487058	0.6877948188985599	0.3297150525076304	T	T	T
0.4365137411526661	0.9377218319794451	0.3295869592100829	T	T	T
0.6885759774608076	0.1897426637569737	0.3290298662350182	T	T	T

0.6868209653623580	0.4397617841674304	0.3298837644813517	T	T	T
0.6886764498271845	0.6895690491861188	0.3297708090890339	T	T	T
0.6867309702544588	0.9395514435333112	0.3296085188035462	T	T	T
0.9385110303102380	0.1878593037116545	0.3288289489675833	T	T	T
0.9370427841454330	0.4379035848778230	0.3300806177777957	T	T	T
0.9387111510550099	0.6877868626181609	0.3297204316702178	T	T	T
0.9365211965086573	0.9377176615480423	0.3296095420439613	T	T	T
0.1820964359334596	0.1838542412376398	0.4335477870763143	T	T	T
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0.1918881580012197	0.9347906013221348	0.4354427511375789	T	T	T
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0.4331961188141804	0.6937476217539214	0.4349649373908946	T	T	T
0.4421495694822397	0.9425649466245503	0.4351345504723412	T	T	T
0.6821080540929785	0.1838241801791156	0.4335336939154217	T	T	T
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0.6834417964346642	0.6841084849753898	0.4348146210388677	T	T	T
0.6918909933581574	0.9347822186058536	0.4354375979240785	T	T	T
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0.7328293214245107	0.7279825918239737	0.5355747383669041	T	T	T
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0.9035855613787547	0.9009827165093753	0.5363081732866988	T	T	T
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0.4829777282676062	0.1482504509560130	0.5320388288634206	T	T	T
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0.4445056799193523	0.9306639582300775	0.6387540087329029	T	T	T
0.9441283760537900	0.6811516759178815	0.6360363170243772	T	T	T

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0.7976891502257075	0.2917444511934093	0.5416573725843392	T	T	T
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0.1717233368260196	0.9612548660351123	0.5743549756379807	T	T	T
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0.0466903616111765	0.0851448084234221	0.5398976535078006	T	T	T
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0.7962637876395391	0.7941251404344030	0.5392962155106886	T	T	T
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0.9218482857253889	0.9196183652099990	0.5732376611055159	T	T	T
0.1994314450804495	0.6934984327615439	0.5961255087929160	T	T	T
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0.1969198575015270	0.8452658110601590	0.6422343605455012	T	T	T
0.2796883340012570	0.9610459460592864	0.6464637930116126	T	T	T
0.6102808032397817	0.6655332066254189	0.6437281495167895	T	T	T
0.6993669751118574	0.6931930665300925	0.5961101627635159	T	T	T
0.6964693341865953	0.8448850027991597	0.6421348532971436	T	T	T
0.7801492874111418	0.9598424334425033	0.6463561994425859	T	T	T
0.3587239036003282	0.6661525688802712	0.6451392936107396	T	T	T
0.4493676224836776	0.6736588137554094	0.5973578722643396	T	T	T
0.5275126957423240	0.9600387769901317	0.6460221843169549	T	T	T
0.4485521387562628	0.8401549393120291	0.6429952724160870	T	T	T
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0.0274347090902438	0.9580922572599775	0.6462736138515268	T	T	T
0.9486567899164413	0.8379600326900345	0.6431694237623162	T	T	T

P_100_1d

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10.9799995421999999 0.0000000000000000 0.0000000000000000

0.0000000000000000 10.9799995421999999 0.0000000000000000

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Selective dynamics

Direct

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0.3137422377098275	0.5636569945970796	0.3273310843958975	T	T	T
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0.8136276092420291	0.0629076197644530	0.3273223216747851	T	T	T
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0.0642171170542412	0.5640539003255245	0.4518798206037227	T	T	T
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0.9387522795774856	0.1887522792723857	0.1408004422727274	F	F	F
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0.4387960745316066	0.1886013233410204	0.2668573495298751	T	T	T
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0.4384363907891313	0.6881618197081606	0.2660029990485323	T	T	T
0.4385091581856734	0.9385199826986571	0.2633132547055289	T	T	T
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0.6886268025450236	0.4380467202562192	0.2668734262835072	T	T	T
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0.9388197117877650	0.1883997904797231	0.2668447014192583	T	T	T
0.9388640360930307	0.4384701893325593	0.2633566635579606	T	T	T
0.9384337242712391	0.6885027007266102	0.2666565645671559	T	T	T
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0.1889345139676373	0.1890137380021334	0.3852126797529465	T	T	T
0.1892510522502844	0.4389442813883805	0.3947547601389126	T	T	T
0.1880285556437993	0.6885824410987010	0.3854729059189038	T	T	T
0.1880981059721296	0.9394106079147854	0.3940427184420778	T	T	T
0.4388618773697043	0.1883094350988611	0.3945497198480788	T	T	T
0.4385114150960077	0.4382144965906979	0.3872057151278599	T	T	T
0.4383288609725260	0.6880115663436874	0.3921504816676605	T	T	T
0.4385300112017055	0.9383169933516881	0.3848397230569189	T	T	T
0.6890932717052659	0.1873682381937754	0.3853654634976429	T	T	T
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0.6880827002262587	0.6874801228351360	0.3850450539338524	T	T	T
0.6878263267314244	0.9369793500492840	0.3942049047237272	T	T	T
0.9392843024523947	0.1883734856417278	0.3941470002950844	T	T	T
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0.1904475976462993	0.4425273592478544	0.5268699885466798	T	T	T
0.1889465313499048	0.6917698485833650	0.5062843426500097	T	T	T
0.1858134503308292	0.9411092514489425	0.5261525641370940	T	T	T
0.4404783839933198	0.1868411748601746	0.5245552919219478	T	T	T
0.4422118651247659	0.4356749475973083	0.5104235794502434	T	T	T
0.4375000659654742	0.6875597456439091	0.5196244769097399	T	T	T
0.4357994608858773	0.9371491582709092	0.5052866751066288	T	T	T
0.6897507969390042	0.1850981015004902	0.5054148357940056	T	T	T
0.6922146471052574	0.4344066790926165	0.5257886356786671	T	T	T
0.6870081202022994	0.6843132555186450	0.5053180963686774	T	T	T
0.6864502033678526	0.9352596548499198	0.5264094611938832	T	T	T
0.9392404213921286	0.1878292322527531	0.5255210123496230	T	T	T
0.9409726542553254	0.4379180999791540	0.5048728913658859	T	T	T
0.9378927852968852	0.6886221366115771	0.5237772540874249	T	T	T
0.9360837649011364	0.9385616663586285	0.5053324478910087	T	T	T
0.1906287752166088	0.1908764937219758	0.6253197510536724	T	T	T
0.1695242012839017	0.6894244203462913	0.6253830949066650	T	T	T
0.4395589257007095	0.4302077519323671	0.6332213850242020	T	T	T
0.4434790815157685	0.9524573155224972	0.6249346129812814	T	T	T
0.6898382712412638	0.1922416594254963	0.6253072227645736	T	T	T
0.7053377257947503	0.6917051391253897	0.6240396029924603	T	T	T
0.9412858838701539	0.4355424375283736	0.6252169281472827	T	T	T
0.9361243529806884	0.9443426322897083	0.6255671503430048	T	T	T
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0.3788797293189667	0.7498859069108612	0.6695436987651106	T	T	T

P_100_1m

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0.0000000000000000	10.9799995421999999	0.0000000000000000
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Selective dynamics

Direct

0.0637522795251186	0.3137522799303980	0.0784041136363669	F	F	F
0.0637522795251186	0.8137522798302186	0.0784041136363669	F	F	F
0.3137522799303980	0.0637522795251186	0.0784041136363669	F	F	F
0.3137522799303980	0.5637522794249321	0.0784041136363669	F	F	F
0.5637522794249321	0.3137522799303980	0.0784041136363669	F	F	F
0.5637522794249321	0.8137522798302186	0.0784041136363669	F	F	F
0.8137522798302186	0.0637522795251186	0.0784041136363669	F	F	F
0.8137522798302186	0.5637522794249321	0.0784041136363669	F	F	F

0.0633027043384679	0.0632046500894309	0.2029714470222451	T	T	T
0.0633423853854970	0.5632255454244930	0.2029515305305125	T	T	T
0.3133462135293069	0.3132360770589250	0.2029655100558845	T	T	T
0.3132883509405086	0.8132396782757070	0.2029639035451999	T	T	T
0.5633011960860141	0.0632038945849651	0.2029755696716643	T	T	T
0.5633426116560734	0.5631695033065079	0.2029554135462855	T	T	T
0.8133217890445487	0.3131682578850939	0.2029719208238199	T	T	T
0.8133256546460694	0.8131755462058139	0.2029519215807825	T	T	T
0.0627888863870405	0.3123656115844513	0.3273190028394072	T	T	T
0.0624628140851217	0.8124672394399881	0.3273983520480473	T	T	T
0.3126422006604772	0.0625538867781527	0.3274234677803232	T	T	T
0.3127973555745656	0.5624609711995459	0.3273217094888491	T	T	T
0.5628160543830415	0.3121475363056701	0.3274638581031677	T	T	T
0.5626329603442241	0.8122613899932019	0.3272794444043717	T	T	T
0.8126192300284951	0.0622369126469126	0.3274766120140584	T	T	T
0.8127940648724643	0.5622718189271529	0.3273480879427617	T	T	T
0.0616052921459398	0.0613796261981266	0.4521283669730470	T	T	T
0.0621832903932016	0.5616010840489895	0.4519000373787673	T	T	T
0.3121709232384935	0.3117569077705105	0.4521996772711155	T	T	T
0.3124783924373907	0.8119661466763204	0.4518418847425788	T	T	T
0.5616299209342432	0.0607350741737280	0.4526032365166082	T	T	T
0.5621250300653922	0.5616952570087294	0.4519535500682569	T	T	T
0.8118836345432566	0.3110617408897166	0.4520671539495006	T	T	T
0.8110303086930382	0.8109123843536236	0.4524756611294406	T	T	T
0.0624058095148787	0.3106607661880593	0.5780456685352152	T	T	T
0.0606780985627794	0.8118057388768690	0.5780903247643310	T	T	T
0.3117590015275413	0.0616877394595046	0.5776722300326050	T	T	T
0.3124017137470782	0.5640887730976460	0.5765732082405425	T	T	T
0.5627870922906343	0.3110785726922329	0.5784332493879969	T	T	T
0.5602093651968609	0.8079613965014155	0.5805251365034932	T	T	T
0.8110999057075162	0.0605698859077572	0.5779762315620792	T	T	T
0.8139808432874411	0.5597120851353231	0.5775064652917192	T	T	T
0.4421816268435343	0.6779642580887874	0.6620012382607946	T	T	T
0.1887522792723857	0.1887522792723857	0.0160252236363618	F	F	F
0.1887522792723857	0.6887522791722063	0.0160252236363618	F	F	F
0.4387522796776651	0.4387522796776651	0.0160252236363618	F	F	F
0.4387522796776651	0.9387522795774856	0.0160252236363618	F	F	F
0.6887522791722063	0.1887522792723857	0.0160252236363618	F	F	F
0.6887522791722063	0.6887522791722063	0.0160252236363618	F	F	F
0.9387522795774856	0.4387522796776651	0.0160252236363618	F	F	F
0.9387522795774856	0.9387522795774856	0.0160252236363618	F	F	F
0.1887522792723857	0.1887522792723857	0.1408004422727274	F	F	F
0.1887522792723857	0.4387522796776651	0.1408004422727274	F	F	F
0.1887522792723857	0.6887522791722063	0.1408004422727274	F	F	F
0.1887522792723857	0.9387522795774856	0.1408004422727274	F	F	F
0.4387522796776651	0.1887522792723857	0.1408004422727274	F	F	F

0.4387522796776651	0.4387522796776651	0.1408004422727274	F	F	F
0.4387522796776651	0.6887522791722063	0.1408004422727274	F	F	F
0.4387522796776651	0.9387522795774856	0.1408004422727274	F	F	F
0.6887522791722063	0.1887522792723857	0.1408004422727274	F	F	F
0.6887522791722063	0.4387522796776651	0.1408004422727274	F	F	F
0.6887522791722063	0.6887522791722063	0.1408004422727274	F	F	F
0.6887522791722063	0.9387522795774856	0.1408004422727274	F	F	F
0.9387522795774856	0.1887522792723857	0.1408004422727274	F	F	F
0.9387522795774856	0.4387522796776651	0.1408004422727274	F	F	F
0.9387522795774856	0.6887522791722063	0.1408004422727274	F	F	F
0.9387522795774856	0.9387522795774856	0.1408004422727274	F	F	F
0.1881271803168156	0.1879072878143953	0.2633928261528471	T	T	T
0.1879989566725251	0.4377846364089404	0.2668621545522932	T	T	T
0.1881143117439226	0.6878938067194231	0.2634782601779425	T	T	T
0.1878707093788124	0.9378341305700828	0.2669339560892228	T	T	T
0.4379585808013840	0.1877477526613115	0.2669692922984976	T	T	T
0.4381141218346444	0.4378329652929826	0.2635445114100428	T	T	T
0.4379641243888236	0.6877367118586286	0.2666804891390722	T	T	T
0.4380341175551379	0.9378910581704306	0.2634201402818779	T	T	T
0.6880693983326116	0.1877287901036912	0.2634506312063880	T	T	T
0.6879753725468402	0.4376214285226798	0.2668877898548748	T	T	T
0.6881192972080545	0.6877901812154276	0.2634049807969833	T	T	T
0.6879136488920827	0.9376928305881034	0.2670263612147833	T	T	T
0.9379343919602000	0.1876456892872092	0.2669555314580251	T	T	T
0.9381283631400889	0.4378006524460510	0.2633594432657861	T	T	T
0.9379702063643338	0.6877118354281549	0.2668795855991352	T	T	T
0.9379850710407160	0.9377947452541628	0.2634152162848595	T	T	T
0.1872455677462380	0.1871347348822902	0.3851258299758428	T	T	T
0.1876177289768945	0.4371353090508917	0.3945186030220246	T	T	T
0.1870006237329112	0.6870727357861414	0.3852525812864763	T	T	T
0.1871609988666419	0.9372415380050964	0.3945634807473055	T	T	T
0.4373125663911327	0.1866087472962506	0.3948119987500365	T	T	T
0.4374421622208595	0.4365583923614059	0.3854621035408046	T	T	T
0.4372048845514355	0.6867468840913817	0.3938761105603877	T	T	T
0.4372515077063310	0.9366655329417301	0.3851656291071331	T	T	T
0.6872680429431776	0.1866995757768483	0.3852146987851959	T	T	T
0.6875836835806339	0.4366660984810612	0.3944711458848166	T	T	T
0.6870858961156432	0.6867521563834679	0.3851196124843219	T	T	T
0.6870668711234502	0.9366540920313144	0.3950625888044850	T	T	T
0.9373082789187048	0.1867614300000960	0.3946022843175140	T	T	T
0.9375333806929055	0.4367842008391736	0.3850586904775495	T	T	T
0.9370065663828511	0.6867778732933369	0.3945510737788968	T	T	T
0.9370889782831024	0.9367862823920882	0.3851905781094984	T	T	T
0.1870127699389224	0.1860169528806361	0.5052958944662769	T	T	T
0.1867891093619430	0.4360901543412619	0.5262166780181002	T	T	T
0.1884005755456542	0.6856402321716542	0.5056816400119465	T	T	T

0.1857260677102487	0.9362166457182984	0.5263856188381700	T	T	T
0.4369462938353506	0.1872390704154494	0.5263383899368411	T	T	T
0.4357037436935757	0.4377503170974340	0.5061954886342855	T	T	T
0.4373447876308627	0.6872607568578309	0.5241566761632385	T	T	T
0.4352158377667985	0.9371610339775150	0.5055828492449342	T	T	T
0.6874450135715497	0.1848043301307572	0.5054804798330359	T	T	T
0.6871254758673421	0.4349875851010441	0.5259607619983199	T	T	T
0.6866457471406050	0.6849529406657054	0.5054557068477510	T	T	T
0.6853993141992146	0.9347075429873708	0.5277781051795261	T	T	T
0.9368623957548091	0.1857784311657268	0.5263484771334511	T	T	T
0.9370287570327992	0.4361633416792688	0.5052152980900751	T	T	T
0.9377923801741193	0.6860448177115419	0.5255915138706712	T	T	T
0.9355500387870026	0.9363997887016388	0.5054568208011290	T	T	T
0.1884549747768930	0.1866246621079300	0.6253104959093726	T	T	T
0.1847232361462604	0.6866372802119669	0.6257490098350772	T	T	T
0.4443089493050072	0.4384626809518298	0.6269449412443240	T	T	T
0.4373446855020711	0.9387739922308690	0.6254358954898236	T	T	T
0.6874833518561960	0.1864093682952077	0.6254169413075871	T	T	T
0.6960054849142592	0.6856906114596872	0.6249619638571270	T	T	T
0.9388459218496740	0.4340630587378720	0.6253125723917181	T	T	T
0.9375871593753599	0.9364478920990444	0.6253578417964073	T	T	T
0.4707281160770421	0.5970265106884380	0.6754755075892754	T	T	T
0.3772252120429789	0.7084896500557513	0.6881400416908071	T	T	T

P_100_24

1.0

10.9799995421999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.9799995421999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.0000000000000000

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Selective dynamics

Direct

0.0637522795251186	0.3137522799303980	0.0663419423076945	F	F	F
0.0637522795251186	0.8137522798302186	0.0663419423076945	F	F	F
0.3137522799303980	0.0637522795251186	0.0663419423076945	F	F	F
0.3137522799303980	0.5637522794249321	0.0663419423076945	F	F	F
0.5637522794249321	0.3137522799303980	0.0663419423076945	F	F	F
0.5637522794249321	0.8137522798302186	0.0663419423076945	F	F	F
0.8137522798302186	0.0637522795251186	0.0663419423076945	F	F	F
0.8137522798302186	0.5637522794249321	0.0663419423076945	F	F	F
0.0639374716139827	0.0635613298675466	0.1717032438816233	T	T	T
0.0639809867022336	0.5636079490101196	0.1716927789445606	T	T	T
0.3139771701005429	0.3135851346598386	0.1717162598317543	T	T	T
0.3139461736322673	0.8135448261730431	0.1716998226237507	T	T	T
0.5639763915617522	0.0635909012726117	0.1717151011766447	T	T	T

0.5639324378386945	0.5635737508808276	0.1717155642132226	T	T	T
0.8139272447690971	0.3135405051283087	0.1717034173003711	T	T	T
0.8139719293262146	0.8135812420067765	0.1717176124333193	T	T	T
0.0643882548327852	0.3131726467594333	0.2768911581019537	T	T	T
0.0642749052470037	0.8132248245493514	0.2768785323379461	T	T	T
0.3142715338230531	0.0632879332137222	0.2768910680509151	T	T	T
0.3143248520665054	0.5632320447841579	0.2768838984946242	T	T	T
0.5643455142068063	0.3132762034196475	0.2769109394528542	T	T	T
0.5643320585671887	0.8132503186214279	0.2769083633597802	T	T	T
0.8142919944734146	0.0632030502867735	0.2768923060650721	T	T	T
0.8142851650473730	0.5632409847435014	0.2769061554501846	T	T	T
0.0644839821142824	0.0628746594832705	0.3820264143868286	T	T	T
0.0645190947295475	0.5629475480015316	0.3820290653737501	T	T	T
0.3146577965902750	0.3128187316307560	0.3820721020454556	T	T	T
0.3145732626100894	0.8128546334628339	0.3820935891575559	T	T	T
0.5644938151088255	0.0629916272152045	0.3820986764924612	T	T	T
0.5645610190325456	0.5629889304876841	0.3821064426071814	T	T	T
0.8146360116649376	0.3127322330677345	0.3821043892650238	T	T	T
0.8145342599512944	0.8127128085901063	0.3821095629853701	T	T	T
0.0662743029702781	0.3127056626219158	0.4871461785999642	T	T	T
0.0659934677542182	0.8125767545738256	0.4871787369645446	T	T	T
0.3161392957435822	0.0625263508657241	0.4871086353114649	T	T	T
0.3162418910038127	0.5624748575580796	0.4871829732808806	T	T	T
0.5662923171433505	0.3128874643049500	0.4873550526570654	T	T	T
0.5659996198063482	0.8128206052657845	0.4873470599826462	T	T	T
0.8159719451896095	0.0622546362926499	0.4871735302512903	T	T	T
0.8160885176357766	0.5622958507438796	0.4871638431074246	T	T	T
0.1887522792723857	0.1887522792723857	0.0135598046153831	F	F	F
0.1887522792723857	0.6887522791722063	0.0135598046153831	F	F	F
0.4387522796776651	0.4387522796776651	0.0135598046153831	F	F	F
0.4387522796776651	0.9387522795774856	0.0135598046153831	F	F	F
0.6887522791722063	0.1887522792723857	0.0135598046153831	F	F	F
0.6887522791722063	0.6887522791722063	0.0135598046153831	F	F	F
0.9387522795774856	0.4387522796776651	0.0135598046153831	F	F	F
0.9387522795774856	0.9387522795774856	0.0135598046153831	F	F	F
0.1887522792723857	0.1887522792723857	0.1191388357692276	F	F	F
0.1887522792723857	0.4387522796776651	0.1191388357692276	F	F	F
0.1887522792723857	0.6887522791722063	0.1191388357692276	F	F	F
0.1887522792723857	0.9387522795774856	0.1191388357692276	F	F	F
0.4387522796776651	0.1887522792723857	0.1191388357692276	F	F	F
0.4387522796776651	0.4387522796776651	0.1191388357692276	F	F	F
0.4387522796776651	0.6887522791722063	0.1191388357692276	F	F	F
0.4387522796776651	0.9387522795774856	0.1191388357692276	F	F	F
0.6887522791722063	0.1887522792723857	0.1191388357692276	F	F	F
0.6887522791722063	0.4387522796776651	0.1191388357692276	F	F	F
0.6887522791722063	0.6887522791722063	0.1191388357692276	F	F	F

0.6887522791722063	0.9387522795774856	0.1191388357692276	F	F	F
0.9387522795774856	0.1887522792723857	0.1191388357692276	F	F	F
0.9387522795774856	0.4387522796776651	0.1191388357692276	F	F	F
0.9387522795774856	0.6887522791722063	0.1191388357692276	F	F	F
0.9387522795774856	0.9387522795774856	0.1191388357692276	F	F	F
0.1890424762797949	0.1881911966650023	0.2243667101236042	T	T	T
0.1892782337735994	0.4382564543678882	0.2241733316937342	T	T	T
0.1890537890906572	0.6881863413744114	0.2243704807074778	T	T	T
0.1892648175145553	0.9382417675186829	0.2241520876936463	T	T	T
0.4389935964991167	0.1886211706254599	0.2241350040076071	T	T	T
0.4393349239034592	0.4385599771775119	0.2244424505916669	T	T	T
0.4389825403993584	0.6886355494214200	0.2241420491708652	T	T	T
0.4393334843920513	0.9385576560214588	0.2244321477412541	T	T	T
0.6890273710573140	0.1881681233839956	0.2244016249892056	T	T	T
0.6892989653216901	0.4382589127510599	0.2242118498388592	T	T	T
0.6890274450009315	0.6881767213823693	0.2243867508025659	T	T	T
0.6892441267960834	0.9382712134308377	0.2241935259855126	T	T	T
0.9389604346300189	0.1885856917445494	0.2241232536888944	T	T	T
0.9393305253019477	0.4385144460476837	0.2244054986789763	T	T	T
0.9389668219340450	0.6885719888046040	0.2241344665816598	T	T	T
0.9393138734449309	0.9385360553551081	0.2244215729718135	T	T	T
0.1904675165684324	0.1889847415318684	0.3294218633225228	T	T	T
0.1885788743921211	0.4389589467014119	0.3295298495238583	T	T	T
0.1904296895592950	0.6889748647711045	0.3294312498861487	T	T	T
0.1885153056832891	0.9389355634221417	0.3295063280932240	T	T	T
0.4404870079551841	0.1871673203083901	0.3294046169079365	T	T	T
0.4385132489947594	0.4372010197823570	0.3296239282088749	T	T	T
0.4404314690884945	0.6871775974786800	0.3294382297174678	T	T	T
0.4384906197270908	0.9372110531531348	0.3296034349319470	T	T	T
0.6904237077138617	0.1889504977931438	0.3294947318590360	T	T	T
0.6885728199189387	0.4389561105208486	0.3296104739764800	T	T	T
0.6903963185217350	0.6889652900741936	0.3294302823823969	T	T	T
0.6884958725549168	0.9389650829948479	0.3295899794260180	T	T	T
0.9404460883496739	0.1870785432850113	0.3293815853525146	T	T	T
0.9385024592699480	0.4370995067678010	0.3295526373978817	T	T	T
0.9404304222317137	0.6870734286239752	0.3293812638236275	T	T	T
0.9384581846766551	0.9371125775745242	0.3295723744915051	T	T	T
0.1847948825332679	0.1830061329355246	0.4344847175932216	T	T	T
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0.6532562895495825	0.1530119376210331	0.6086717310703605	T	T	T

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P_111_0

1.0

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-7.7589412887 13.4388805245 0.0000000000
0.0000000000 0.0000000000 19.0000000000

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Ce O

48 96

Selective

Cartesian

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+7.7587161217 +6.7193953603 +7.4578300000 T T T
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+0.0000899586 +2.2404700717 +4.3219700000 T T T
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+1.9402231614	+5.6005407910	+1.9780800000	F	F	F

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P_111_1d

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Ce O H

48 97 2

Selective dynamics

Direct

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0.2472380990305914 0.2471073485569656 0.3921428584043816 T T T
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0.0012270593002608 0.7506508080197222 0.3915080314693869 T T T
0.2472379215584180 0.5002253500246556 0.3921389225741575 T T T
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0.5005215994533714 0.0003165350033302 0.3923317225429619 T T T

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0.1667378647324753	0.8334122399822519	0.0625011046315791	F	F	F
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0.4167378647324753	0.8334122399854706	0.0625011046315791	F	F	F
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P_111_1m

1.0

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Selective dynamics

Direct

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0.6794957172227587	0.5890471100860776	0.4385840269842445	T	T	T
0.6667607546826105	0.8335999608367867	0.4327677656624755	T	T	T
0.9175947055984642	0.5836404349164770	0.4331896911382289	T	T	T
0.9175175448122919	0.8337801306298651	0.4333702468641622	T	T	T
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0.0828602695362474	0.4166714644449798	0.3504191682772648	T	T	T
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0.0837681156892341	0.9169495634102622	0.3504808975750076	T	T	T
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0.8331950998236315	0.1666648167798876	0.3505734791735100	T	T	T
0.8336978997298061	0.4166157779876050	0.3505986915575757	T	T	T
0.5840018112352326	0.6634885580062087	0.3527064638576419	T	T	T
0.5833912091886110	0.9169461481713835	0.3504577691674934	T	T	T
0.8353531973993646	0.6677471827142107	0.3493013044154967	T	T	T
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0.0011256992099075	0.7505525523043968	0.2692821594274753	T	T	T
0.2501130135600236	0.4996459396499644	0.2699616221169818	T	T	T
0.2500363414349779	0.7505360503589141	0.2692865983159972	T	T	T
0.5002361396680874	0.0002269297438984	0.2695800508842572	T	T	T
0.5008160161889772	0.2514767626701112	0.2702860325924284	T	T	T
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0.5009548175300639	0.7493472920585197	0.2705765552385928	T	T	T
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0.7497636828695593	0.7501095562058986	0.2699313224238582	T	T	T

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0.6666165162943878	0.8332896675203917	0.1853105613593408	T	T	T
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P_111_2

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Selective dynamics

Direct

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0.0013350570172908	0.7505300561603284	0.3915145692912395	T	T	T
0.2476334849569057	0.5003163703381464	0.3919462632805211	T	T	T
0.2510267789808497	0.7507049056451993	0.3919413620487832	T	T	T
0.5008854759855025	0.0007958209072245	0.3926358794010820	T	T	T
0.4959788413679422	0.2481923343481284	0.3962774928859885	T	T	T
0.7503033032158811	0.0010162231174228	0.3925795615562790	T	T	T
0.7518187306548705	0.2507787074527784	0.3928302798797509	T	T	T
0.4879140284368751	0.4935949851163995	0.3958236698655508	T	T	T
0.5001394394793549	0.7497110837296681	0.3931338504948526	T	T	T
0.7565343894661652	0.4993086284598879	0.3926991243515012	T	T	T
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0.4167378647324753	0.3334122399854706	0.0625011046315791	F	F	F
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0.8334045314289042	0.1667455732789165	0.1041092327105275	F	F	F
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0.5834045314289042	0.6667455732821352	0.1041092327105275	F	F	F
0.8334045314289042	0.4167455732789165	0.1041092327105275	F	F	F

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0.2500711981253403	0.5000789065787998	0.0208851243684194	F	F	F
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0.5864413605341250	0.6601863869790372	0.3563913134329339	T	T	T

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p_111_4

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Ce O H
12 28 8
Selective dynamics
Direct
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0.0389902842810889	0.5875447572177210	0.5533223029454576	T	T	T
0.3225411674991574	0.0138708908949883	0.5493315023549692	T	T	T
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p_111_7

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12 31 14

Selective dynamics

Direct

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0.6127118076753177	0.0618332299891264	0.3914496756979204	T	T	T
0.6065183017462985	0.5698170061718955	0.3927430432189141	T	T	T
0.2716051946214861	0.3973284959769217	0.2280170687450607	T	T	T
0.2701108886066663	0.8995660158049361	0.2279168457369281	T	T	T
0.7701827145284668	0.3986979724171462	0.2272555545637758	T	T	T
0.7725432281073878	0.8988234766220558	0.2265156881552102	T	T	T
0.4376510733424723	0.2318005082241115	0.0625011046315791	F	F	F
0.4376510733424723	0.7318005082241115	0.0625011046315791	F	F	F
0.9376510733424723	0.2318005082305561	0.0625011046315791	F	F	F
0.9376510733424723	0.7318005082305561	0.0625011046315791	F	F	F
0.2709844067353373	0.3984671748238782	0.1041092327105275	F	F	F
0.7709844067353373	0.3984671748174335	0.1041092327105275	F	F	F
0.2709844067353373	0.8984671748238782	0.1041092327105275	F	F	F
0.7709844067353373	0.8984671748303228	0.1041092327105275	F	F	F
0.6043177401282023	0.0651338414172002	0.0208851243684194	F	F	F
0.6043177401282023	0.5651338414172002	0.0208851243684194	F	F	F
0.1043177401282023	0.0651338414236449	0.0208851243684194	F	F	F
0.1043177401282023	0.5651338414236449	0.0208851243684194	F	F	F
0.4560999893011441	0.2275583627455546	0.4493324214554448	T	T	T
0.4321861338030786	0.7352859550255104	0.4171961027601228	T	T	T
0.9409053876972351	0.2487420212344063	0.4222413439300112	T	T	T
0.9262880520166163	0.7101666249156864	0.4411268003356739	T	T	T
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0.2652354365669609	0.9147954728150580	0.3524277939326836	T	T	T
0.7537926243562083	0.3969803141596344	0.3485752725458511	T	T	T
0.7834749957305220	0.8967406267054088	0.3530926057004393	T	T	T
0.1006614084439690	0.0655886218790087	0.2655503090203268	T	T	T

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0.4399291869138509	0.2316615013054104	0.1858713041055893	T	T	T
0.4346708052855917	0.7318144233969761	0.1845541355242659	T	T	T
0.9369390080944271	0.2352228444136486	0.1848954527709310	T	T	T
0.9392100387437878	0.7290385909679458	0.1851639279588824	T	T	T
0.0736941903500679	0.0758214678554054	0.5228732695793852	T	T	T
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0.1999398607708684	0.8774949965973420	0.5935214328170986	T	T	T
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