

Supplementary Materials for
On the Mechanism of Methanol Synthesis from CO₂ Hydrogenation over
Pt₈/In₂O₃ Catalysts:

A Combined Study on Density Functional Theory and Microkinetic Modeling

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S1: The XYZ coordinations of all calculated adsorbates and transition states.

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cONTCAR\5)      h+co2-pt4
1.00000000000000
 10.2175998688000007    0.0000000000000000    0.0000000000000000
 0.0000000000000000    14.4497995377000006    0.0000000000000000
 0.0000000000000000    0.0000000000000000    20.9857006073000001

O   In   Pt   C   H
50  32   4    1   1

```

Selective dynamics

Direct

0.1819400070000015	0.5179200199999983	0.1152000000000015	F	F	F
0.6819400070000015	0.0179200010000002	0.1152000000000015	F	F	F
0.6795349610000017	0.0317670000000021	0.2518329840000035	T	T	T
0.1794640020000031	0.5183029800000014	0.2622090099999994	T	T	T
0.9183799970000024	0.3758610000000004	0.3583169939999991	T	T	T
0.4084239860000025	0.8819649630000015	0.3576740070000000	T	T	T
0.4254840190000024	0.6725980089999979	0.3517940070000023	T	T	T
0.9183309949999980	0.1617740020000014	0.3497880170000016	T	T	T
0.9545099699999966	0.3958000000000013	0.1866899999999987	F	F	F
0.4545100160000004	0.8957999670000021	0.1866899999999987	F	F	F
0.6423570059999975	0.7837669580000011	0.2660990159999983	T	T	T
0.1458420020000020	0.2863459730000031	0.2731930079999998	T	T	T
0.4545100160000004	0.1542000070000000	0.1726800109999971	F	F	F
0.9545099699999966	0.6542000230000014	0.1726800109999971	F	F	F
0.1454900069999994	0.7638599679999984	0.1037499959999977	F	F	F
0.6454899840000010	0.2638599839999998	0.1037499959999977	F	F	F
0.1903399939999986	0.2862900060000015	0.1125700079999987	F	F	F
0.6903399589999992	0.7862899730000024	0.1125700079999987	F	F	F
0.9096599470000015	0.8817800340000019	0.1725899979999994	F	F	F
0.4096599940000019	0.3817800010000028	0.1725899979999994	F	F	F
0.4096599940000019	0.6682199560000015	0.1867800019999990	F	F	F
0.9096599470000015	0.1682200059999985	0.1867800019999990	F	F	F
0.6900830040000017	0.2665229999999994	0.2532990079999990	T	T	T
0.1866659920000018	0.7614599750000011	0.2534469960000010	T	T	T
0.4180599930000000	0.7820899849999989	0.0870100030000032	F	F	F
0.9180600400000003	0.2820900179999981	0.0870100030000032	F	F	F
0.9151170490000027	0.7649319920000011	0.2874130049999977	T	T	T
0.4189080009999984	0.2674680080000016	0.2827900090000028	T	T	T
0.6819400070000015	0.4224300249999970	0.1752299990000026	F	F	F
0.1819400070000015	0.9224299589999987	0.1752299990000026	F	F	F
0.1819400070000015	0.1275800049999987	0.1841400010000029	F	F	F
0.6819400070000015	0.6275799969999980	0.1841400010000029	F	F	F
0.6449750000000023	0.3885569899999979	0.3506140080000009	T	T	T

0.1362400049999977	0.8966400039999982	0.3518660129999986	T	T	T
0.9572399669999996	0.0116190000000032	0.2701899999999995	T	T	T
0.4554730150000026	0.5140450130000005	0.2719370040000015	T	T	T
0.1519750109999976	0.6505040059999985	0.3636380100000025	T	T	T
0.6440490089999997	0.1508329950000018	0.3627519879999994	T	T	T
0.4545100160000004	0.5361400390000028	0.0984700050000029	F	F	F
0.9545099699999966	0.0361399980000030	0.0984700050000029	F	F	F
0.4096599940000019	0.0137100000000032	0.0896599969999983	F	F	F
0.9096599470000015	0.5137100339999989	0.0896599969999983	F	F	F
0.7083369969999964	0.9189570180000004	0.3600470020000017	T	T	T
0.3171359859999967	0.3984469939999968	0.3942170320000002	T	T	T
0.2022740020000029	0.1315979999999968	0.3575119990000033	T	T	T
0.6874589900000032	0.6324040060000016	0.3527610100000018	T	T	T
0.9006829429999996	0.5373659730000000	0.2826890099999986	T	T	T
0.4070350000000005	0.0383120010000013	0.2783080029999994	T	T	T
0.7211280080000009	0.7638080259999995	0.4547419960000028	T	T	T
0.5510929699999991	0.7378609929999982	0.5230370210000004	T	T	T
0.7999999999999972	0.7581899819999975	0.1902599909999978	F	F	F
0.3000000230000026	0.7918100090000024	0.1691199950000026	F	F	F
0.3000000230000026	0.2581899979999989	0.1902599909999978	F	F	F
0.7999999999999972	0.2918100090000024	0.1691199950000026	F	F	F
0.8336300499999965	0.0250000010000022	0.1796899989999972	F	F	F
0.7741730159999989	0.2652699900000002	0.3493959950000018	T	T	T
0.3336300030000032	0.5249999790000004	0.1796899989999972	F	F	F
0.2642619929999981	0.7754599760000005	0.3509489979999998	T	T	T
0.5483459849999974	0.9170359809999979	0.2815040119999992	T	T	T
0.5499999999999972	0.1331900059999995	0.0905399970000005	F	F	F
0.0344269969999971	0.4115309929999995	0.2777810119999984	T	T	T
0.0499999999999972	0.6331899899999982	0.0905399970000005	F	F	F
0.7936700169999966	0.0449090019999971	0.3403450030000030	T	T	T
0.2820009790000029	0.9990399770000025	0.3537909980000009	T	T	T
0.3003909859999965	0.5452160099999972	0.3451530009999999	T	T	T
0.7979819729999988	0.4975579990000014	0.3677900240000014	T	T	T
0.7593270160000003	0.7800970090000021	0.3528270170000027	T	T	T
0.8336300499999965	0.5249999790000004	0.1796899989999972	F	F	F
0.2740240039999975	0.2663800130000027	0.3534420109999985	T	T	T
0.3336300030000032	0.0250000010000022	0.1796899989999972	F	F	F
0.0470990020000031	0.8807659570000013	0.2586269990000005	T	T	T
0.0499999999999972	0.1668099999999981	0.1116699999999966	F	F	F
0.5489579919999983	0.3820760070000020	0.2564390069999973	T	T	T
0.5499999999999972	0.6668099509999976	0.1116699999999966	F	F	F
0.5499999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0491270010000022	0.1470210000000023	0.2712369839999980	T	T	T
0.5499999999999972	0.8999999540000019	0.1011099950000016	F	F	F

0.0484780009999994	0.6472949959999994	0.2723709939999992	T	T	T
0.0499999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0499999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.5488839759999991	0.6501029949999975	0.2659719780000032	T	T	T
0.5516539679999966	0.1496369919999978	0.2690930039999984	T	T	T
0.3391810010000000	0.5188360220000021	0.4741110040000009	T	T	T
0.5153120279999968	0.4264680169999977	0.4207790079999967	T	T	T
0.5472400419999985	0.6133379770000005	0.4225340110000033	T	T	T
0.6986430279999993	0.5035199980000016	0.4821799959999993	T	T	T
0.6164500329999996	0.7259269629999991	0.4751920260000020	T	T	T
0.3883239860000032	0.5993470180000031	0.5171359810000027	T	T	T

CONTCAR(5) h+co2-pdpt3

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0.0000000000000000	0.0000000000000000	20.9857006073000001

O	In	Pd	Pt	C	H
50	32	1	3	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6793022729810403	0.0325017735061550	0.2516459749950144	T	T	T
0.1790921805372534	0.5177045559681588	0.2627485321848937	T	T	T
0.9113962616250717	0.3775937211866349	0.3586831194457218	T	T	T
0.4081075405460126	0.8826005485290622	0.3576920713664649	T	T	T
0.4246295467599381	0.6751492867787263	0.3513730620147015	T	T	T
0.9157075931600005	0.1630515619290946	0.3496462115844921	T	T	T
0.9545099696828743	0.395799996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6428187612763736	0.7845601261232105	0.2654338436408068	T	T	T
0.1435260302638355	0.2863727862366758	0.2733954866296600	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F

0.6899878406662197	0.2677827539385902	0.2539473545301334	T	T	T
0.1864246135165786	0.7610229304383651	0.2534676066423884	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9163896883337088	0.7646066749156262	0.2870270828514947	T	T	T
0.4178618110869934	0.2670117363081346	0.2818623507818998	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6360274919899709	0.3897884022969862	0.3527359847107832	T	T	T
0.1358334034768873	0.8966357181629050	0.3517457027719146	T	T	T
0.9568735807349285	0.0117830801777359	0.2703242863461668	T	T	T
0.4553497239173794	0.5147382312958442	0.2711249757242413	T	T	T
0.1532654635514135	0.6492039613883591	0.3644801076329713	T	T	T
0.6416856587125324	0.1511145704685504	0.3629832930552368	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7082657841890381	0.9188670362668461	0.3594554153828682	T	T	T
0.3092106555920111	0.3973500304775968	0.3924283960151911	T	T	T
0.2006939633017524	0.1311926384102620	0.3572637509352319	T	T	T
0.6859083151591321	0.6332229101782048	0.3516999922908468	T	T	T
0.8995959882247320	0.5373126850909458	0.2828468338556007	T	T	T
0.4067777482766104	0.0385739743527154	0.2781594921077399	T	T	T
0.7336967013264015	0.7637825458633714	0.4540828195986890	T	T	T
0.5545116121239886	0.7660660339084799	0.5190476397365273	T	T	T
0.799999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7702005657044069	0.2663411468072141	0.3505362902687352	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2635050975184257	0.7756799815971007	0.3508609212448732	T	T	T
0.5481359557800332	0.9173374281775750	0.2816501755689913	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0322368587261153	0.4115374564187562	0.2787233589842515	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7925842774928640	0.0455294258120702	0.3402861967705064	T	T	T
0.2817817531530196	0.9991472635729295	0.3536184024693654	T	T	T
0.3025280285204985	0.5440283458778765	0.3455498072734287	T	T	T
0.7902505885027225	0.4993677144008259	0.3673192792197923	T	T	T

0.7606989036945890	0.7797976959303199	0.3517707872903202	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2738213983194342	0.2654375516040375	0.3528837502867077	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0470663154734083	0.8808151224689524	0.2585287227737254	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5481831052378183	0.3824277999790979	0.2565934574382496	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0477995858928395	0.1474200372462562	0.2715402014888042	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0489818499675962	0.6463814118930600	0.2726722114397830	T	T	T
0.0499999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5492226851235458	0.6506004840264268	0.2661094428354076	T	T	T
0.5513468000705046	0.1500372091061806	0.2687384668240540	T	T	T
0.3331038251939518	0.5326204901321319	0.4772030381931955	T	T	T
0.4998620458556289	0.4343948179416799	0.4196184653118991	T	T	T
0.5453701082493012	0.6229493446396219	0.4255454789184299	T	T	T
0.6883939804656833	0.5057628761225672	0.4822131634072022	T	T	T
0.6211329770925218	0.7394867955885402	0.4747915255707440	T	T	T
0.4380980786268225	0.6255820940392027	0.4873869378497346	T	T	T

CONTCAR h+co2-pd2pt2

1.0000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O	In	Pd	Pt	C	H
50	32	2	2	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6792452261025446	0.0319602302091866	0.2518217538134095	T	T	T
0.1790162003688494	0.5182363554959650	0.2623472614396221	T	T	T
0.9155550706407638	0.3777165278064132	0.3591655701668941	T	T	T
0.4080943595481301	0.8824619398344851	0.3577181334211730	T	T	T
0.4243573626621213	0.6738742375205860	0.3516990917728862	T	T	T
0.9163328864208893	0.1631127238267567	0.3494068190261572	T	T	T
0.9545099696828743	0.3957999996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6424276637610546	0.7844912546116944	0.2656655154946606	T	T	T

0.1439826762055674	0.2866317057030727	0.2727034060273184	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6895168587652165	0.2665366878389293	0.2531992334674058	T	T	T
0.1863506220327125	0.7611296806542711	0.2535053366052509	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9161375472280113	0.7647486556841656	0.2871862248304495	T	T	T
0.4177541619269789	0.2671825760124094	0.2822025836942075	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6412616902923602	0.3905743296920647	0.3506083436775853	T	T	T
0.1360070256926349	0.8965681078860896	0.3518526505045401	T	T	T
0.9570459935808273	0.0117440231280881	0.2703265381858557	T	T	T
0.4550568614739205	0.5143904187350472	0.2718414258021511	T	T	T
0.1526863837424273	0.6493834986254186	0.3644295015200214	T	T	T
0.6428348739195897	0.1517189772130436	0.3629180180090970	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7086997671112769	0.9187639655245690	0.3601707353372845	T	T	T
0.3086670579715545	0.3982020497203465	0.3931661395635189	T	T	T
0.2013858256509451	0.1318660684512167	0.3570275587310405	T	T	T
0.6862576717814406	0.6334600897627922	0.3520211482136943	T	T	T
0.8994701326930468	0.5375211079985576	0.2827795136905280	T	T	T
0.4067698425187487	0.0383250607331505	0.2781654092899686	T	T	T
0.7307014077703258	0.7627092718229420	0.4550121438196939	T	T	T
0.5491033868423187	0.7633988280544841	0.5188051177092561	T	T	T
0.7999999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.7999999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F

0.7720392546436798	0.2671036918155281	0.3493552873002841	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2638643762214272	0.7753447119337693	0.3508998212834626	T	T	T
0.5480789482973947	0.9172262328245466	0.2816732044309234	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0328486629692080	0.4120706299761494	0.2785072207780246	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7926434525067876	0.0457066474577843	0.3403407086080890	T	T	T
0.2815272648225502	0.9993702475227337	0.3535618392783135	T	T	T
0.3013043760081331	0.5433036394675383	0.3455303167874604	T	T	T
0.7913191349012720	0.4985886244528714	0.3674015110376061	T	T	T
0.7603710118088500	0.7797865223758080	0.3519868100397048	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2725448937552173	0.2671339311636913	0.3529199065618727	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0470427397790871	0.8807891449556493	0.2586277958055447	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5485561521066060	0.3822506915835859	0.2566387409918605	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0482023326174854	0.1474942032648840	0.2713784060751294	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0488123842800405	0.6465368983757855	0.2727388789744012	T	T	T
0.0499999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5491574830457537	0.6502640557793029	0.2664142447158966	T	T	T
0.5510142184125826	0.1499247989762367	0.2690838952359726	T	T	T
0.3347596394729493	0.5264965106308424	0.4742807889944061	T	T	T
0.5060304991619375	0.4301347469704453	0.4201013502605875	T	T	T
0.5454815859360238	0.6206919343476400	0.4252250713725303	T	T	T
0.6918171979980272	0.5065071177319282	0.4828243469527465	T	T	T
0.6189568920856061	0.7378984747976673	0.4755663405875907	T	T	T
0.4376499298394592	0.6193961577522842	0.4876038833753782	T	T	T

CONTCAR\3) h+co2-pd3pt

1.0000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O	In	Pd	Pt	C	H
50	32	3	1	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6791774977193654	0.0315311850833240	0.2522231859225670	T	T	T
0.1794215487606081	0.5180746897476709	0.2624589497265788	T	T	T
0.9143937654308942	0.3786826433797827	0.3593151711235265	T	T	T
0.4084058182553676	0.8833502123908161	0.3582090644017981	T	T	T
0.4223292404284749	0.6750250710323229	0.3497393727605385	T	T	T
0.9155475860447595	0.1637614061911421	0.3492412122096411	T	T	T
0.9545099696828743	0.395799996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6424739691472965	0.7854907537225131	0.2649463067680102	T	T	T
0.1434029964612407	0.2867331356802296	0.2726016491956003	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6894138681783559	0.2665339935830175	0.2531671154634552	T	T	T
0.1858927053509092	0.7613819428613837	0.2531064537968533	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9166237510677178	0.7651598487809963	0.2865355792643669	T	T	T
0.4176702680549269	0.2670581851675351	0.2820242124879542	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6410743542615052	0.3915396129010489	0.3504664805447533	T	T	T
0.1364582437292867	0.8968665251887060	0.3515629487766248	T	T	T
0.9568214459690410	0.0119432207777379	0.2703723079860509	T	T	T
0.4556196384778417	0.5144687134328265	0.2714104794516743	T	T	T
0.1511837687961872	0.6497994561117579	0.3643564736871596	T	T	T
0.6427510248490691	0.1518587333010899	0.3629941997782851	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7097346408295238	0.9181606813459666	0.3613502594601314	T	T	T
0.3082098848897346	0.3981697556086274	0.3927803006078463	T	T	T

0.2012165328259528	0.1322545345860959	0.3569375444222445	T	T	T
0.68911111747819920	0.6362487361239602	0.3513828985255643	T	T	T
0.8995068593723161	0.5374931062634829	0.2825333484303485	T	T	T
0.4066540695148007	0.0385734493574574	0.2780651911751448	T	T	T
0.5553544392822829	0.7578931157275406	0.5231603605128186	T	T	T
0.7370844058867974	0.7609475311124498	0.4576687812794589	T	T	T
0.799999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7713133838552864	0.2680772999201579	0.3497165790885859	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2640618073085221	0.7753802057488741	0.3503501665970461	T	T	T
0.5474991493329497	0.9172703807698142	0.2818128100801403	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0323602658760365	0.4122884560006526	0.2788907485424801	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7926454953220698	0.0457852992308148	0.3405246110696751	T	T	T
0.2814824516825354	0.9997483088090249	0.3535162663570546	T	T	T
0.3023997001840470	0.5445089151538838	0.3457040447073609	T	T	T
0.7903945694471304	0.5005671708109318	0.3677038291960812	T	T	T
0.7607874771092469	0.7797181907744459	0.3510503494392836	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2724722673944413	0.2675703997023220	0.3528046984889244	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0471926435984145	0.8809895372261494	0.2585265699088524	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5484273505061310	0.3824636126977197	0.2569062766365846	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0480702108047097	0.1477597137313325	0.2715035347909520	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0489257477487683	0.6464503417627512	0.2727630160737817	T	T	T
0.0499999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5495360426892120	0.6505107914232227	0.2668884876395623	T	T	T
0.5511324890353038	0.1500700543550053	0.2691438578052114	T	T	T
0.3323357907751401	0.5262381439656565	0.4742281673001543	T	T	T
0.5052748523771058	0.4321968592713219	0.4197069422206923	T	T	T
0.5454713632436565	0.6253045572841955	0.4250124384772178	T	T	T
0.6892557894681772	0.5086452565716542	0.4824923484471668	T	T	T
0.6283007411372026	0.7385268886748051	0.4801108020834235	T	T	T
0.4304307439497066	0.6162951354812947	0.4866087162699770	T	T	T

CONTCAR\4) h+co2-pd4

1.000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O In Pd C H

50 32 4 1 1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6794797029872797	0.0311218317433273	0.2522144154003101	T	T	T
0.1800602524076567	0.5180701758735680	0.2625031020104700	T	T	T
0.9151201150516997	0.3782816478090893	0.3592357893395217	T	T	T
0.4085608003186465	0.8831319533351518	0.3582884155498363	T	T	T
0.4221936282730567	0.6741097956651600	0.3494902754050457	T	T	T
0.9168252414841618	0.1628059579683168	0.3495360930198714	T	T	T
0.9545099696828743	0.395799996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6425538973799974	0.7849543471352831	0.2651810431846258	T	T	T
0.1436101823853804	0.2866323149870738	0.2725723641422988	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6894289499328679	0.2655515535164028	0.2527992462667825	T	T	T
0.1857305894771386	0.7612488954617191	0.2529630417455522	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9164255867240598	0.7650180845561252	0.2865025059711144	T	T	T
0.4177357499024978	0.2667687599497768	0.2820883291704277	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6436645117728546	0.3900113691249061	0.3489825199619503	T	T	T
0.1368504180133812	0.8964364500493005	0.3515545134192664	T	T	T

0.9572183517445794	0.0117856215034280	0.2702622660935390	T	T	T
0.4559704264567515	0.5137925266654904	0.2712038722846444	T	T	T
0.1510540394862403	0.6493232262401776	0.3643752054683915	T	T	T
0.6437925377512812	0.1511586517315280	0.3628915831141484	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.013709999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7099143363666087	0.9176449990600588	0.3612418441689229	T	T	T
0.3082420933028089	0.3982315095058695	0.3934202816302061	T	T	T
0.2020970398022897	0.1323101906039028	0.3568462074405119	T	T	T
0.6897809955978857	0.6351406824131800	0.3511084444390704	T	T	T
0.8997111911571309	0.5370666490507716	0.2822519036983451	T	T	T
0.4068423707207174	0.0382479116785959	0.2780160871995321	T	T	T
0.7478986497882261	0.7567889843733084	0.4567590995021931	T	T	T
0.6018661400309426	0.7249902138330313	0.5370454831879812	T	T	T
0.799999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7727683461065027	0.2669251890243700	0.3491788820284114	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2646715931500481	0.7746739879522409	0.3501377873750897	T	T	T
0.5478433701086942	0.9168200773415762	0.2819521252915749	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0331041314619256	0.4125113972861101	0.2787164642356572	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7933661736052926	0.0449758729613663	0.3405389972757789	T	T	T
0.2815694036731458	0.9995349838684220	0.3534923364720512	T	T	T
0.3030191295901190	0.5443543871790197	0.3460442102087740	T	T	T
0.7893259045236718	0.4998346149123094	0.3671211941428894	T	T	T
0.7608690015835649	0.7790228864559765	0.3515264305310097	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2724696327588489	0.2680369010387338	0.3529445335901116	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0471394220370911	0.8806512088586516	0.2586367196066206	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5485402314746466	0.3818805124876761	0.2564139178565981	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0484863971220548	0.1475904434045106	0.2714912600697588	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0487076951083196	0.6463222971791467	0.2730131137738567	T	T	T

0.049999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.049999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5489528017223719	0.6502180345149924	0.2670288064694191	T	T	T
0.5512928051176686	0.1495276785606379	0.2692368938167391	T	T	T
0.3379791460188102	0.5236154751959816	0.4742473649537970	T	T	T
0.5105285278323208	0.4329000734921493	0.4177555317927784	T	T	T
0.6946445868638449	0.5063245017120295	0.4843198010034158	T	T	T
0.5500641037982135	0.6242720472861336	0.4260979709920463	T	T	T
0.6525057578269227	0.7201447548864195	0.4850152905691516	T	T	T
0.4354005606693576	0.6136396345439294	0.4885040856331386	T	T	T

O	In	Pt	C	H	TS1
1.000000000000000					
10.2175998688000007				0.0000000000000000	0.0000000000000000
0.0000000000000000				14.4497995377000006	0.0000000000000000
0.0000000000000000				0.0000000000000000	20.9857006073000001
O	In	Pt	C	H	
50	32	4		1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6801855913206367	0.0265644821108424	0.2537084664974500	F	F	F
0.1770398405254667	0.5199441786263748	0.2629542544046544	F	F	F
0.9105599250436214	0.3767538001420974	0.3590504468156652	F	F	F
0.4082206698485962	0.8827636948597686	0.3586746241011483	F	F	F
0.4285238298423906	0.6762794095794860	0.3507439099751721	F	F	F
0.9159699063817186	0.1622136980906959	0.3501397300921738	F	F	F
0.9545099696828743	0.3957999996524819	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520351	0.1866900003632566	F	F	F
0.6414285207961612	0.7854200679465251	0.2649204930081552	F	F	F
0.1458446906550321	0.2861836681569301	0.2750738209023424	F	F	F
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827731	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295112	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476740	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264438	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6901701288685942	0.2677381112512478	0.2540861600052011	F	F	F

0.1877327791272734	0.7613576196650271	0.2534812229719918	F	F	F
0.4180599929386020	0.7820899854364995	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9171381413232922	0.7651113140790784	0.2851633727870251	F	F	F
0.4196480132020426	0.2630097040070325	0.2803571540177003	F	F	F
0.6819400070927131	0.4224300249338739	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225851	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6330337574245277	0.3888882214173961	0.3542169598127032	F	F	F
0.1351966902427790	0.8960299592552659	0.3519472591763417	F	F	F
0.9564060093562290	0.0113173260273740	0.2705234173631794	F	F	F
0.4561412013131729	0.5160705049059686	0.2715775989121667	F	F	F
0.1504001735510698	0.6530576787810389	0.3644796790677347	F	F	F
0.6439252445430768	0.1478261519530690	0.3619073151665830	F	F	F
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7130675855637065	0.9155812889708344	0.3679977977878153	F	F	F
0.3191329449794935	0.4009183324680308	0.3745505776686073	F	F	F
0.1967848979761584	0.1284445725256447	0.3538634516600325	F	F	F
0.6959445149525365	0.6404943048915044	0.3571781669891791	F	F	F
0.8969967951029361	0.5369118688288026	0.2837842546685962	F	F	F
0.4071831667869716	0.0373112527366430	0.2780817493719212	F	F	F
0.3983440710875428	0.2415204259302399	0.4467374102096073	T	T	T
0.5709952666814502	0.2947256157458256	0.5048227115720820	T	T	T
0.7999999999960821	0.7581899815576207	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159594	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.7999999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7701844146296537	0.2648476798336858	0.3505825048031355	F	F	F
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2635359023093429	0.7761500605062892	0.3508537741860067	F	F	F
0.5438185518968695	0.9162198581797867	0.2812821890334689	F	F	F
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0335842325614877	0.4107040063689027	0.2791160078593222	F	F	F
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7954049545742095	0.0431976984068783	0.3414998479561007	F	F	F
0.2802645377181605	0.9990650655815614	0.3534739390039263	F	F	F
0.2953704449178360	0.5458857248756033	0.3487306230309528	F	F	F
0.7883808510543915	0.4963698186527594	0.3684324499962059	F	F	F
0.7615123682125784	0.7814930357631482	0.3487986394793339	F	F	F

0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2823372506155835	0.2599474772544710	0.3549829187353097	F	F	F
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0488154085237369	0.8812367435913657	0.2579410843971743	F	F	F
0.049999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5452009400096216	0.3819229267580226	0.2577271655328488	F	F	F
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871358	0.1011099948343812	F	F	F
0.0489307517146997	0.1478007827257386	0.2722372441523930	F	F	F
0.5500000000156575	0.8999999537758470	0.1011099948343812	F	F	F
0.0485709359758175	0.6461582185940742	0.2721299810542064	F	F	F
0.049999999569383	0.4000000197871358	0.1011099948343812	F	F	F
0.049999999569383	0.8999999537758470	0.1011099948343812	F	F	F
0.5485632864223362	0.6501001568147871	0.2655397918847910	F	F	F
0.5538274902505194	0.1481812440047605	0.2680832383477139	F	F	F
0.3503658883481009	0.5456156448939566	0.4822388044014190	F	F	F
0.4888450448327006	0.4293020104606313	0.4238902062971377	F	F	F
0.6841459099235934	0.5043299204499263	0.4875334514949756	F	F	F
0.5389206273882792	0.6099502464087507	0.4187912007007384	F	F	F
0.4816246787700109	0.3009457401121907	0.4635388698556042	T	T	T
0.6265686410961564	0.3971338657157731	0.4953528594117769	T	T	T

O	In	Pd	Pt	C	H	TS1
1.000000000000000						
10.2175998688000007				0.0000000000000000		0.0000000000000000
0.0000000000000000				14.4497995377000006		0.0000000000000000
0.0000000000000000				0.0000000000000000		20.9857006073000001

O	In	Pd	Pt	C	H
50	32	1	3	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6793983911516506	0.0323426238926530	0.2517494839278598	F	F	F
0.1794432648739459	0.5177206537400849	0.2632929214139565	F	F	F
0.9102614599956738	0.3765061410573765	0.3581934031434670	F	F	F
0.4085216585878868	0.8821119602781877	0.3580020448009762	F	F	F
0.4261859710090619	0.6732078914896533	0.3505980423321802	F	F	F
0.9152868401161456	0.1636569790924511	0.3495553686541584	F	F	F
0.9545099696828743	0.395799996524819	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520422	0.1866900003632566	F	F	F
0.6430456642134317	0.7851466862601200	0.2656003788121950	F	F	F
0.1433595366034126	0.2865368847346517	0.2732298611497086	F	F	F

0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827873	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295254	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476811	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264438	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6897533106013256	0.2681403869919166	0.2541253580343223	F	F	F
0.1868164451064587	0.7607439180304212	0.2536720248371154	F	F	F
0.4180599929386020	0.7820899854365138	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9172750580298725	0.7647995634501257	0.2875813498875601	F	F	F
0.4180858255205848	0.2663929376547927	0.2813376485542705	F	F	F
0.6819400070927131	0.4224300249338810	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225922	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6307859396612372	0.3890952216812167	0.3542981800771159	F	F	F
0.1364339348710075	0.8963565824999620	0.3518773594936135	F	F	F
0.9572954868270713	0.0118559451219227	0.2704568261186040	F	F	F
0.4561405633261728	0.5149192979046120	0.2715106285838189	F	F	F
0.1555630990567920	0.6484799823282188	0.3649755363952494	F	F	F
0.6409531634357961	0.1506866852109212	0.3630408420109319	F	F	F
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7087574789685505	0.9199424413417532	0.3600623453282594	F	F	F
0.3102368209708786	0.3988850536976685	0.3903813977484631	F	F	F
0.2016118613338449	0.1319960332406893	0.3574292543411701	F	F	F
0.6928340689337134	0.6358061225096421	0.3506144938399842	F	F	F
0.8997712845672723	0.5367808849143145	0.2830896668537193	F	F	F
0.4067672707677374	0.0381987574656506	0.2782908164478428	F	F	F
0.7075155639593760	0.7756365385164870	0.4566343918851814	T	T	T
0.5357231886290492	0.7361854753216406	0.5205446533601119	T	T	T
0.799999999960821	0.7581899815576350	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159736	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7681692430607399	0.2663152863995961	0.3507575753084922	F	F	F

0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2644817041810015	0.7751525432821680	0.3506263553899984	F	F	F
0.5477936907092840	0.9175216028576187	0.2814955797500716	F	F	F
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0323388966921954	0.4116080823183026	0.2785567217958302	F	F	F
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7932749963141745	0.0461636350781305	0.3401423284774125	F	F	F
0.2815975345470747	0.9993033559023488	0.3536624792659353	F	F	F
0.3022645851454939	0.5421879014351632	0.3472938683601825	F	F	F
0.7900213721908216	0.4973285559750380	0.3672514823825850	F	F	F
0.7609405007434447	0.7819620985293056	0.3520405495523136	F	F	F
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2744062998167820	0.2666029118207121	0.3522170646833658	F	F	F
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0475353639121181	0.8808837242944421	0.2584316304838126	F	F	F
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5476943483896903	0.3825685311373164	0.2569537006698184	F	F	F
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871358	0.1011099948343812	F	F	F
0.0478290567517234	0.1476868970460785	0.2715422071919846	F	F	F
0.5500000000156575	0.8999999537758541	0.1011099948343812	F	F	F
0.0495005916108084	0.6460010844220889	0.2729472303299332	F	F	F
0.0499999999569383	0.4000000197871358	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537758541	0.1011099948343812	F	F	F
0.5495422310586378	0.6507745844759398	0.2653720268398132	F	F	F
0.5514056342344134	0.1499096465264955	0.2685213710346588	F	F	F
0.3638859170223157	0.5547727209757412	0.4924565799199172	F	F	F
0.4965338926513496	0.4391936937159926	0.4233128020949550	F	F	F
0.5499244049328382	0.6181260935454844	0.4212950332786889	F	F	F
0.6908991147571442	0.5059334904548223	0.4829856154208017	F	F	F
0.6083102166023124	0.7290088873356524	0.4714279484928809	T	T	T
0.4641654379743300	0.6521951639630289	0.5042358529284199	T	T	T

pd2pt2 TS1

1.0000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O	In	Pd	Pt	C	H
50	32	2	2	1	1

Selective dynamics

Direct

0.1819400070169976	0.5179200200151755	0.1152000000009252	F	F	F
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0.6819400070463573	0.0179200012018939	0.1152000000009252	F	F	F
0.6792494959680866	0.0322083097390049	0.2518082108922286	F	F	F
0.1796084945591474	0.5182330194678570	0.2630290938429596	F	F	F
0.9138259486675793	0.3767687756019029	0.3585129246987862	F	F	F
0.4083171794238467	0.8821932402865613	0.3579118869817393	F	F	F
0.4257788003405025	0.6727700884498304	0.3499152812339617	F	F	F
0.9152141652039631	0.1641770646507226	0.3491794135909956	F	F	F
0.9545099698414390	0.3957999998262451	0.1866900001816276	F	F	F
0.4545100162030877	0.8957999668260399	0.1866900001816276	F	F	F
0.6429289788306249	0.7852956340658963	0.2654087044705307	F	F	F
0.1435033341477734	0.2865175279853744	0.2722493636550425	F	F	F
0.4545100162030877	0.1542000069701785	0.1726800108877526	F	F	F
0.9545099698414390	0.6542000232107696	0.1726800108877526	F	F	F
0.1454900069787115	0.7638599677414035	0.1037499961175854	F	F	F
0.6454899838125741	0.2638599840062099	0.1037499961175854	F	F	F
0.1903399941604107	0.2862900058149904	0.1125700078034555	F	F	F
0.6903399591220492	0.7862899728147710	0.1125700078034555	F	F	F
0.9096599471898728	0.8817800338738593	0.1725899977654990	F	F	F
0.4096599940025882	0.3817800008632233	0.1725899977654990	F	F	F
0.4096599940025882	0.6682199561975537	0.1867800021095292	F	F	F
0.9096599471898728	0.1682200059331933	0.1867800021095292	F	F	F
0.6892491121112556	0.2672669487234529	0.2534077760961537	F	F	F
0.1865840364612694	0.7608985061502906	0.2535882872568607	F	F	F
0.4180599929692974	0.7820899852182563	0.0870100031954095	F	F	F
0.9180600397917971	0.2820900182184687	0.0870100031954095	F	F	F
0.9171316996332166	0.7649393519151815	0.2874828371356983	F	F	F
0.4179921239401594	0.2667685975803948	0.2815745433059007	F	F	F
0.6819400070463573	0.4224300249669426	0.1752299989658965	F	F	F
0.1819400070169976	0.9224299589613025	0.1752299989658965	F	F	F
0.1819400070169976	0.1275800051637148	0.1841400009091316	F	F	F
0.6819400070463573	0.6275799970165963	0.1841400009091316	F	F	F
0.6357774438545931	0.3908405918994404	0.3526798062312437	F	F	F
0.1365359798522974	0.8964886009411899	0.3518622892963208	F	F	F
0.9572987663313626	0.0119211780823392	0.2704056664483403	F	F	F
0.4556627067620695	0.5148549992418552	0.2718495547612534	F	F	F
0.1551800274597568	0.6487192732919027	0.3650002055571946	F	F	F
0.6416171211067621	0.1514800718968630	0.3629655666168929	F	F	F
0.4545100162030877	0.5361400390455131	0.0984700049111495	F	F	F
0.9545099698414390	0.0361399979172035	0.0984700049111495	F	F	F
0.4096599940025882	0.0137099999771024	0.0896599968929479	F	F	F
0.9096599471898728	0.5137100339721385	0.0896599968929479	F	F	F
0.7093010976468719	0.9198690250531243	0.3603549709463181	F	F	F
0.3065105935431021	0.3994224820932502	0.3908023775253824	F	F	F
0.2020367986793090	0.1326501464667231	0.3569688344669686	F	F	F

0.6933656278161706	0.6359870805644761	0.3501448408393273	F	F	F
0.8998689349253723	0.5369213668831350	0.2829016276169298	F	F	F
0.4068651059864834	0.0381464243597733	0.2782175403611831	F	F	F
0.7062062201707349	0.7729775946829207	0.4568123367174906	T	T	T
0.5331386967898339	0.7337715776282963	0.5199572298014417	T	T	T
0.7999999999980432	0.7581899817788198	0.1902599908171680	F	F	F
0.3000000231641877	0.7918100087579916	0.1691199952197238	F	F	F
0.3000000231641877	0.2581899980436262	0.1902599908171680	F	F	F
0.7999999999980432	0.2918100087873938	0.1691199952197238	F	F	F
0.8336300499262208	0.0250000011075358	0.1796899988537035	F	F	F
0.7689622166189451	0.2676789458402880	0.3499278281277682	F	F	F
0.3336300031037212	0.5249999787630841	0.1796899988537035	F	F	F
0.2645202581487212	0.7749548595775053	0.3505833668048766	F	F	F
0.5478532046092113	0.9175020399258926	0.2815491365946770	F	F	F
0.5500000000078273	0.1331900061686895	0.0905399971422867	F	F	F
0.0331071571423749	0.4120172559078554	0.2784414776720396	F	F	F
0.0499999999784677	0.6331899899038689	0.0905399971422867	F	F	F
0.7930106668209547	0.0466244415044912	0.3401431830788297	F	F	F
0.2813446765079775	0.9996297656682458	0.3534713200001676	F	F	F
0.3011729241331338	0.5409293908169772	0.3479735666711079	F	F	F
0.7906702916689525	0.4968076848681449	0.3674021142450954	F	F	F
0.7606007904235312	0.7817501695280669	0.3519453381895303	F	F	F
0.8336300499262208	0.5249999787630841	0.1796899988537035	F	F	F
0.2729726122220129	0.2681858899498124	0.3521014390396644	F	F	F
0.3336300031037212	0.0250000011075358	0.1796899988537035	F	F	F
0.0473472205157037	0.8808596615536715	0.2585479361369636	F	F	F
0.0499999999784677	0.1668100001424335	0.1116700002187869	F	F	F
0.5482685640109537	0.3829733774164197	0.2574204615967446	F	F	F
0.5500000000078273	0.6668099509068028	0.1116700002187869	F	F	F
0.5500000000078273	0.4000000198935751	0.1011099949171879	F	F	F
0.0479564341846768	0.1478502881090904	0.2714678460261837	F	F	F
0.5500000000078273	0.8999999538879351	0.1011099949171879	F	F	F
0.0493019820611522	0.6459903187037810	0.2732096260700132	F	F	F
0.0499999999784677	0.4000000198935751	0.1011099949171879	F	F	F
0.0499999999784677	0.8999999538879351	0.1011099949171879	F	F	F
0.5495461053671846	0.6505382093929200	0.2653345716143392	F	F	F
0.5511254598543616	0.1501276915916350	0.2687875510000453	F	F	F
0.3613102660802596	0.5558759956322206	0.4898920242647549	F	F	F
0.4973456743286988	0.4358106464076172	0.4242981701625155	F	F	F
0.5493863213467876	0.6165008878343841	0.4199743031309993	F	F	F
0.6914307978147463	0.5072558210686822	0.4831357758786083	F	F	F
0.6071901529925725	0.7263590119105601	0.4715382058132676	T	T	T
0.4586522925621566	0.6517857097744512	0.5047198120621301	T	T	T

pd3pt TS1

1.0000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O In Pd Pt C H

50 32 3 1 1 1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6793226838283104	0.0314989645363539	0.2521820629655664	F	F	F
0.1798827561397616	0.5182684975247653	0.2630542321848779	F	F	F
0.9126452132429677	0.3775570014703220	0.3585282280168016	F	F	F
0.4085856258336307	0.8827376282138175	0.3582994036998883	F	F	F
0.4228308745903817	0.6732540768798998	0.3485631417940382	F	F	F
0.9149351096408864	0.1642322694969423	0.3492116548380864	F	F	F
0.9545099696828743	0.395799996524819	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520422	0.1866900003632566	F	F	F
0.6426909175262097	0.7857964322848119	0.2650348888403755	F	F	F
0.1432081392621640	0.2867232286260588	0.2724576457482115	F	F	F
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827873	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295254	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476811	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264438	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6891034925539543	0.2669479048453383	0.2533088844473212	F	F	F
0.1861830881624584	0.7610319305587367	0.2533245343752881	F	F	F
0.4180599929386020	0.7820899854365138	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9175116303118784	0.7652723061391882	0.2869472450788280	F	F	F
0.4178445780126978	0.2664984822926471	0.2814929127287300	F	F	F
0.6819400070927131	0.4224300249338739	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225922	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6353633208852401	0.3909946231128529	0.3523380860892900	F	F	F
0.1369232456318201	0.8965663279940372	0.3517177146327555	F	F	F

0.9573238020918708	0.0120383808231992	0.2704444120075351	F	F	F
0.4560704434781258	0.5146765573500431	0.2714946824008351	F	F	F
0.1532811212321405	0.6487237291766661	0.3651805606899785	F	F	F
0.6419215070061668	0.1512161915187988	0.3629892427264778	F	F	F
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7104115361064842	0.9188365328532129	0.3614004782209577	F	F	F
0.3061719319720453	0.3998606560552957	0.3905988694604403	F	F	F
0.2022373457394337	0.1329274736775687	0.3570645976026228	F	F	F
0.6957702739802158	0.6370627453010300	0.3492424316935754	F	F	F
0.9000328461133975	0.5367667967839722	0.2826376764972593	F	F	F
0.4067526316534966	0.0381853911064383	0.2781465170026678	F	F	F
0.7081750852079836	0.7696123859190607	0.4593352007755414	T	T	T
0.5374252935880648	0.7257365504994482	0.5232300427280521	T	T	T
0.799999999960821	0.7581899815576350	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159736	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7688263364584245	0.2680175105860272	0.3498982437407818	F	F	F
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2646046914096019	0.7747483808625262	0.3502214072068526	F	F	F
0.5474494202350613	0.9173036878913479	0.2817188881929980	F	F	F
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0328222615215878	0.4123816234511040	0.2786418702877285	F	F	F
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7932182045427183	0.0461608439930430	0.3403695098654467	F	F	F
0.2814524352516159	0.9998367675724040	0.3535512175426803	F	F	F
0.3018298419573711	0.5421476136447723	0.3478994233808450	F	F	F
0.7891960021937194	0.4981527382477822	0.3674059126987785	F	F	F
0.7608585479507894	0.7810275170690986	0.3512857395974436	F	F	F
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2732230143519701	0.2685144312829308	0.3522023773164591	F	F	F
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0475570004484140	0.8809621364599920	0.2584881960159322	F	F	F
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5480699567992531	0.3828128172872240	0.2573445781015309	F	F	F
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871358	0.1011099948343812	F	F	F
0.0477134733167190	0.1481542905145616	0.2715796398322041	F	F	F
0.5500000000156575	0.8999999537758541	0.1011099948343812	F	F	F
0.0492100786884677	0.6459315250551825	0.2732568749275757	F	F	F

0.049999999569383	0.4000000197871358	0.1011099948343812	F	F	F
0.049999999569383	0.8999999537758541	0.1011099948343812	F	F	F
0.5494814806051451	0.6506297171171340	0.2658015400517115	F	F	F
0.5511917998982838	0.1498921000958120	0.2689239069800564	F	F	F
0.3646286548641058	0.5551715607551273	0.4908531195534707	F	F	F
0.4968856082226054	0.4364599405993488	0.4237515441765751	F	F	F
0.5493520105658334	0.6189175709125081	0.4192850476833172	F	F	F
0.6890151741990280	0.5076391424448232	0.4830156442086206	F	F	F
0.6112016159570004	0.7227374469016610	0.4745941765750885	T	T	T
0.4617484047546227	0.6474443524127196	0.5094431732641125	T	T	T

PD4 TS1

1.000000000000000

10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9857006073000001

O	In	Pd	C	H
50	32	4	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6795395119927079	0.0312698010497172	0.2523167868147738	F	F	F
0.1796824503498513	0.5178703413607195	0.2626937577842625	F	F	F
0.9110837475653497	0.3781135593084173	0.3592187208020619	F	F	F
0.4086811856454275	0.8825554752476918	0.3581612666781524	F	F	F
0.4225282964052468	0.6720645460549477	0.3486793375466846	F	F	F
0.9149047489356121	0.1640593058308042	0.3492447477562237	F	F	F
0.9545099696828743	0.3957999996524890	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520493	0.1866900003632566	F	F	F
0.6432354298106873	0.7859618912843018	0.2651487774965275	F	F	F
0.1425004091007978	0.2868641706405128	0.2725979158146217	F	F	F
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827873	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295254	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476882	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264509	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6890467711653443	0.2665540532704114	0.2532249042751360	F	F	F

0.1861574618738828	0.7608053517858338	0.2532109680395607	F	F	F
0.4180599929386020	0.7820899854365138	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9179744599270947	0.7651413360018609	0.2868161963419524	F	F	F
0.4174858897127720	0.2662661961089867	0.2814289151515013	F	F	F
0.6819400070927131	0.4224300249338810	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225993	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6348886570648276	0.3905545516179885	0.3518144148174827	F	F	F
0.1374281677738693	0.8960533020763251	0.3516982590367661	F	F	F
0.9575116115734374	0.0118738666496512	0.2705185159518493	F	F	F
0.4564079697764996	0.5143340475327065	0.2709128637289595	F	F	F
0.1540614676539249	0.6474583903140214	0.3650926333949513	F	F	F
0.6419278452027655	0.1509738631059463	0.3630643184035378	F	F	F
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7101770507768137	0.9185382402867006	0.3619170424522551	F	F	F
0.3056355905596533	0.4008464588978029	0.3906028821684941	F	F	F
0.2028848375622516	0.1331486130778856	0.3568902583219185	F	F	F
0.6960820998004991	0.6369361069982631	0.3477443604964563	F	F	F
0.8996999771119931	0.5364176256795474	0.2825171066942715	F	F	F
0.4067945138110787	0.0380427277943198	0.2780942080112396	F	F	F
0.7340928442328334	0.7603167055949811	0.4593637662434134	T	T	T
0.5825289784619585	0.7113955618957419	0.5318068185734077	T	T	T
0.7999999999960821	0.7581899815576350	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159736	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.7999999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7686286646403815	0.2677234639233603	0.3499487626401674	F	F	F
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2654253165352856	0.7738069681191178	0.3500485312448163	F	F	F
0.5476292606122541	0.9170874555735509	0.2818288132770235	F	F	F
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0319446296211296	0.4124557860933891	0.2791020743397112	F	F	F
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7932885975596022	0.0457551214965832	0.3405691330754124	F	F	F
0.2814569384244550	0.9996192507273705	0.3535090024163026	F	F	F
0.3031384187694854	0.5415283779196045	0.3473037816316307	F	F	F
0.7858481556742589	0.4984822336104600	0.3669576809091311	F	F	F
0.7622211889254586	0.7808670226661221	0.3515666109883568	F	F	F

0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2729622726891492	0.2693596968887846	0.3522311934512814	F	F	F
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0477754419436707	0.8807011429554734	0.2586032543206542	F	F	F
0.049999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5478448395279045	0.3823535047076163	0.2570966570369038	F	F	F
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871429	0.1011099948343812	F	F	F
0.0480675609118251	0.1479302050901623	0.2717421841394341	F	F	F
0.5500000000156575	0.8999999537758612	0.1011099948343812	F	F	F
0.0493426524584635	0.6455877730908242	0.2734757698352226	F	F	F
0.049999999569383	0.4000000197871429	0.1011099948343812	F	F	F
0.049999999569383	0.8999999537758612	0.1011099948343812	F	F	F
0.5491428937662661	0.6508287734470315	0.2658900804490401	F	F	F
0.5511320157017465	0.1496254853330967	0.2690139934648812	F	F	F
0.3859641960132478	0.5552491810487226	0.4997029592277116	F	F	F
0.4989113380053354	0.4388151042014528	0.4232979129347001	F	F	F
0.6926361354153272	0.5064638060183739	0.4854072435320447	F	F	F
0.5553008311368970	0.6204541348473214	0.4204367283479797	F	F	F
0.6403758843128244	0.7118637773456342	0.4781423273547603	T	T	T
0.4972217040936399	0.6367359111562011	0.5194800168486423	T	T	T

CONTCAR(5) trans-cooh-pt4

1.000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O In Pt C H

50 32 4 1 1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6800440273306023	0.0270020576185104	0.2539718256025836	T	T	T
0.1775681117160062	0.5201400447678068	0.2629753522472669	T	T	T
0.9128984158882005	0.3764925342302234	0.3587597480126874	T	T	T
0.4078566117130435	0.8829183142148409	0.3588786813308573	T	T	T
0.4251164734765993	0.6749677139492860	0.3492909784966756	T	T	T
0.9168146031045055	0.1621774184579436	0.3501143775886320	T	T	T
0.9545099696828743	0.395799996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6412786719547157	0.7864667325528032	0.2644861453656446	T	T	T
0.1458501395787835	0.2867115705290786	0.2743298632292550	T	T	T

0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6900528415833449	0.2680750552274631	0.2540685141991830	T	T	T
0.1874464652505097	0.7614546802391331	0.2535559965993812	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9173220399919657	0.7652813624758465	0.2852132157510923	T	T	T
0.4202110205231264	0.2635849205369851	0.2804451845081175	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6353266745331183	0.3894971387486805	0.3547788878194353	T	T	T
0.1351104205086244	0.8963735457745443	0.3519534055478672	T	T	T
0.9565084860625319	0.0113823278926120	0.2705024667229949	T	T	T
0.4566301128301831	0.5158528673856750	0.2713784945323496	T	T	T
0.1501504842503536	0.6522672755027230	0.3649645321825687	T	T	T
0.6446624004243944	0.1489328665753860	0.3622869317214068	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7131018643421214	0.9162106935155094	0.3686406038944128	T	T	T
0.3218583099288921	0.4023732598482752	0.3762228669062608	T	T	T
0.1982474823085951	0.1299110342138334	0.3539674165011704	T	T	T
0.6939049856742656	0.6419810976498255	0.3551090760851281	T	T	T
0.8972405644165278	0.5371980215494361	0.2840845371992273	T	T	T
0.4071101721025201	0.0376521815343267	0.2781824057900693	T	T	T
0.3953342043584342	0.2441233649862014	0.4474690834570509	T	T	T
0.5460138720832859	0.2874669456172825	0.5171214823662211	T	T	T
0.799999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7720287564174839	0.2654903267725999	0.3496970356068090	T	T	T

0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2630216500493958	0.7759628893627877	0.3508766215191486	T	T	T
0.5431334768423781	0.9166477509111317	0.2814245443221068	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0338229454805727	0.4115336532651241	0.2787296976764608	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7955132577423498	0.0434664116510604	0.3414934773220466	T	T	T
0.2799693928187281	0.9995464789774360	0.3534674377844169	T	T	T
0.2962666247139154	0.5454349893949697	0.3491048799990182	T	T	T
0.7919506309245818	0.4972120441342085	0.3697371221594423	T	T	T
0.7612546987264182	0.7825002030938748	0.3483206546397568	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2810971074266959	0.2626459720026517	0.3538412291844324	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0488501168709874	0.8812598306124357	0.2578129319355966	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5456569515243217	0.3826245330230336	0.2580689857212235	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0494006617103651	0.1477021756661543	0.2721019721682154	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0488053681236167	0.6461868678672502	0.2723076531417163	T	T	T
0.0499999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5486339605949411	0.6503443791692973	0.2653722318384197	T	T	T
0.5538366690862873	0.1485220717345186	0.2682737028861553	T	T	T
0.3595260504724536	0.5455978337644609	0.4857713820227758	T	T	T
0.4966981462554756	0.4294462271271442	0.4270591762332572	T	T	T
0.6862585164206934	0.5090806479465400	0.4855123164117359	T	T	T
0.5403875477507540	0.6104590247464543	0.4173092376255738	T	T	T
0.4722408680813714	0.3053174590963934	0.4654953582230021	T	T	T
0.5987314643862902	0.3438812369185840	0.5247811307069696	T	T	T

CONTCAR(4) trans-cooh-pdpt3

1.0000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O In Pd Pt C H
50 32 1 3 1 1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6793741845017891	0.0317885188763398	0.2518994003621984	T	T	T

0.1786425046348512	0.5176235179920354	0.2638762891441289	T	T	T
0.9096343570464001	0.3774773492669610	0.3591110034151797	T	T	T
0.4083119485245277	0.8814833653094425	0.3583395222108905	T	T	T
0.4248070954004746	0.6723696425552745	0.3519458592158600	T	T	T
0.9149732169665086	0.1636012599228351	0.3495961884914678	T	T	T
0.9545099696828743	0.3957999996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6414345421324015	0.7845968079451850	0.2653187086177908	T	T	T
0.1429541102879668	0.2861131377838717	0.2733745089477324	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6899220670981521	0.2680805840549141	0.2541395462618397	T	T	T
0.1867514885165136	0.7607122190683597	0.2534943919849013	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9172120854921957	0.7650012571684996	0.2866908474282468	T	T	T
0.4186012469964169	0.2657176309213085	0.2808650283673728	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6319728328618410	0.3900357996522388	0.3537069059978251	T	T	T
0.1358622696798975	0.8960791468025491	0.3518824937203036	T	T	T
0.9569216475051476	0.0117785150291922	0.2705008637690085	T	T	T
0.4545890871115219	0.5148035528098731	0.2716888365870673	T	T	T
0.1520580292269145	0.6498121292187236	0.3649236382101719	T	T	T
0.6410119397708414	0.1506854472213774	0.3630601277912930	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7092258236052942	0.9187964235980814	0.3601143927532746	T	T	T
0.3105872521888742	0.3962115148213599	0.3891349060764426	T	T	T
0.2006432765104194	0.1308259613769565	0.3575362917218854	T	T	T
0.6933585349101321	0.6356176849677055	0.3507053680965768	T	T	T
0.8991551814623975	0.5365422517322358	0.2828871264654467	T	T	T

0.4069101293757100	0.0378825807250038	0.2784406567045821	T	T	T
0.7091695622341376	0.7736095110759322	0.4557473550336653	T	T	T
0.5455330717573972	0.7538730501591360	0.5235756163214731	T	T	T
0.7999999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.7999999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7684147085996003	0.2666052004776205	0.3507475174449937	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2636159063900863	0.7747405471153570	0.3504084970215757	T	T	T
0.5474128944503178	0.9171096724764212	0.2814979702145308	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0313530077515054	0.4113217950709398	0.2789914444285131	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7930762345938618	0.0457478295711979	0.3402943530938956	T	T	T
0.2813694565288927	0.9985990500236923	0.3535962635505285	T	T	T
0.2987350872994625	0.5421918944932642	0.3486701808677566	T	T	T
0.7885137883790705	0.4986268743938851	0.3674879400896103	T	T	T
0.7608937978226891	0.7806534929840012	0.3507119644567069	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2753843498570987	0.2643326626906202	0.3517729867783288	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0476880787689353	0.8809455425183046	0.2582305073497295	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5474448843853850	0.3827615935732425	0.2569267296650324	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0471477410023553	0.1476693970725762	0.2713667032593534	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0488683845396096	0.6458213519815814	0.2725963104780789	T	T	T
0.0499999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5495884214216105	0.6494233356731058	0.2661721518646303	T	T	T
0.5520837562088516	0.1496093420518321	0.2682802511681359	T	T	T
0.3521580763884344	0.5489967511935561	0.4862025486429715	T	T	T
0.4948261642309788	0.4392903465675886	0.4216917250004641	T	T	T
0.5446984282302481	0.6190913762891981	0.4247700965208168	T	T	T
0.6863418681195199	0.5054946364402895	0.4839539243761593	T	T	T
0.6088255128982780	0.7292884188653801	0.4700557297037022	T	T	T
0.4744186284317990	0.7081756374474324	0.5288658385674054	T	T	T

1.0000000000000000
 10.2175998688000007 0.0000000000000000 0.0000000000000000
 0.0000000000000000 14.4497995377000006 0.0000000000000000
 0.0000000000000000 0.0000000000000000 20.9857006073000001

O In Pd Pt C H
 50 32 2 2 1 1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.115200000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.115200000018631	F	F	F
0.6790485345003177	0.0318859679049481	0.2519299029751565	T	T	T
0.1791627679881955	0.5182828073891059	0.2635191790479610	T	T	T
0.9127792588380572	0.3778432053848277	0.3591591875447051	T	T	T
0.4078885911255199	0.8818087832719002	0.3582530389293126	T	T	T
0.4251918499207292	0.6720493447800635	0.3515098312610405	T	T	T
0.9149303241430147	0.1642268891329408	0.3492192813433093	T	T	T
0.9545099696828743	0.3957999996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6412570690643591	0.7847346559817296	0.2651812236235003	T	T	T
0.1426102262870117	0.2863552355483279	0.2722210095565103	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6892350248293297	0.2672568515560414	0.2534904846549964	T	T	T
0.1868095740990157	0.7609867399481800	0.2534840549179407	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9172045817789893	0.7651506479186807	0.2866558352956545	T	T	T
0.4177488523637436	0.2662049075372579	0.2813264462330380	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6361254940871248	0.3914748466628382	0.3521907232756405	T	T	T
0.1357374916848073	0.8961447832951563	0.3519311291899783	T	T	T
0.9568366233980541	0.0118513040506016	0.2704965134543755	T	T	T
0.4545010136174312	0.5145765559729654	0.2721427318854381	T	T	T

0.1524240359410172	0.6498708767367347	0.3649865680659090	T	T	T
0.6416119143614836	0.1516242442280813	0.3630344739546203	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7092640218136808	0.9191201071130379	0.3604765955762446	T	T	T
0.3066721080428607	0.3971348720430967	0.3899361896292106	T	T	T
0.2006000916159323	0.1316533489978795	0.3568446354673824	T	T	T
0.6940511550931348	0.6361326259156357	0.3503552755261126	T	T	T
0.8995950333490441	0.5369770892905095	0.2827447422570728	T	T	T
0.4067258105314409	0.0378683038987546	0.2783959603305917	T	T	T
0.7099599131135008	0.7718487349352188	0.4562288139986705	T	T	T
0.5514250214092584	0.7452734049109182	0.5261308796330653	T	T	T
0.799999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7691308259909917	0.2679249933211523	0.3499259761715265	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2639575352249182	0.7746504334303665	0.3504345043536432	T	T	T
0.5472880627965537	0.9172600488647404	0.2815666052190551	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0324648997529238	0.4120395893631823	0.2787070901908280	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7926713812167847	0.0464361786223577	0.3401991758016578	T	T	T
0.2804952409963235	0.9990720264346464	0.3533617312906188	T	T	T
0.2978486438344063	0.5407401236813740	0.3494246734997901	T	T	T
0.7893695009015715	0.4983360471536500	0.3674072680996687	T	T	T
0.7606990705581751	0.7811533854352959	0.3505422676418704	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2723054103973297	0.2665800456673466	0.3517568192473917	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0475635696377452	0.8810380583117308	0.2583469953811104	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5476210197010332	0.3827264690755996	0.2571851779187284	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0472593848610288	0.1478174927770297	0.2712666456643333	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0492517520396447	0.6459876705276173	0.2727204677904780	T	T	T
0.0499999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537758328	0.1011099948343812	F	F	F

0.5497038185833887	0.6490132638250472	0.2660158120135563	T	T	T
0.5511865521657668	0.1499720961659321	0.2687397435417154	T	T	T
0.3544014841262992	0.5488867100698300	0.4849129090854518	T	T	T
0.4964093415271904	0.4363905758123749	0.4217756002606734	T	T	T
0.5456200998496712	0.6183681448639291	0.4235083361638132	T	T	T
0.6872935916302652	0.5064274949141563	0.4838682864613730	T	T	T
0.6122661255729440	0.7253591491438129	0.4711469495360632	T	T	T
0.4817897611543316	0.6979340561722438	0.5307674655850292	T	T	T

CONTCAR(2) trans-cooh-pd3pt

1.0000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O	In	Pd	Pt	C	H
50	32	3	1	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6793385133490446	0.0312777768095458	0.2522357731524139	T	T	T
0.1794188328393034	0.5183715402373181	0.2636229502622172	T	T	T
0.9115569093378184	0.3784470679302032	0.3591838691641627	T	T	T
0.4083187012512610	0.8825293523216970	0.3585954795899653	T	T	T
0.4221685596845575	0.6728858223189889	0.3499083329658106	T	T	T
0.9147557853753483	0.1640795455847197	0.3493226162088874	T	T	T
0.9545099696828743	0.3957999996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6413026657450658	0.7853481338683608	0.2649095026092567	T	T	T
0.1425382481146684	0.2864457092920034	0.2724442022343183	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6893392486662933	0.2670745955615885	0.2534573989056241	T	T	T
0.1860885913921280	0.7611260978099850	0.2531908449567339	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F

0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9170134063129112	0.7655046750285663	0.2864569591336661	T	T	T
0.4178967643158344	0.2659861674262416	0.2811545804937055	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6356729584711331	0.3912476106402778	0.3520175069943932	T	T	T
0.1364272224282601	0.8965048028046141	0.3517084425086097	T	T	T
0.9568584683422685	0.0119470829083497	0.2704758820939901	T	T	T
0.4549821142407922	0.5144596207026879	0.2717435153089056	T	T	T
0.1504151001757847	0.6502293074442633	0.3651962982713925	T	T	T
0.6419043916942186	0.1512696648168088	0.3630264406029511	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7103487004012408	0.9182605413136500	0.3613394273155279	T	T	T
0.3057419127882142	0.3974656556691727	0.3899045522631823	T	T	T
0.2011064567908463	0.1320152582090870	0.3568715650673795	T	T	T
0.6961411748853124	0.6364857352733821	0.3490996908255113	T	T	T
0.9001267439157061	0.5365327503705259	0.2823884230046971	T	T	T
0.4069174454872595	0.0380401165079221	0.2782120153232199	T	T	T
0.7069357752347400	0.7703562616694910	0.4586504445780406	T	T	T
0.5474885367766120	0.7404849377023197	0.5281692171526302	T	T	T
0.799999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7690771841589381	0.2680748747810071	0.3501255761773407	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2640626864219016	0.7746348060967563	0.3500737209512224	T	T	T
0.5470738247832116	0.9170915645807085	0.2817212241406537	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0322545058283907	0.4122715074681125	0.2790390735285015	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7929489000247543	0.0459170884879683	0.3404785349440971	T	T	T
0.2811417661982745	0.9994321405872881	0.3533693250448806	T	T	T
0.2987595058446928	0.5423967066668069	0.3491565604014255	T	T	T
0.7878388067885069	0.4994282305179496	0.3671494429088042	T	T	T
0.7600521072246096	0.7801580335683838	0.3505739386291111	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2733070269230069	0.2669214965349553	0.3518113549171389	T	T	T

0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0473794765944078	0.8809484814142436	0.2584206504828046	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5476449328040331	0.3827517470013291	0.2571694105378057	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0472078991656772	0.1479864555164525	0.2714620112116677	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0487356636076228	0.6460356531552307	0.2731061618425912	T	T	T
0.0499999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5496424141370255	0.6494233339988966	0.2666412322389249	T	T	T
0.5517416019722106	0.1498059856468359	0.2687344214962266	T	T	T
0.3527689246736614	0.5476429004726242	0.4840369269455707	T	T	T
0.4955590018046649	0.4360276776442760	0.4212597028618958	T	T	T
0.5447053175442775	0.6197769612627368	0.4229076328230121	T	T	T
0.6846999420442756	0.5063425664420507	0.4835523125814802	T	T	T
0.6107107326240211	0.7233155665493243	0.4735399828058107	T	T	T
0.4787802518812470	0.6921547511172221	0.5314772024446341	T	T	T

CONTCAR(3) trans-cooh-pd4

1.0000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O In Pd C H

50 32 4 1 1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6795257221083659	0.0307742060194300	0.2525395698127255	T	T	T
0.1800093995871208	0.5182315088619802	0.2640019352849308	T	T	T
0.9110838881392738	0.3791820126277869	0.3595298204122912	T	T	T
0.4084612869772570	0.8824330841158599	0.3584262527655326	T	T	T
0.4216400560130822	0.6724793649043548	0.3482734394144842	T	T	T
0.9149304258512814	0.1641102896948681	0.3492293881981041	T	T	T
0.9545099696828743	0.3957999996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6426140022806806	0.7857025331991636	0.2651976593074394	T	T	T
0.1424451047103190	0.2865287279595421	0.2725965278281492	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F

0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6890605783082933	0.2668588782770058	0.2533420431689137	T	T	T
0.1860655686823733	0.7610407867886195	0.2529901525736875	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9177894975857299	0.7654214748144454	0.2862740935699506	T	T	T
0.4177918638652400	0.2658614157857357	0.2812351247566625	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6362940655023408	0.3909849219934927	0.3519826211529562	T	T	T
0.1369184785546551	0.8963385751510842	0.3515415600499452	T	T	T
0.9570600322817313	0.0118909717485494	0.2704949514170281	T	T	T
0.4554826693655087	0.5141645544934548	0.2713391714744873	T	T	T
0.1507867373287510	0.6497369072926489	0.3653492099347417	T	T	T
0.6423432580485766	0.1510552167851742	0.3630978387890735	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7107865208476341	0.9178164911808224	0.3625097725957787	T	T	T
0.3058787463764290	0.3977744934554437	0.3907766048766419	T	T	T
0.2018292065254457	0.1321853148763310	0.3567551818160482	T	T	T
0.6965579996136384	0.6370714563709470	0.3478093182454174	T	T	T
0.8998543939852581	0.5364869558455609	0.2820485126988075	T	T	T
0.4070839020821992	0.0378972717929216	0.2781293243923457	T	T	T
0.7401064408082831	0.7565278672979261	0.4602690566044458	T	T	T
0.6025651818380950	0.7187729957809452	0.5384416338278726	T	T	T
0.799999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7692920201261941	0.2680436802584296	0.3498765007297422	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2645255297817783	0.7741609569758410	0.3498682631120289	T	T	T

0.5473068345119785	0.9166663102680275	0.2818710804296174	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0325240863297509	0.4125359080446600	0.2791568894555496	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7932140611452496	0.0455448291434521	0.3407213355145302	T	T	T
0.2813465522897687	0.9993747917113467	0.3533757970196021	T	T	T
0.3002456170158467	0.5422975231310829	0.3501590695312942	T	T	T
0.7857217160918495	0.4998629164466948	0.3662403335098716	T	T	T
0.7626748905377099	0.7802750663427105	0.3511864229322939	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2732615858223184	0.2676136574001475	0.3521356482856675	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0476732155484143	0.8808502481976390	0.2584286336882684	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5473935266461822	0.3826206446928495	0.2572412646688136	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0478592557494295	0.1478036484448495	0.2716369525685707	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0492889149833857	0.6457495256996566	0.2732391286241125	T	T	T
0.0499999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5491652214324176	0.6499291365303250	0.2661432171523543	T	T	T
0.5516129524474067	0.1495510426260367	0.2690075409236883	T	T	T
0.3643749353608357	0.5535828958050288	0.4868407227058356	T	T	T
0.4972720106572197	0.4395111567246417	0.4208828648140184	T	T	T
0.6884870329933932	0.5092110421139964	0.4847958414764975	T	T	T
0.5500039859092354	0.6254866038708187	0.4222284620072188	T	T	T
0.6471837919352339	0.7077785600008966	0.4785872028923990	T	T	T
0.5304476940589424	0.6733609332113417	0.5430213709692779	T	T	T

pt4 TS2

1.0000000000000000

10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9857006073000001

O In Pt C H

50 32 4 1 1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F

0.6798090047260530	0.0275063224283159	0.2542841313811905	F	F	F
0.1780098421634548	0.5200444886732143	0.2630883406356190	F	F	F
0.9134533905919042	0.3764019880093556	0.3588019343677189	F	F	F
0.4076206555910105	0.8830989591293985	0.3588483055103140	F	F	F
0.4249969939219937	0.6747904549018102	0.3490334642160988	F	F	F
0.9165908587371518	0.1621378967874776	0.3501674247753357	F	F	F
0.9545099696828743	0.3957999996524890	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520564	0.1866900003632566	F	F	F
0.6413272975210731	0.7868379755559687	0.2644230339457323	F	F	F
0.1453218786575405	0.2866869311473295	0.2739855580450765	F	F	F
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674828015	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295396	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476953	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264509	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6897769157931180	0.2678870629422576	0.2540570917399734	F	F	F
0.1872982642365741	0.7613507782165740	0.2535311809858456	F	F	F
0.4180599929386020	0.7820899854365280	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9172949181685226	0.7652058890960234	0.2851939455469079	F	F	F
0.4200643661501928	0.2636765617471681	0.2806042214375637	F	F	F
0.6819400070927131	0.4224300249338810	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589226064	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6350489636822871	0.3890546670578061	0.3552372338855108	F	F	F
0.1349247567467060	0.8961760996335215	0.3519402846549013	F	F	F
0.9562449650316296	0.0112941172036116	0.2705564017384532	F	F	F
0.4567655849486059	0.5158183666120024	0.2712585463650186	F	F	F
0.1503397554103429	0.6519849546374559	0.3650500187677181	F	F	F
0.6446150239404673	0.1496270597956695	0.3633474914778816	F	F	F
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7133087981623518	0.9163335790037621	0.3690018076924844	F	F	F
0.3217534469883745	0.4023106448015739	0.3764439881169324	F	F	F
0.1979397747050555	0.1300736042714945	0.3538783806028931	F	F	F
0.6943316843169640	0.6421539905081062	0.3545627595946073	F	F	F

0.8972458430293528	0.5369573208084262	0.2843244987331417	F	F	F
0.4069458084613728	0.0378406273531411	0.2783007263103201	F	F	F
0.3881507203494650	0.2461273570623419	0.4493790989310682	T	T	T
0.5240579920221720	0.2927617562392797	0.5267337307825812	T	T	T
0.799999999960821	0.7581899815576492	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159878	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7724749494329899	0.2659948889419752	0.3492384775401902	F	F	F
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2632283548016119	0.7756691901513619	0.3508153770973976	F	F	F
0.5428821851778096	0.9167228389723476	0.2814325582484543	F	F	F
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0338993692632599	0.4118486644806723	0.2786628032342762	F	F	F
0.049999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7954926206237261	0.0434620994355797	0.3415612534441337	F	F	F
0.2793184242289684	0.9995133016892197	0.3533805590541945	F	F	F
0.2972453118680107	0.5452929389114090	0.3493516358703630	F	F	F
0.7926376388229883	0.4972647798474341	0.3706081031271040	F	F	F
0.7611920648902739	0.7825888399116678	0.3482849973138897	F	F	F
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2798342130236620	0.2632356352066907	0.3534176285655874	F	F	F
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0487677799839332	0.8810909700804928	0.2577710604652665	F	F	F
0.049999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5456208222094290	0.3828254901534720	0.2582940055367473	F	F	F
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871429	0.1011099948343812	F	F	F
0.0492258351322192	0.1476338841432678	0.2719962471514421	F	F	F
0.5500000000156575	0.8999999537758683	0.1011099948343812	F	F	F
0.0488231738431324	0.6459711554993675	0.2724941283669295	F	F	F
0.049999999569383	0.4000000197871429	0.1011099948343812	F	F	F
0.049999999569383	0.8999999537758683	0.1011099948343812	F	F	F
0.5487533501650077	0.6504042964874586	0.2653943883083016	F	F	F
0.5534730243955437	0.1487094103917528	0.2686771586555992	F	F	F
0.3615931226804392	0.5457001685285192	0.4859617710517412	F	F	F
0.4968522136726534	0.4271993191707395	0.4285079004065793	F	F	F
0.6855331984029007	0.5078787213543592	0.4854758955725345	F	F	F
0.5420575477353538	0.6097928886446624	0.4167851195505605	F	F	F
0.4644252947566088	0.3067702046846748	0.4687738062879774	T	T	T
0.6094675804502714	0.2634997913756934	0.5202644058883434	T	T	T

Pdpt3 ts2

1.0000000000000000
10.2175998688000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 14.4497995377000006 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.9857006073000001

O In Pd Pt C H
50 32 1 3 1 1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6795260695792962	0.0313458965436837	0.2520427887277563	F	F	F
0.1788807061398501	0.5176111626340969	0.2642778813835918	F	F	F
0.9100681016446899	0.3778399069229721	0.3593602537095535	F	F	F
0.4085254511212426	0.8814333758898414	0.3582233181475942	F	F	F
0.4241457919899574	0.6720988359760227	0.3514539868682860	F	F	F
0.9149780073292106	0.1637676528952241	0.3495333356256864	F	F	F
0.9545099696828743	0.3957999996524890	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520493	0.1866900003632566	F	F	F
0.6415855286453720	0.7846285178524326	0.2651603563291047	F	F	F
0.1430577339926202	0.2861703850766233	0.2733964919438776	F	F	F
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827873	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295254	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476882	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264509	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6899394610658831	0.2680307811576483	0.2540722905563726	F	F	F
0.1873065464236348	0.7607533227381467	0.2536269441301684	F	F	F
0.4180599929386020	0.7820899854365138	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9180422196155433	0.7650489869496155	0.2863343187118872	F	F	F
0.4188732829056292	0.2656207668778450	0.2808163210184276	F	F	F
0.6819400070927131	0.4224300249338810	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225993	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6328240795743625	0.3905105995632070	0.3536297506543065	F	F	F
0.1360202995261446	0.8962013869934822	0.3519723606738694	F	F	F
0.9571342560323330	0.0117560355225805	0.2705324791108339	F	F	F

0.4544214431064262	0.5146942031258703	0.2717725472505563	F	F	F
0.1514684219271416	0.6500155196832083	0.3651959209257924	F	F	F
0.6414138715535813	0.1506587091849241	0.3629882167221439	F	F	F
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7099941981571902	0.9184476384251212	0.3606060824365542	F	F	F
0.3111497396419338	0.3957242243026045	0.3892561282308620	F	F	F
0.2008012740201224	0.1307963428604921	0.3576156418625018	F	F	F
0.6939830395559312	0.6366611761686016	0.3506358636082894	F	F	F
0.8992089207382179	0.5366735426359170	0.2828802734520295	F	F	F
0.4070632187748302	0.0379026572066294	0.2784105774552543	F	F	F
0.7038563926202386	0.7750525477136847	0.4564504433942673	T	T	T
0.5176194808790129	0.7685183010838230	0.5139163133147449	T	T	T
0.799999999960821	0.7581899815576350	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159736	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7685481311331728	0.2669780690140939	0.3506408570489867	F	F	F
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2635263146257074	0.7747362054192450	0.3507709297371591	F	F	F
0.5472415245794693	0.9169014143148360	0.2814637819338017	F	F	F
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0315091231679077	0.4114647461636949	0.2791298736025780	F	F	F
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7932577340022888	0.0457145772002505	0.3402971495768981	F	F	F
0.2815956769579415	0.9986357638985979	0.3536187187076365	F	F	F
0.2979720587348922	0.5418668142249459	0.3497356307682438	F	F	F
0.7883856556600861	0.4989574887114827	0.3674720051513987	F	F	F
0.7620762131211194	0.7807517705798332	0.3501578339911831	F	F	F
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2757071657685941	0.2642144339590260	0.3517480270898332	F	F	F
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0484389835755223	0.8810125273698404	0.2581562237577160	F	F	F
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5473861370843878	0.3829040316895203	0.2570830372895188	F	F	F
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871429	0.1011099948343812	F	F	F
0.0470348480707656	0.1477982480552029	0.2713527694680238	F	F	F
0.5500000000156575	0.8999999537758612	0.1011099948343812	F	F	F
0.0495199600671867	0.6456907779275269	0.2726098925322233	F	F	F
0.0499999999569383	0.4000000197871429	0.1011099948343812	F	F	F

0.0499999999569383	0.8999999537758612	0.1011099948343812	F	F	F
0.5496656926116827	0.6490331144576444	0.2660924211784703	F	F	F
0.5525110810661999	0.1495598317490661	0.2681969917786731	F	F	F
0.3544874717817876	0.5507435815487938	0.4866636486320743	F	F	F
0.4944617569037248	0.4405255980371905	0.4218971903770949	F	F	F
0.5437947243240231	0.6210996736919157	0.4246797661436617	F	F	F
0.6857742664551623	0.5078334213029052	0.4839676016904875	F	F	F
0.5992381562060487	0.7340971181677176	0.4675696120693331	T	T	T
0.5417144195862987	0.7445161352883363	0.5551048423002412	T	T	T

Pd2pt2 ts2

1.000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O	In	Pd	Pt	C	H
50	32	2	2	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6791341587016788	0.0313190605357079	0.2521660414370999	F	F	F
0.1792440966870643	0.5180824957240944	0.2637522084415878	F	F	F
0.9125613765016354	0.3780241699183122	0.3595020917751270	F	F	F
0.4082590560136339	0.8817429954376337	0.3582791967490664	F	F	F
0.4248152323125467	0.6720344506515232	0.3511613069447961	F	F	F
0.9147750251150626	0.1641434986361716	0.3492341249014288	F	F	F
0.9545099696828743	0.395799996524819	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520422	0.1866900003632566	F	F	F
0.6417524972863973	0.7847635296904656	0.2651041003487293	F	F	F
0.1425866236769906	0.2862838888287271	0.2723823076344516	F	F	F
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827873	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295254	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476811	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264438	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6892359045373126	0.2670684786530799	0.2534792209463888	F	F	F
0.1875018212789854	0.7609908902046811	0.2536240332704409	F	F	F

0.4180599929386020	0.7820899854365138	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9183224016519631	0.7650538375053912	0.2862477083432182	F	F	F
0.4180075370052307	0.2659896751701396	0.2812072347033592	F	F	F
0.6819400070927131	0.4224300249338810	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225922	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6363729753942522	0.3915780042300625	0.3522202044856044	F	F	F
0.1359557678980465	0.8962169357457270	0.3519702273439691	F	F	F
0.9569452065201105	0.0117408330642306	0.2705314761710227	F	F	F
0.4545751100495252	0.5145938577702083	0.2721305701880681	F	F	F
0.1522824444988444	0.6500117390530136	0.3651164227238723	F	F	F
0.6416912976354467	0.1512050216625695	0.3630612624382579	F	F	F
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7102048399488439	0.9184263223318467	0.3610057814699772	F	F	F
0.3064304077027273	0.3967508283720065	0.3898921755640714	F	F	F
0.2007585205253193	0.1315683787885007	0.3568887156312144	F	F	F
0.6944566706570683	0.6370050060273158	0.3505892119020118	F	F	F
0.8995629196813937	0.5370295749548575	0.2828172299091776	F	F	F
0.4068186229714783	0.0377214657660261	0.2783458460170962	F	F	F
0.7065839827299811	0.7725879770403310	0.4569773699614146	T	T	T
0.5225366079046765	0.7630952831245637	0.5161200848709200	T	T	T
0.7999999999960821	0.7581899815576350	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159736	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.7999999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7689701922724765	0.2679042743849749	0.3499336049061057	F	F	F
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2639133658688522	0.7746995417059495	0.3507809382236786	F	F	F
0.5472137191439543	0.9169139991079263	0.2815179178765987	F	F	F
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0321480997428694	0.4119078756495185	0.2789846293535589	F	F	F
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7928980039983742	0.0460746545579482	0.3403248085544632	F	F	F
0.2808209577012590	0.9990787481896177	0.3533731607459600	F	F	F
0.2977698178776507	0.5406311353575077	0.3498329580951278	F	F	F
0.7888701217965917	0.4985263011569927	0.3674498354874274	F	F	F
0.7624905825769730	0.7809432398804219	0.3500480732794102	F	F	F
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F

0.2729860439631295	0.2663470589790862	0.3517625840493892	F	F	F
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0483103273681422	0.8810557869930236	0.2581877973843874	F	F	F
0.049999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5476724542638962	0.3827176886721091	0.2572474764250998	F	F	F
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871358	0.1011099948343812	F	F	F
0.0472390004328958	0.1478186478797667	0.2713049388123068	F	F	F
0.5500000000156575	0.8999999537758541	0.1011099948343812	F	F	F
0.0502257599315570	0.6457638587748917	0.2726399481427677	F	F	F
0.049999999569383	0.4000000197871358	0.1011099948343812	F	F	F
0.049999999569383	0.8999999537758541	0.1011099948343812	F	F	F
0.5497667663444474	0.6489725565187072	0.2659859450099731	F	F	F
0.5513295484812915	0.1497144980094802	0.2687292278689100	F	F	F
0.3552180119600763	0.5502890318023432	0.4846880317892897	F	F	F
0.4951385892472402	0.4376788046083533	0.4216928842892855	F	F	F
0.5445265343756276	0.6207037912204783	0.4238846177796560	F	F	F
0.6855964895835385	0.5083454138987591	0.4840100059976891	F	F	F
0.6028821424298414	0.7310571223733646	0.4686134975833198	T	T	T
0.5490227512417647	0.7381617330687292	0.5567206129731401	T	T	T

Pd3pt ts2

1.0000000000000000

10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9857006073000001

O	In	Pd	Pt	C	H
50	32	3	1	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6793560695200469	0.0309760709053108	0.2523550003065012	F	F	F
0.1795312384351817	0.5182439221497290	0.2638390175403842	F	F	F
0.9117805907133558	0.3789126468279420	0.3593927335248281	F	F	F
0.4085617290202421	0.8824411458828649	0.3584735615607073	F	F	F
0.4216612370040735	0.6728524640945324	0.3497572191655181	F	F	F
0.9148823994206765	0.1642831923644152	0.3491944044281681	F	F	F
0.9545099696828743	0.3957999996524890	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520564	0.1866900003632566	F	F	F
0.6412772962140423	0.7854284877464792	0.2646701035017713	F	F	F
0.1426194180417752	0.2864163123245049	0.2724587020018490	F	F	F
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F

0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674828015	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295396	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476953	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264509	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6893027407123142	0.2670463340897768	0.2533997459607207	F	F	F
0.1864724886043589	0.7611395353238422	0.2532043975471794	F	F	F
0.4180599929386020	0.7820899854365280	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9177667748014713	0.7655714458333662	0.2859402825301132	F	F	F
0.4181931248491750	0.2659438125126741	0.2810947222686764	F	F	F
0.6819400070927131	0.4224300249338810	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589226064	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6363818452990699	0.3916680488165625	0.3519338362266140	F	F	F
0.1364963294820427	0.8965058168973457	0.3517200939949348	F	F	F
0.9570412052332671	0.0119651630731639	0.2704587021614415	F	F	F
0.4548054541141298	0.5145130010854828	0.2717698072186678	F	F	F
0.1497696050173616	0.6504144018795657	0.3652181766678595	F	F	F
0.6422965557544202	0.1512559289138764	0.3630143469955343	F	F	F
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7112176245793194	0.9178522153020552	0.3616063215643024	F	F	F
0.3058721250472090	0.3968564082108799	0.3899448827662582	F	F	F
0.2011331924876103	0.1318296379841328	0.3569024743720561	F	F	F
0.6965942720817253	0.6373486999945612	0.3492042908870090	F	F	F
0.8999326384960327	0.5366467457043882	0.2822740488433126	F	F	F
0.4069728869159093	0.0380409795287093	0.2781910051793588	F	F	F
0.7032991527108763	0.7716061191208539	0.4591930976186447	T	T	T
0.5232480415546945	0.7552544424377103	0.5211576448261042	T	T	T
0.7999999999960821	0.7581899815576492	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159878	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.7999999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7693732714730430	0.2684125574357878	0.3498975663563257	F	F	F
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F

0.2639210287234945	0.7746036435771941	0.3501791643787513	F	F	F
0.5470204451759244	0.9169430747627842	0.2816195780713002	F	F	F
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0322359586919703	0.4122721130282514	0.2790924307522928	F	F	F
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7932005439455310	0.0458930794316004	0.3404314247500508	F	F	F
0.2813017280969845	0.9993637178979213	0.3533827898761643	F	F	F
0.2981417993343740	0.5421963280987825	0.3498667911870825	F	F	F
0.7876125894729711	0.5000249606369778	0.3670989652986663	F	F	F
0.7612024486938296	0.7801305826269598	0.3498201587521237	F	F	F
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2735345464867436	0.2665883437888894	0.3517743545864320	F	F	F
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0479428575986915	0.8810910247384598	0.2582999775718022	F	F	F
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5477122211668828	0.3830193347274786	0.2572790620250416	F	F	F
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871429	0.1011099948343812	F	F	F
0.0474098488460299	0.1479949046906128	0.2713921072413115	F	F	F
0.5500000000156575	0.8999999537758683	0.1011099948343812	F	F	F
0.0492072378527553	0.6458657591217474	0.2728156637914978	F	F	F
0.0499999999569383	0.4000000197871429	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537758683	0.1011099948343812	F	F	F
0.5495513548049118	0.6493537952562818	0.2667095968916300	F	F	F
0.5518701313575178	0.1497292175323253	0.2687715444367669	F	F	F
0.3530907144262443	0.5479299855088584	0.4835265982601769	F	F	F
0.4950256464638443	0.4370154749633244	0.4209706847903334	F	F	F
0.5433708515549682	0.6222153637224395	0.4237077439235293	F	F	F
0.6837831176819691	0.5078958617479117	0.4835736192255666	F	F	F
0.6024086347471780	0.7285781985267121	0.4718697180742097	T	T	T
0.5542793926241103	0.7291714871334137	0.5607140471561207	T	T	T

Pd4 ts2

1.0000000000000000

10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9857006073000001

O	In	Pd	C	H
50	32	4	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F

0.6797783178500083	0.0297850647675801	0.2532096452840022	F	F	F
0.1797381106816900	0.5177925680939310	0.2646256897408890	F	F	F
0.9093520013828069	0.3803364106831140	0.3598781817538566	F	F	F
0.4078627434939222	0.8828598745274974	0.3590927389338319	F	F	F
0.4194345676885618	0.6746159567071857	0.3466525761544119	F	F	F
0.9141767562845260	0.1640971680708248	0.3494675499492530	F	F	F
0.9545099696828743	0.395799996524890	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520422	0.1866900003632566	F	F	F
0.6432316753690372	0.7863073204643669	0.2653041803275755	F	F	F
0.1427321047243666	0.2866941254650470	0.2733602318291020	F	F	F
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827873	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295254	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476811	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264509	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6890429459240792	0.2672081207045025	0.2536403537166620	F	F	F
0.1859416795214841	0.7614723420386795	0.2528771872841347	F	F	F
0.4180599929386020	0.7820899854365138	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9177853477708666	0.7653559869813762	0.2859821415131307	F	F	F
0.4179042457054152	0.2656234813257825	0.2811043813874505	F	F	F
0.6819400070927131	0.4224300249338810	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225922	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6355993937116935	0.3915018376844159	0.3531271201969872	F	F	F
0.1359941057138627	0.8972483626604841	0.3514569407210644	F	F	F
0.9567298600230103	0.0121229977731616	0.2705893948915730	F	F	F
0.4545757625573188	0.5142046969829153	0.2711476973501448	F	F	F
0.1490697300607380	0.6508309718239218	0.3651528928543897	F	F	F
0.6420571503687711	0.1504186298115329	0.3632286993445248	F	F	F
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7124866056130870	0.9159103355529510	0.3644182845416353	F	F	F
0.3102628215651677	0.3956013242701459	0.3934484053536380	F	F	F
0.2017423215263818	0.1322743151946639	0.3566412392319336	F	F	F
0.6939832630105016	0.6362844248975676	0.3449089835533528	F	F	F

0.9001352059395202	0.5364606692665390	0.2813001966580302	F	F	F
0.4073958230185468	0.0376799676660156	0.2780752645295763	F	F	F
0.7677991348856992	0.7318017332481119	0.4594650386998822	T	T	T
0.6527888840042380	0.6873935526457515	0.5469181550492195	T	T	T
0.799999999960821	0.7581899815576350	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159736	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7684241791739410	0.2680702655779257	0.3503565283826404	F	F	F
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2622733907856158	0.7750801700555883	0.3501239945867951	F	F	F
0.5471323906128873	0.9160558459663548	0.2821829924249357	F	F	F
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0318730546718271	0.4121412045988961	0.2794467086064074	F	F	F
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7932042523042995	0.0446220208667114	0.3414066742359267	F	F	F
0.2812955268399051	0.9997498747682556	0.3532914162647387	F	F	F
0.2996370281479344	0.5424033993074886	0.3504009282512328	F	F	F
0.7826840236544612	0.5008238742126423	0.3639122855018755	F	F	F
0.7638587390323011	0.7781300745033590	0.3519133939587320	F	F	F
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2747505436758928	0.2675030821427384	0.3528342112973348	F	F	F
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0470927083214860	0.8809581885200473	0.2583381167047847	F	F	F
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5468798123665835	0.3828171977332957	0.2578420112810420	F	F	F
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871429	0.1011099948343812	F	F	F
0.0477089539719628	0.1480681024164952	0.2719546642216883	F	F	F
0.5500000000156575	0.8999999537758541	0.1011099948343812	F	F	F
0.0492735017394210	0.6459266176778158	0.2731177369805948	F	F	F
0.0499999999569383	0.4000000197871429	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537758541	0.1011099948343812	F	F	F
0.5487242526002376	0.6502340638635076	0.2654617820189102	F	F	F
0.5520178588214435	0.1493247621291189	0.2689177057259684	F	F	F
0.3530201103321886	0.5625374458904631	0.4804222541108629	F	F	F
0.4973236190778181	0.4482929550492472	0.4211470206642218	F	F	F
0.6983555720618355	0.5296368354945002	0.4844746436403256	F	F	F
0.5445513040949024	0.6371321977778592	0.4201626102027163	F	F	F
0.6835799675571081	0.6768059341178869	0.4821991338777707	T	T	T
0.5810626811280954	0.7318514579125620	0.5508553340922928	T	T	T

CONTCAR\4 cis-cooh-pt4

1.000000000000000

10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9857006073000001

O	In	Pt	C	H
50	32	4	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6794919931856143	0.0311643712542207	0.2519220414253383	T	T	T
0.1787013743565353	0.5179588071831489	0.2648392965621937	T	T	T
0.9113749447549182	0.3771148710716261	0.3589508881336556	T	T	T
0.4083087364410432	0.8816378140990651	0.3589905647920659	T	T	T
0.4238808415722701	0.6720168359979439	0.3518413030745080	T	T	T
0.9154083698816535	0.1632488204276612	0.3497225489892486	T	T	T
0.9545099696828743	0.3957999996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6407141161688372	0.7842177459595518	0.2654171777192289	T	T	T
0.1432702235110526	0.2858966681712545	0.2730472088295741	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6902761371372890	0.2679688028022369	0.2541170125004442	T	T	T
0.1873307415944439	0.7611047214439282	0.2536026553529425	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9169486257256096	0.7651800456192746	0.2861848628008445	T	T	T
0.4194602300831463	0.2650508929414670	0.2804080398711335	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6339606631414370	0.3897315992059802	0.3535763741883500	T	T	T
0.1355730129203465	0.8964084239991763	0.3519252500876675	T	T	T

0.9570155673158496	0.0116745411631243	0.2704817891033358	T	T	T
0.4538737419910461	0.5146861908288116	0.2721382702387416	T	T	T
0.1494393497237638	0.6513644228536890	0.3648504048460026	T	T	T
0.6415623842046188	0.1504593841279487	0.3630441087676957	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.013709999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7089238403184268	0.9188103021958227	0.3607024350479691	T	T	T
0.3152121879005989	0.3946933522540021	0.3867128749607716	T	T	T
0.2005087742513822	0.1307616286499922	0.3576927268288728	T	T	T
0.6920345835523847	0.6362583756578672	0.3521197359662054	T	T	T
0.8985623189182164	0.5369821037149762	0.2829746798062303	T	T	T
0.4070609939246523	0.0377166748516444	0.2784234989684649	T	T	T
0.7103723645060498	0.7735178418084985	0.4557453602955945	T	T	T
0.5358860171605926	0.7582248816958455	0.5192636675364568	T	T	T
0.799999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7692549438210179	0.2665417109255159	0.3506248076253726	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2632168784488229	0.7748557351697301	0.3509193962718697	T	T	T
0.5468179190041766	0.9168492809459394	0.2814944872912548	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0322551445382544	0.4115089776573981	0.2788711780212623	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7932455886876610	0.0455986148355549	0.3401670478356067	T	T	T
0.2811252296369844	0.9986826253370324	0.3534570003319004	T	T	T
0.2955828903046012	0.5422656047330747	0.3515836016766016	T	T	T
0.7902528532076474	0.4982756267478479	0.3677562038284918	T	T	T
0.7613657485536862	0.7809886008187092	0.3501682216261841	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2761332058894581	0.2636622022427346	0.3511875721305486	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0482477934678158	0.8809734643343745	0.2580815572822459	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5471601843619069	0.3830873034741913	0.2572031916115520	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0469318196087585	0.1477756119106886	0.2712521047841818	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0491855587716401	0.6459644340945232	0.2725161621056955	T	T	T

0.049999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.049999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5482754200044724	0.6488656592137190	0.2661795778085363	T	T	T
0.5529416146144257	0.1494935732659215	0.2681177667415113	T	T	T
0.3586257894674105	0.5500909825170197	0.4852819101377719	T	T	T
0.4975729298094080	0.4387117081493344	0.4213192073569161	T	T	T
0.5458240801758691	0.6199213281762042	0.4243129063010969	T	T	T
0.6877290700405894	0.5067376386875395	0.4837725128009183	T	T	T
0.6067456529164943	0.7311119048126855	0.4686125433794928	T	T	T
0.5794935947940161	0.8132872572789367	0.5371798270436869	T	T	T

CONTCAR(4) cis- cooh-pdpt3

1.000000000000000

10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9857006073000001

O	In	Pd	Pt	C	H
50	32	1	3	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6794569748901722	0.0313173821022943	0.2520033679800022	T	T	T
0.1787544225555564	0.5177461122283518	0.2642737805676418	T	T	T
0.9101233006852496	0.3775282710766916	0.3592296404003079	T	T	T
0.4083973443048876	0.8816766784852703	0.3588673459389184	T	T	T
0.4243274430944766	0.6719099802262178	0.3521488586423729	T	T	T
0.9149768872287538	0.1636208010458304	0.3495855738028268	T	T	T
0.9545099696828743	0.3957999996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6410080784761547	0.7846100858559524	0.2654192364632593	T	T	T
0.1429449206925071	0.2860479457576375	0.2732624893589488	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6899116859569858	0.2677998765679561	0.2540001599415262	T	T	T

0.1871510444749234	0.7608151777947043	0.2536585642145610	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9172159423003734	0.7651628105958324	0.2864933424538165	T	T	T
0.4187667655922311	0.2655461546273301	0.2807981072502699	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6326846641890498	0.3899703444384812	0.3533767140700235	T	T	T
0.1357557689902151	0.8960830901994683	0.3519405278489884	T	T	T
0.9570284107418914	0.0117418180702700	0.2705493089384490	T	T	T
0.4541081644925526	0.5145852028637421	0.2718225839291577	T	T	T
0.1511622596579016	0.6502227783789465	0.3651337194438540	T	T	T
0.6412674742956455	0.1505916854402187	0.3630204534147978	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7093155224358014	0.9187677242536623	0.3609680501023647	T	T	T
0.3101371769922849	0.3955862595316617	0.3890606716180045	T	T	T
0.2005512131055127	0.1307449981562456	0.3576748074378102	T	T	T
0.6938444992393613	0.6356445241718731	0.3502863074058737	T	T	T
0.8992810551980526	0.5364598300363710	0.2828551093233145	T	T	T
0.4068993325713208	0.0378090189390363	0.2784320897288879	T	T	T
0.7084451464432107	0.7727381590649216	0.4557073644161278	T	T	T
0.5344514515217327	0.7579969216008493	0.5195009631769238	T	T	T
0.7999999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.7999999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7685819996010608	0.2668095822791727	0.3505718230308545	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2636681074332401	0.7746678541491292	0.3507835669166184	T	T	T
0.5471224437059377	0.9169761938565628	0.2815695188418630	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0317158367265478	0.4114658773189674	0.2790899816588635	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7932187301968057	0.0456452074230000	0.3402294116109559	T	T	T
0.2810647119834613	0.9985975457125278	0.3534907144064690	T	T	T
0.2975070727399043	0.5420365817000601	0.3497978778753890	T	T	T
0.7884794696226081	0.4986282620925166	0.3674508804970316	T	T	T
0.7610521359582236	0.7805636710939936	0.3504415800088125	T	T	T

0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2754377895131555	0.2640564419915208	0.3516373708933997	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0479531539897167	0.8809048776274295	0.2581669360794123	T	T	T
0.049999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5473579900062759	0.3828024824630560	0.2569778027336724	T	T	T
0.550000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.550000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0468555905633110	0.1478123770757236	0.2712659323117492	T	T	T
0.550000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0490082124930851	0.6458537032697436	0.2726703112033704	T	T	T
0.049999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.049999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5494144296320584	0.6488593970811110	0.2663093052134400	T	T	T
0.5524206088070542	0.1495176726751879	0.2681882293994633	T	T	T
0.3544126240238654	0.5489261438488029	0.4866773490777234	T	T	T
0.4940804256264855	0.4391713764940803	0.4214323374341973	T	T	T
0.5443367553891960	0.6186985041671349	0.4249535012881367	T	T	T
0.6859158858319816	0.5051896010227850	0.4838740142923754	T	T	T
0.6048548279042194	0.7301125326931839	0.4688002236962490	T	T	T
0.5780359172544038	0.8134092677367022	0.5368141917226978	T	T	T

CONTCAR cis-cooh-pd2pt2

1.000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O	In	Pd	Pt	C	H
50	32	2	2	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6791755109424287	0.0312813900176963	0.2521421713342420	T	T	T
0.1790867407799652	0.5181796016456275	0.2637548039374664	T	T	T
0.9125482059337031	0.3777513568753150	0.3593699436282947	T	T	T
0.4081201596056232	0.8819346807886248	0.3588419563972138	T	T	T
0.4249145016382059	0.6719431749628484	0.3518286682497873	T	T	T
0.9146704815977316	0.1640053468381382	0.3492611319411481	T	T	T
0.9545099696828743	0.395799996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6410267880282206	0.7847683884345145	0.2652896697691247	T	T	T
0.1424195137814550	0.2861553344027286	0.2722006610579655	T	T	T

0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6892184325948492	0.2668664337898790	0.2534347548918063	T	T	T
0.1870754943351827	0.7609440236369238	0.2536572516385434	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9172514070497115	0.7651745764902955	0.2864189212710784	T	T	T
0.4179149001839235	0.2659025619989492	0.2811767728915981	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6361981463773603	0.3911911233026473	0.3520053245111043	T	T	T
0.1357707738395106	0.8960735407739620	0.3519668242269560	T	T	T
0.9567737355144814	0.0117137922568915	0.2705549476455218	T	T	T
0.4542983606900535	0.5145168972817373	0.2722095354475300	T	T	T
0.1518391853517613	0.6501007444275828	0.3651281286270773	T	T	T
0.6415995118533928	0.1510845535834804	0.3631137897074481	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7095608426936764	0.9187029280569234	0.3613568823867084	T	T	T
0.3059560747346879	0.3964561115843495	0.3897474661705331	T	T	T
0.2003211042104454	0.1315036003847325	0.3569623875084105	T	T	T
0.6941781354720860	0.6360146808132470	0.3502913275340802	T	T	T
0.8994581988360579	0.5368039932847424	0.2827828097351457	T	T	T
0.4067502080081624	0.0376654459303936	0.2784238785622577	T	T	T
0.7103337069094593	0.7705260999136030	0.4564504322988014	T	T	T
0.5406513448040400	0.7509368507526872	0.5226330599298592	T	T	T
0.799999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7689221433420030	0.2677480195328670	0.3498800794010108	T	T	T

0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2639269830271687	0.7746050751525217	0.3507366497774527	T	T	T
0.5470410587957275	0.9170073387081885	0.2816642256892194	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0322287443090801	0.4119204108838161	0.2789401634834974	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7927828173311369	0.0459865593085951	0.3402646007618131	T	T	T
0.2803579722306537	0.9990078969778082	0.3533111314304307	T	T	T
0.2971398970750840	0.5407135070636713	0.3499364073811577	T	T	T
0.7889398254930242	0.4982253984980787	0.3674930970400041	T	T	T
0.7610905327988178	0.7807320770593833	0.3504262317508093	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2725306900898232	0.2661267075898905	0.3515765500706607	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0478612084029209	0.8809337539173256	0.2582449316692248	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5475981119173667	0.3826575372081749	0.2571306991181288	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0468886633978087	0.1478117147249591	0.2712404239163604	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0492655470447971	0.6458634241415950	0.2728007018897713	T	T	T
0.0499999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5496520141511709	0.6487535783982779	0.2662195267640826	T	T	T
0.5513486470993030	0.1496714280056395	0.2686903918539869	T	T	T
0.3548855330340785	0.5483835872098268	0.4846235530099037	T	T	T
0.4950525251277185	0.4366289474639728	0.4211325435955189	T	T	T
0.5447010103263779	0.6185009408410238	0.4241433181082712	T	T	T
0.6857895619205223	0.5059403128051727	0.4839234219945965	T	T	T
0.6085722060712797	0.7265484945187737	0.4702901142800897	T	T	T
0.5844146165099957	0.8057406290754727	0.5407550726734414	T	T	T

CONTCAR(2) cis- cooh-pd3pt

1.0000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O	In	Pd	Pt	C	H
50	32	3	1	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
--------------------	--------------------	--------------------	---	---	---

0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6792646831016640	0.0311970125886560	0.2522241297618351	T	T	T
0.1794189376192818	0.5183827764781128	0.2638238368443666	T	T	T
0.9118377082909177	0.3785784811892015	0.3592016991274036	T	T	T
0.4084860519336431	0.8826294450061667	0.3589357458417552	T	T	T
0.4219412956970388	0.6726360654429797	0.3504334657803625	T	T	T
0.9148941553750447	0.1640697741309154	0.3492351938170870	T	T	T
0.9545099696828743	0.3957999996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6406740373933175	0.7852098168280577	0.2648858240889496	T	T	T
0.1425929510155086	0.2863280176877296	0.2723827209687144	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6893321890388719	0.2669437172158950	0.2533514614590047	T	T	T
0.1863007559513505	0.7611324434422571	0.2532565520302796	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9168055477764057	0.7655279808587565	0.2861701413696451	T	T	T
0.4180897774107208	0.2659494047671060	0.2811366612099846	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6362264828471069	0.3912810783804517	0.3516915427134535	T	T	T
0.1363888189359059	0.8963731436501305	0.3517277599949082	T	T	T
0.9570293713461737	0.0119395157664073	0.2704125614838944	T	T	T
0.4544298217841529	0.5143591959731140	0.2718270444339339	T	T	T
0.1495985471575452	0.6505327840471580	0.3652885268619031	T	T	T
0.6422300900908411	0.1511744146653413	0.3630548296269751	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7107176848204020	0.9179155382682325	0.3614015100785295	T	T	T
0.3052619291629668	0.3967541566506014	0.3900399886270307	T	T	T
0.2009474106873341	0.1317522196590986	0.3569440270099449	T	T	T

0.6961937552432147	0.6360937395341182	0.3486220128274908	T	T	T
0.9001884018702739	0.5364533067448463	0.2822278387105968	T	T	T
0.4069644909727472	0.0379623063573149	0.2781981474689559	T	T	T
0.7076143358717317	0.7693568615725326	0.4583489600449582	T	T	T
0.5429782026674843	0.7438171200591057	0.5270491623509557	T	T	T
0.799999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7694314345314197	0.2681712904831102	0.3498688671207404	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2640674594487891	0.7745476812933134	0.3502024577572129	T	T	T
0.5470715280899228	0.9170037922743788	0.2817404274675681	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0323702980784688	0.4122825540434931	0.2790058383163512	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7931213368221250	0.0457748899878965	0.3402941261056185	T	T	T
0.2810148100591121	0.9992964633121062	0.3532400564279143	T	T	T
0.2978001967936876	0.5422564244482260	0.3498656366741741	T	T	T
0.7879609071766538	0.4997260694356456	0.3670192672388950	T	T	T
0.7598839012722820	0.7795112033206024	0.3503445421805651	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2732207140506304	0.2664959033673995	0.3517286124668786	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0473476677067453	0.8808490684354879	0.2583778699187320	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5476522376199284	0.3829780794569402	0.2571488620117961	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0473319457506207	0.1479802613812424	0.2713249274151295	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0486882233752510	0.6460065469040401	0.2730480288440376	T	T	T
0.0499999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5491627672404391	0.6492127062206379	0.2667776331629383	T	T	T
0.5518000255792685	0.1498018594882282	0.2687265371800365	T	T	T
0.3530039983451161	0.5460644698464279	0.4832540684935793	T	T	T
0.4952815136131719	0.4357024201115181	0.4203933232936947	T	T	T
0.5437906395953647	0.6197657792005344	0.4237047756392514	T	T	T
0.6842307742898939	0.5060823099387264	0.4833344216056190	T	T	T
0.6088496230206815	0.7237445413515076	0.4733590064376756	T	T	T
0.5851896434110344	0.7984397986738330	0.5465017672432069	T	T	T

CONTCAR\2) cis- cooh-pd4

1.0000000000000000

10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9857006073000001

O	In	Pd	C	H
50	32	4	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6790500778130806	0.0310778401659420	0.2522666374831815	T	T	T
0.1797455764450930	0.5183871981502648	0.2641839438687157	T	T	T
0.9112425247165774	0.3792462429876480	0.3598169012118078	T	T	T
0.4081519912832405	0.8827763883738697	0.3588152614361988	T	T	T
0.4215379419964265	0.6726604380191219	0.3488261881940318	T	T	T
0.9147204130459201	0.1642011858090200	0.3492085374781624	T	T	T
0.9545099696828743	0.395799996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6417522332757457	0.7856801351374543	0.2650721111124525	T	T	T
0.1420649651683945	0.2865453939304743	0.2725169118981157	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6889973918420651	0.2668935106843904	0.2533210509155026	T	T	T
0.1862000112834821	0.7611754028326487	0.2530684389658333	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9174628323874856	0.7654961835854053	0.2860519634520315	T	T	T
0.4177181230789060	0.2661033864262379	0.2811045880103435	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6365527003629836	0.3911298801979868	0.3518680602752511	T	T	T
0.1362539623298318	0.8962314010811525	0.3516616854401704	T	T	T

0.9568557133436570	0.0119445068345101	0.2704816630739089	T	T	T
0.4550953761647492	0.5142402981673015	0.2714239606211351	T	T	T
0.1497169884154843	0.6503774545568817	0.3654190941368327	T	T	T
0.6419279984997601	0.1513253000405541	0.3631423768879216	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7107077444372365	0.9182165172376173	0.3621288349501199	T	T	T
0.3051855335726401	0.3973520574967040	0.3906927673377183	T	T	T
0.2010404545671634	0.1321262767746276	0.3567570529992139	T	T	T
0.6966828001415735	0.6368470963416399	0.3484700473271829	T	T	T
0.8995502621865725	0.5364437039822505	0.2821504656115295	T	T	T
0.4066395315174844	0.0379165069984424	0.2782080781161298	T	T	T
0.7248229019429360	0.7647644334442987	0.4588445053055068	T	T	T
0.5614408251244143	0.7441046183297360	0.5287288669383727	T	T	T
0.799999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7693558948263188	0.2683029489021465	0.3498011578736495	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2643536057307401	0.7741915877645482	0.3500724131621880	T	T	T
0.5469520956678480	0.9168753942210373	0.2819220948826526	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0322421015825540	0.4126454475045662	0.2793241172848298	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7928564731420948	0.0458828903966264	0.3403431154837193	T	T	T
0.2804110743656381	0.9993814403230843	0.3532642904635992	T	T	T
0.2992127671855727	0.5424173176067129	0.3505781498570784	T	T	T
0.7859124193205318	0.5000444277357801	0.3669442060741872	T	T	T
0.7618773587677197	0.7802179523146435	0.3505927687108610	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2729605938681061	0.2673741513057806	0.3519642268544914	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0475799079667922	0.8808408497075817	0.2583640543635397	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5474580833406435	0.3829806719524953	0.2572119504505253	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0475314542928658	0.1480027440167149	0.2714997795624257	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0491615500112985	0.6457713490347530	0.2732407724969832	T	T	T

0.049999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.049999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5489663776761162	0.6496984000711095	0.2666001528442195	T	T	T
0.5511794952699347	0.1497391838226534	0.2689705812326793	T	T	T
0.3609029436211770	0.5509995072486831	0.4851595945376204	T	T	T
0.4971412267963018	0.4386641685308561	0.4202728771054041	T	T	T
0.5484507091676463	0.6225062363205325	0.4234491752061302	T	T	T
0.6869484407466544	0.5076807813438151	0.4854294916943687	T	T	T
0.6247925230720170	0.7205237339433950	0.4748371287439213	T	T	T
0.6044248840511699	0.8002409391538023	0.5455232478857326	T	T	T

Pt4 ts3

1.000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O	In	Pt	C	H
50	32	4	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6804879854503199	0.0297978544360404	0.2527704978646241	F	F	F
0.1820716773659186	0.5184934719569014	0.2664396679774867	F	F	F
0.9106118695950016	0.3762719420434095	0.3582183839112858	F	F	F
0.4110058478259759	0.8839549497454868	0.3584263916122197	F	F	F
0.4336091057482534	0.6774755983189351	0.3502932649298600	F	F	F
0.9151732183978680	0.1629820748407127	0.3495449883633484	F	F	F
0.9545099696828743	0.3957999996526098	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666523193	0.1866900003632566	F	F	F
0.6422909360384779	0.7861620845651700	0.2641380998301557	F	F	F
0.1433232887342371	0.2852998732426570	0.2730158053732552	F	F	F
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674830289	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726297670	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337479582	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007265717	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6898609878087569	0.2681791926548840	0.2539735717123435	F	F	F

0.1862459186191074	0.7612822714128455	0.2526514407707054	F	F	F
0.4180599929386020	0.7820899854367553	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9152476420241129	0.7647141898670071	0.2874432899596115	F	F	F
0.4189977814067660	0.2639580377636221	0.2797188224380633	F	F	F
0.6819400070927131	0.4224300249340089	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589228693	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6326014678521616	0.3893700456555109	0.3545525024946699	F	F	F
0.1385587562504398	0.8959365710129461	0.3510907623832793	F	F	F
0.9567462608343789	0.0112916122366542	0.2702935023798076	F	F	F
0.4538780217472720	0.5142162872928182	0.2711553924809067	F	F	F
0.1558274026100861	0.6537362388406152	0.3645339586735830	F	F	F
0.6419860313312711	0.1499012838048870	0.3626127190435326	F	F	F
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7104825967943498	0.9188489640776396	0.3643965969353005	F	F	F
0.3196410550566142	0.3885884061800198	0.3864762630065641	F	F	F
0.1984146418011079	0.1290063827128805	0.3567127174967624	F	F	F
0.6942011685021754	0.6282981053710159	0.3426021131850732	F	F	F
0.9014634796825831	0.5357120819597085	0.2827502859842852	F	F	F
0.4072334059797456	0.0385216081289741	0.2778501630931984	F	F	F
0.7542993320340585	0.6801078796922013	0.5418987765561809	T	T	T
0.5164309772817006	0.6942791444137342	0.5121006269669337	T	T	T
0.7999999999960821	0.7581899815578765	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085162152	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.7999999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150764	0.1796899987074170	F	F	F
0.7688936668364263	0.2663035942314451	0.3508283445477431	F	F	F
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2692247371362058	0.7754548654278750	0.3495477145060804	F	F	F
0.5469278726331339	0.9170079441640340	0.2814096548106022	F	F	F
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0348788434852310	0.4123600712046738	0.2791661908052916	F	F	F
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7942972706014544	0.0448973606231107	0.3413680084211705	F	F	F
0.2823115094754840	0.9987019828246417	0.3534203934238320	F	F	F
0.3061611321030142	0.5462737801259863	0.3538488764293888	F	F	F
0.7878788731473065	0.4957616393153330	0.3677926619119560	F	F	F
0.7563692706548011	0.7809812512814673	0.3509569635642293	F	F	F

0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2765411427300677	0.2605473479320537	0.3514767882618131	F	F	F
0.3336300032074320	0.0250000012150764	0.1796899987074170	F	F	F
0.0469542277066637	0.8798553685403476	0.2590245420387305	F	F	F
0.049999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5458954598301133	0.3828184356136646	0.2582190826075248	F	F	F
0.550000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.550000000156575	0.4000000197872637	0.1011099948343812	F	F	F
0.0467848945065938	0.1474565931883944	0.2714182098325821	F	F	F
0.550000000156575	0.8999999537761312	0.1011099948343812	F	F	F
0.0505312737096162	0.6455524593406707	0.2743035831448708	F	F	F
0.049999999569383	0.4000000197872637	0.1011099948343812	F	F	F
0.049999999569383	0.8999999537761312	0.1011099948343812	F	F	F
0.5473501331982291	0.6491433218602012	0.2647640264613784	F	F	F
0.5536106614551457	0.1491549445855398	0.2680478277648461	F	F	F
0.3344597675871910	0.5287804804891252	0.4835892383778102	F	F	F
0.4950309675418936	0.4369170586636812	0.4234722110736868	F	F	F
0.6788664740971839	0.5144928593226012	0.4841544706438583	F	F	F
0.5884107281182978	0.6688252955825860	0.4199889864878372	F	F	F
0.6729553796538568	0.6563672437053683	0.5036709042368486	T	T	T
0.4519814444390917	0.6385641740072857	0.5125575664087263	T	T	T

Pdpt3 ts3

1.0000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O	In	Pd	Pt	C	H
50	32	1	3	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6798915616832133	0.0311763409605703	0.2524872630089803	F	F	F
0.1814034179431872	0.5182860524335808	0.2644184830079581	F	F	F
0.9073911535430668	0.3770309978948703	0.3587887715401834	F	F	F
0.4107221080102974	0.8844229264388730	0.3585370148437619	F	F	F
0.4316551693730446	0.6766385415077565	0.3489553886358863	F	F	F
0.9151878091725294	0.1641358188129445	0.3493129148252052	F	F	F
0.9545099696828743	0.395799996525388	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666521630	0.1866900003632566	F	F	F
0.6441443792884129	0.7868814087664902	0.2644468234808954	F	F	F
0.1414801803826151	0.2866587592643981	0.2728664624288371	F	F	F

0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674828939	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726296320	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337478019	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007265006	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6893518698626764	0.2676963334697007	0.2538688298127525	F	F	F
0.1851121421170845	0.7604519980367357	0.2529874285625340	F	F	F
0.4180599929386020	0.7820899854366203	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9157073156774658	0.7646978485166116	0.2886715595630278	F	F	F
0.4169613846379363	0.2656159437137831	0.2810073686387540	F	F	F
0.6819400070927131	0.4224300249339308	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589227130	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6293235619895299	0.3888557242176560	0.3536627260583813	F	F	F
0.1391952812663675	0.8954354359260819	0.3512432274548374	F	F	F
0.9572246403566567	0.0115974607423013	0.2704316597044851	F	F	F
0.4564969009102811	0.5141465274375747	0.2693843010337389	F	F	F
0.1609373182057325	0.6487382181574972	0.3655677715260879	F	F	F
0.6409813884220341	0.1506682892449405	0.3629506728967797	F	F	F
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7093428138973508	0.9216601589052402	0.3641483660669991	F	F	F
0.3093881114463528	0.3965928855174425	0.3887683084744751	F	F	F
0.2001747249902763	0.1314314536435788	0.3566799780395797	F	F	F
0.6935813085299145	0.6269261796762393	0.3435803395605532	F	F	F
0.9003512226987169	0.5359139053716362	0.2835187503129077	F	F	F
0.4065342637255824	0.0386200845481994	0.2778336978149198	F	F	F
0.8220573391403789	0.6577407387485081	0.5137929882499819	T	T	T
0.6057857722475930	0.7055660118434304	0.5345681620208680	T	T	T
0.799999999960821	0.7581899815577415	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085160802	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150764	0.1796899987074170	F	F	F
0.7675130936415115	0.2664274489806502	0.3509482103137387	F	F	F

0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2700802433701881	0.7744955554088193	0.3490462433990018	F	F	F
0.5473461414544261	0.9176001341970945	0.2816376802013210	F	F	F
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0324755704725703	0.4130686092617424	0.2793483688700178	F	F	F
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7941401238061090	0.0464614814438775	0.3408366296584617	F	F	F
0.2816563356113591	0.9995375678385869	0.3534457947481329	F	F	F
0.3123332925062812	0.5448831316229672	0.3480944086535658	F	F	F
0.7849130636181130	0.4960633582362632	0.3696171403877671	F	F	F
0.7569689772442985	0.7836429515386811	0.3523307076379609	F	F	F
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2724931235463046	0.2658779296745664	0.3520096915647244	F	F	F
0.3336300032074320	0.0250000012150764	0.1796899987074170	F	F	F
0.0466760926194425	0.8797938667433485	0.2592453611704713	F	F	F
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5468946439506794	0.3821950540436703	0.2569011809272226	F	F	F
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871927	0.1011099948343812	F	F	F
0.0473220056099208	0.1478334907078249	0.2713544164904746	F	F	F
0.5500000000156575	0.8999999537759749	0.1011099948343812	F	F	F
0.0497604744717108	0.6451309012504964	0.2751741728262544	F	F	F
0.0499999999569383	0.4000000197871927	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537759749	0.1011099948343812	F	F	F
0.5489776459622959	0.6506312226995874	0.2649471752857551	F	F	F
0.5513667295828810	0.1496526203601363	0.2687467888892314	F	F	F
0.3966616973992103	0.5702265568825808	0.4832244857029124	F	F	F
0.4936771837512239	0.4374611445146357	0.4211803148189333	F	F	F
0.5938248123633301	0.6752273078945805	0.4212958919926848	F	F	F
0.6755579726105339	0.5110297599075508	0.4859732012563782	F	F	F
0.7073056246014318	0.6558663032187795	0.4960801748532333	T	T	T
0.5365748384107292	0.6591177337920443	0.5432142628800589	T	T	T

Pd2pt2 ts3

1.0000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O	In	Pd	Pt	C	H
50	32	2	2	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
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0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6798680929876397	0.0311921774501442	0.2524535922911539	T	T	T
0.1810240422431093	0.5186047280153332	0.2638274162691019	T	T	T
0.9094663719330995	0.3772811940827410	0.3592284586009029	T	T	T
0.4106895111854882	0.8844070853790740	0.3584322793566983	T	T	T
0.4317766659548496	0.6757715580445733	0.3496543750157883	T	T	T
0.9153943295004154	0.1645218261793175	0.3492199337419279	T	T	T
0.9545099696828743	0.3957999996525388	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666521701	0.1866900003632566	F	F	F
0.6439510367054666	0.7866680682181979	0.2645726312194014	T	T	T
0.1416402872425380	0.2867616130226907	0.2723858237392562	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674829010	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726296391	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337478090	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007265006	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6892238595159199	0.2669893807549641	0.2534656394872101	T	T	T
0.1853113972044866	0.7604485773587015	0.2530680370125395	T	T	T
0.4180599929386020	0.7820899854366274	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9158701777005192	0.7648047833811162	0.2885836902562247	T	T	T
0.4170484203548313	0.2657920988926250	0.2810833647468485	T	T	T
0.6819400070927131	0.4224300249339308	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589227201	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6324969629528709	0.3888951541215633	0.3527007043011423	T	T	T
0.1395101543850572	0.8954734806574791	0.3512727408554923	T	T	T
0.9574762128482917	0.0117061887114929	0.2704814162582849	T	T	T
0.4561687747870451	0.5139091178345652	0.2700180879773626	T	T	T
0.1609662115379891	0.6484583765667153	0.3655388478140011	T	T	T
0.6412772914671976	0.1509608763805304	0.3629863990874895	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7093415274510875	0.9220926590583360	0.3640592419235205	T	T	T
0.3072801175435700	0.3985925266144434	0.3882442137559536	T	T	T
0.2012643063371726	0.1323904588968361	0.3566145522719992	T	T	T

0.6931068124073718	0.6260466799039577	0.3434558500469436	T	T	T
0.9003123713727987	0.5359712880163841	0.2833498217063806	T	T	T
0.4065258927414703	0.0385704561070739	0.2778080519033566	T	T	T
0.8238815570668550	0.6563285699239358	0.5144318611359111	T	T	T
0.6065521941792582	0.7068878129908569	0.5325971550367044	T	T	T
0.799999999960821	0.7581899815577486	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085160873	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150764	0.1796899987074170	F	F	F
0.7678630112508955	0.2669620327220841	0.3506069406572720	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2704717374047476	0.7741826059185257	0.3491167120217327	T	T	T
0.5473485629015187	0.9176674985072992	0.2816240301155801	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0326915649610271	0.4131269690887009	0.2793251881063981	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7942024232954026	0.0469042133603566	0.3407531924096716	T	T	T
0.2816227299737548	0.9998746988842484	0.3534583571963950	T	T	T
0.3107621087669941	0.5433581368682212	0.3480956342857056	T	T	T
0.7840605241297283	0.4951851567485548	0.3689004055432790	T	T	T
0.7575375688058656	0.7842936239958860	0.3521824770630531	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2721774176828333	0.2677085014478138	0.3519413587447886	T	T	T
0.3336300032074320	0.0250000012150764	0.1796899987074170	F	F	F
0.0469664213084187	0.8798998744302864	0.2592633424107973	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5472323385852533	0.3820832525192728	0.2570646439737700	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871927	0.1011099948343812	F	F	F
0.0477271041288674	0.1479864307983121	0.2714180142471392	T	T	T
0.5500000000156575	0.8999999537759820	0.1011099948343812	F	F	F
0.0497635709457214	0.6451260086106743	0.2751024376934978	T	T	T
0.0499999999569383	0.4000000197871927	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537759820	0.1011099948343812	F	F	F
0.5484529615805229	0.6504096678020943	0.2651218041754007	T	T	T
0.5511481611848765	0.1496911431258852	0.2689015833479118	T	T	T
0.4023142804537301	0.5709431845553112	0.4815644771976153	T	T	T
0.4960515277542967	0.4342960858514004	0.4215106823686199	T	T	T
0.5967067926358922	0.6752242768147383	0.4212796499472873	T	T	T
0.6757246993576587	0.5103560349860246	0.4869395653382753	T	T	T
0.7099213469289722	0.6545819864222082	0.4957576077600905	T	T	T
0.5385612477708435	0.6605889908195905	0.5441132693092285	T	T	T

Pd3pt ts3

1.00000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O	In	Pd	Pt	C	H
50	32	3	1	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6797180746198990	0.0283410023738284	0.2539492003530484	F	F	F
0.1789553448427696	0.5183592264686752	0.2623683318456216	F	F	F
0.9115972740842722	0.3794706823234151	0.3590675163643766	F	F	F
0.4090035326404546	0.8838524764589408	0.3585022183400994	F	F	F
0.4192837614662253	0.6741823041414250	0.3469068754176163	F	F	F
0.9153455039789193	0.1637119911431668	0.3495780245541624	F	F	F
0.9545099696828743	0.3957999996525245	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666521346	0.1866900003632566	F	F	F
0.6416920458723752	0.7864383707968514	0.2642304075985678	F	F	F
0.1433293762807608	0.2870865836810665	0.2729676435832786	F	F	F
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674828654	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726296035	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337477735	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264864	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6896019553024786	0.2664352872251570	0.2536013478872690	F	F	F
0.1854100340066580	0.7615696234540295	0.2526983539182837	F	F	F
0.4180599929386020	0.7820899854365919	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9171219044254073	0.7656782232946426	0.2852394975597861	F	F	F
0.4183758140682627	0.2660867613059636	0.2816367836972020	F	F	F
0.6819400070927131	0.4224300249339166	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589226845	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6381765353143578	0.3922592546700088	0.3519893463956123	F	F	F

0.1374307452190635	0.8968552661071243	0.3512028015487729	F	F	F
0.9567079270710437	0.0120008149044324	0.2706625722917053	F	F	F
0.4569774287645529	0.5140755802531842	0.2706187793693857	F	F	F
0.1491027958144500	0.6502293605902167	0.3646316775316478	F	F	F
0.6434960417529965	0.1501806694155974	0.3631246128901182	F	F	F
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7142519266323575	0.9155059079653114	0.3666935983221080	F	F	F
0.3094979821767581	0.3997452752343165	0.3909754717081739	F	F	F
0.2018823550901629	0.1327982847275848	0.3568114287204622	F	F	F
0.6912518449493135	0.6405210354348796	0.3549433944696716	F	F	F
0.8976964482551466	0.5379907496732343	0.2824982755013892	F	F	F
0.4065443624240928	0.0386448346710324	0.2779722118420196	F	F	F
0.7649300064322873	0.6775908268159654	0.5164036557746030	T	T	T
0.5207323738376743	0.6544386400397855	0.5374618156542184	T	T	T
0.799999999960821	0.7581899815577131	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085160518	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7702343255058821	0.2680445027545986	0.3502712882091927	F	F	F
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2644225945641665	0.7746421038916864	0.3498006656072263	F	F	F
0.5447059903883513	0.9166074518130642	0.2816334551000708	F	F	F
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0316567850640226	0.4126556601422990	0.2791994000413922	F	F	F
0.049999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7943964880124668	0.0444262106002498	0.3416611709169217	F	F	F
0.2814291605088002	0.0001911812083719	0.3536839739909610	F	F	F
0.3031282222040730	0.5450612805304118	0.3454078186035900	F	F	F
0.7869416886554674	0.5015710223151473	0.3672185736456015	F	F	F
0.7605604863311584	0.7800304999878023	0.3487728211415941	F	F	F
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2740614961967651	0.2683008039407682	0.3527489189518391	F	F	F
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0482148648974388	0.8812948258221525	0.2581864896575610	F	F	F
0.049999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5482455898833720	0.3822602876692187	0.2572654189321426	F	F	F
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871785	0.1011099948343812	F	F	F
0.0480005819483509	0.1482607006297130	0.2718771147347567	F	F	F
0.5500000000156575	0.8999999537759464	0.1011099948343812	F	F	F

0.0488807458160565	0.6463099709594857	0.2727558684692326	F	F	F
0.0499999999569383	0.4000000197871785	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537759464	0.1011099948343812	F	F	F
0.5488642704141569	0.6504008189576638	0.2673470953162607	F	F	F
0.5522625177536469	0.1492586212864992	0.2692319495987050	F	F	F
0.3364475012005812	0.5449662873291672	0.4727576698567972	F	F	F
0.4995429130704494	0.4367340760529999	0.4215546030235018	F	F	F
0.5442153434017101	0.6499068187204813	0.4322461066153451	F	F	F
0.6957152462152507	0.4942870789506344	0.4868080059562203	F	F	F
0.6750971134304464	0.6297479560968782	0.4984008005435001	T	T	T
0.4945267798548301	0.5922785832709110	0.5511410555102101	T	T	T

Pd4 ts3

1.0000000000000000

10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9857006073000001

O	In	Pd	C	H
50	32	4	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6797152527898049	0.0287206945085998	0.2541427550775239	F	F	F
0.1811133000528784	0.5183679788128757	0.2634123775375272	F	F	F
0.9171957171384832	0.3786158489392619	0.3599276715866893	F	F	F
0.4102475528326792	0.8831519429635435	0.3582541816559868	F	F	F
0.4239918004073076	0.6743279488483012	0.3489260981985112	F	F	F
0.9161137689153094	0.1637559773801698	0.3494762793675932	F	F	F
0.9545099696828743	0.395799996525459	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666521701	0.1866900003632566	F	F	F
0.6421080954417206	0.7870099346617891	0.2642542476573055	F	F	F
0.1436076459277729	0.2854318973198815	0.2725952325468057	F	F	F
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674828939	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726296320	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337478090	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007265078	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F

0.6896620292154765	0.2661961615521022	0.2535217108420795	F	F	F
0.1866910478727917	0.7612546028190295	0.2528186180699237	F	F	F
0.4180599929386020	0.7820899854366203	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9178798648357613	0.7658070982163778	0.2850461425009954	F	F	F
0.4180417672291838	0.2664726479465926	0.2827045502970336	F	F	F
0.6819400070927131	0.4224300249339379	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589227201	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6457682891208236	0.3948183240333378	0.3492239849672529	F	F	F
0.1373107124334823	0.8955897556813497	0.3513893561805190	F	F	F
0.9558806028744087	0.0112592874919173	0.2707530466060675	F	F	F
0.4570435090372698	0.5145856493546788	0.2712289582623058	F	F	F
0.1513257276137381	0.6514061856381730	0.3645343338799876	F	F	F
0.6442221328844653	0.1514951540820277	0.3632487400901354	F	F	F
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7139311335154517	0.9170750408758437	0.3677201265663896	F	F	F
0.3064908678855218	0.3907751854398356	0.3920832545922295	F	F	F
0.1970012263216319	0.1283463512564040	0.3578348686667354	F	F	F
0.6953053509307523	0.6435399871538579	0.3563511582945367	F	F	F
0.8991462251425091	0.5380100425148271	0.2825965213434714	F	F	F
0.4061442096637293	0.0390653756423305	0.2783137276193841	F	F	F
0.7175823463678768	0.6640058974300374	0.5465582765967838	T	T	T
0.4779443945367632	0.6308211289948602	0.5265500822415490	T	T	T
0.799999999960821	0.7581899815577415	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085160802	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150764	0.1796899987074170	F	F	F
0.7725052152759559	0.2687955842892151	0.3500286706996434	F	F	F
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2658607420247847	0.7747680140576065	0.3497012347483803	F	F	F
0.5448005671639393	0.9172757496391384	0.2810909436690494	F	F	F
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0339559264763096	0.4124489789185191	0.2789990932493680	F	F	F
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7942558609920596	0.0451956737644679	0.3420108102124928	F	F	F
0.2814939666272807	0.9982969234060448	0.3538483337988581	F	F	F
0.3059014192865845	0.5480027485953158	0.3466156682489299	F	F	F
0.7931683338496356	0.5019651936649296	0.3688506787347592	F	F	F

0.7619392739266644	0.7827912001117951	0.3485063597721734	F	F	F
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2711185088606385	0.2612560858355835	0.3525084134652019	F	F	F
0.3336300032074320	0.0250000012150764	0.1796899987074170	F	F	F
0.0488343642543825	0.8810576512054595	0.2580072768486588	F	F	F
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5488586721057160	0.3825914288846093	0.2568979705640544	F	F	F
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871998	0.1011099948343812	F	F	F
0.0463627474115427	0.1472851322633417	0.2710105033436108	F	F	F
0.5500000000156575	0.8999999537759820	0.1011099948343812	F	F	F
0.0496150255245453	0.6461703301558614	0.2727330533654140	F	F	F
0.0499999999569383	0.4000000197871998	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537759820	0.1011099948343812	F	F	F
0.5496099525513998	0.6507512003780676	0.2670731004151250	F	F	F
0.5525747767859670	0.1496294457739538	0.2693522657714169	F	F	F
0.2809978334196401	0.4825198137975732	0.4658573532220984	F	F	F
0.5056248780719272	0.4359411992316922	0.4165877957795914	F	F	F
0.6954100624507831	0.4966638386153548	0.4875783706804739	F	F	F
0.5541079233431532	0.6491538427146182	0.4294397509625441	F	F	F
0.6441530606482644	0.6297054295418150	0.5084063543385753	T	T	T
0.4548690940455060	0.5643514802246870	0.5214557241668798	T	T	T

CONTCAR(4) -co+oh-pt4

1.0000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O In Pt C H

50 32 4 1 1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6796110179201236	0.0275511823982413	0.2538056607203174	T	T	T
0.1796232907400608	0.5182748453391639	0.2623545679311832	T	T	T
0.9203454585955129	0.3762226986489949	0.3581784411370492	T	T	T
0.4088211740859364	0.8833819009970227	0.3583514984526701	T	T	T
0.4234096633846249	0.6758481293550176	0.3491157008273049	T	T	T
0.9181744676635404	0.1618129207805126	0.3499775753954708	T	T	T
0.9545099696828743	0.3957999996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6415976293086700	0.7853851907998575	0.2652259453295258	T	T	T

0.1468352209373265	0.2859643775544214	0.2738089571158966	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6897505602931844	0.2646925462477157	0.2529107209108616	T	T	T
0.1864165962261666	0.7621883312669055	0.2528471119657425	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9151807129223002	0.7660941563165267	0.2855906541296775	T	T	T
0.4187806372002498	0.2669377595933682	0.2835734787545405	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6507779683724806	0.3899953761246167	0.3484232354640824	T	T	T
0.1354466146106006	0.8971405860249533	0.3516027360125449	T	T	T
0.9562647479210185	0.0115389597248310	0.2703979475780827	T	T	T
0.4567124921662469	0.5145461060053336	0.2716826497017593	T	T	T
0.1486379320902032	0.6534186155762356	0.3626776531742024	T	T	T
0.6453297355827274	0.1494615195340714	0.3626613348066243	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7122630639211707	0.9168541140625734	0.3675784750383855	T	T	T
0.3203833701056169	0.3839952840417169	0.4034842371818925	T	T	T
0.1982562756989594	0.1292013459048462	0.3580740234802420	T	T	T
0.6896270052204869	0.6441152527659852	0.3631750967660068	T	T	T
0.8973362868750598	0.5390356196857482	0.2832990700432632	T	T	T
0.4061123779200955	0.0388725942738475	0.2782121263994028	T	T	T
0.6961939275194098	0.6506396032636701	0.5495268286270942	T	T	T
0.3736363975153978	0.6316289214472022	0.4900263935980576	T	T	T
0.7999999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.7999999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F

0.7747718924905413	0.2658100240475960	0.3495110695522499	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2629451135670209	0.7766890810247418	0.3505663507678847	T	T	T
0.5445700501755226	0.9166870791262340	0.2812707888532344	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0344238489053410	0.4116312862205262	0.2781884553596328	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7951078842429595	0.0437093025868904	0.3414763235900153	T	T	T
0.2814203105232167	0.9990449835796724	0.3539117933948717	T	T	T
0.3021041551443275	0.5509241871371486	0.3436558796046967	T	T	T
0.7994051692381205	0.4996848515084196	0.3696298085676730	T	T	T
0.7598405171818712	0.7820466628456231	0.3502578895722692	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2740438351169132	0.2618784083337289	0.3544294315143190	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0480385311961484	0.8813103198120018	0.2578520393649057	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5494624246026589	0.3817302730195209	0.2566514634604502	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0480917759168165	0.1473783255773355	0.2712016068024425	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0477094027644114	0.6477705658999184	0.2719281900515185	T	T	T
0.0499999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5487587930746969	0.6508975921346689	0.2665599564479848	T	T	T
0.5527709112106791	0.1489884688415728	0.2691723699419910	T	T	T
0.3184080721501203	0.5011502062753124	0.4625686062370704	T	T	T
0.5176319828965177	0.4250860390119797	0.4184237939641804	T	T	T
0.5418715461913308	0.6476462974688530	0.4304325229116515	T	T	T
0.7061906229577488	0.4866263343638408	0.4850367284291295	T	T	T
0.6563985875073186	0.6177423582249659	0.5002320058296448	T	T	T
0.4006215414020389	0.6338077404287077	0.5346560534171090	T	T	T

CONTCAR\4) cooh-co+oh-pdpt3-1-cc

1.0000000000000000

10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9857006073000001

O	In	Pd	Pt	C	H
50	32	1	3	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F

0.6798305117004162	0.0276527477844226	0.2538586370459868	T	T	T
0.1802647325859184	0.5174250130915894	0.2625500428775993	T	T	T
0.9172483278189816	0.3761375937561340	0.3579206702399418	T	T	T
0.4088607530606367	0.8828749300774774	0.3580287317070656	T	T	T
0.4244633191721121	0.6744663081796176	0.3490819444760618	T	T	T
0.9176289114347611	0.1618800727435072	0.3499880356510516	T	T	T
0.9545099696828743	0.395799996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6419880845417865	0.7853388193598434	0.2652057205239302	T	T	T
0.1460259466647713	0.2858953936833615	0.2735974050810910	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6900163809975979	0.2652358554439829	0.2532768676114330	T	T	T
0.1865031721364403	0.7615759591500222	0.2530623560860477	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9159071179617229	0.7653993662616116	0.2859736525428076	T	T	T
0.4186952751855628	0.2667066833571923	0.2829806904761654	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6451370113646959	0.3907171753335561	0.3495688414282299	T	T	T
0.1362067881760254	0.8961472574120606	0.3517939578200995	T	T	T
0.9567445121679299	0.0112983037204017	0.2705245424309908	T	T	T
0.4573813748167339	0.5144323713312460	0.2708426138281794	T	T	T
0.1515355884763778	0.6505442992532267	0.3631686963160519	T	T	T
0.6448256163832582	0.1494725470353302	0.3627825425283717	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7125779540911594	0.9165455770112558	0.3674581035396969	T	T	T
0.3116555535705743	0.3919043779926596	0.3984260166269138	T	T	T
0.1997971126596383	0.1299681614549826	0.3579752070239124	T	T	T
0.6911603389048011	0.6424265195912611	0.3616214020298685	T	T	T

0.8976051321139948	0.5384891546706712	0.2833969637980047	T	T	T
0.4062783193412898	0.0386398994909314	0.2782336555571163	T	T	T
0.6978360719330325	0.6482658558968026	0.5495714135288452	T	T	T
0.3801016793642233	0.6400996620422035	0.4885913946641480	T	T	T
0.799999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7734183654884745	0.2659521513518115	0.3498583712826218	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2641415195370911	0.7751233371448407	0.3506279157354086	T	T	T
0.5447375463664912	0.9165259229794600	0.2813001181418215	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0339575983125613	0.4115392718210131	0.2783563909572777	T	T	T
0.049999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7952240112996094	0.0436321074772721	0.3415004595019937	T	T	T
0.2812094372450318	0.9987852594689102	0.3538278558930372	T	T	T
0.3051195651921148	0.5471113858513164	0.3442959269486821	T	T	T
0.7967005367587063	0.4993639862948740	0.3694289615223241	T	T	T
0.7597615537782261	0.7814713347966133	0.3503184362862513	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2743652448575560	0.2635233250526881	0.3539597685407685	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0482088150330284	0.8808322390588188	0.2581188986919329	T	T	T
0.049999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5493015789485582	0.3816776776671986	0.2565133225585043	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0481161145303020	0.1473700776705229	0.2713938047139521	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0487100783724514	0.6467477832206754	0.2724856147352526	T	T	T
0.049999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.049999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5490234671085901	0.6506615460528309	0.2663159799493329	T	T	T
0.5526761967688856	0.1489491319855816	0.2691988557326894	T	T	T
0.3114756378910002	0.5066630734253863	0.4661512793884413	T	T	T
0.5069658930039296	0.4287768085852903	0.4176326889089736	T	T	T
0.5446651038314130	0.6482275524777918	0.4297909495962813	T	T	T
0.7001331768396852	0.4843100832901897	0.4843339064302228	T	T	T
0.6571969158626914	0.6168482101452284	0.4999984621479356	T	T	T
0.4081462493773316	0.6454802301507598	0.5329273286379532	T	T	T

1.0000000000000000
 10.2175998688000007 0.0000000000000000 0.0000000000000000
 0.0000000000000000 14.4497995377000006 0.0000000000000000
 0.0000000000000000 0.0000000000000000 20.9857006073000001

O In Pd Pt C H
 50 32 2 2 1 1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.115200000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.115200000018631	F	F	F
0.6793968372498597	0.0278573951071905	0.2540594417224997	T	T	T
0.1795102161577041	0.5179698964269844	0.2618272202719928	T	T	T
0.9193955715660953	0.3763014758098438	0.3583160859379866	T	T	T
0.4082411703837345	0.8831443317052766	0.3582620500098673	T	T	T
0.4235279905653796	0.6737871318875241	0.3492755078331677	T	T	T
0.9174380185718639	0.1623547784982480	0.3496464532288715	T	T	T
0.9545099696828743	0.3957999996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6411268323368454	0.7853586782173578	0.2652888851296388	T	T	T
0.1461597351081205	0.2863815326956697	0.2731912775828869	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6895334945060038	0.2647133939328142	0.2529825901231875	T	T	T
0.1865024080937131	0.7618852392076936	0.2531185006681180	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9154859332052330	0.7656469676760207	0.2857679697409829	T	T	T
0.4183400437794035	0.2670698307042313	0.2832304277906495	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6475261585253308	0.3915730052822760	0.3484859200637180	T	T	T
0.1360669885946960	0.8965499233110841	0.3517874447210219	T	T	T
0.9566466735797893	0.0115194656277060	0.2705370689454007	T	T	T
0.4566826373058867	0.5141422198866599	0.2715257356461273	T	T	T

0.1505105288963812	0.6508334611813995	0.3630344795290009	T	T	T
0.6447588419900122	0.1501533185587289	0.3629560262995464	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7125564126125238	0.9167039541958116	0.3674882712184545	T	T	T
0.3150354531469884	0.3950907273694544	0.3975350083027561	T	T	T
0.2006924920307056	0.1315887176057815	0.3578130685179521	T	T	T
0.6911748783891961	0.6418972838469569	0.3604567632884351	T	T	T
0.8978089729264789	0.5385009249538273	0.2830268025721652	T	T	T
0.4057061304148205	0.0387186173102183	0.2783127636281251	T	T	T
0.7071317196524249	0.6550196496843470	0.5460832477130887	T	T	T
0.3826732683733955	0.6416331394108966	0.4888005100577998	T	T	T
0.799999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7736310253873708	0.2667100193362734	0.3494173402694858	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2639506829868558	0.7752974378177330	0.3507337514759908	T	T	T
0.5440615131049565	0.9166591577579062	0.2814764482833644	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0339344640371110	0.4116309602391012	0.2780718167133296	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7947284459560514	0.0441329711523227	0.3415154134318304	T	T	T
0.2804611244296599	-0.0003579088142354	0.3538867318898110	T	T	T
0.3026250137883858	0.5465967765256303	0.3438566783458347	T	T	T
0.7965666691913441	0.4987646914769987	0.3686714932445608	T	T	T
0.7593562974977522	0.7816170726842543	0.3500702237603014	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2733175916254085	0.2665557964297724	0.3542965538199515	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0480687945405453	0.8811111531971002	0.2581003456614060	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5493474869370784	0.3815676738426196	0.2565771884375065	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0485001667182745	0.1476422994987278	0.2714536453047467	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0483848902797665	0.6470931726585548	0.2722581709958155	T	T	T
0.0499999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537758328	0.1011099948343812	F	F	F

0.5486711491903299	0.6504007555432678	0.2664826744133132	T	T	T
0.5517327819052271	0.1491337020547147	0.2694830574106005	T	T	T
0.3169489717954196	0.5082947683902249	0.4651355986941461	T	T	T
0.5147350627238819	0.4306902699422489	0.4188222509180874	T	T	T
0.5456968212946208	0.6475951995537852	0.4291781872240023	T	T	T
0.7083006067299018	0.4877265009269400	0.4857680191208383	T	T	T
0.6624286832281921	0.6198486969435210	0.4985762720500517	T	T	T
0.4115195022612400	0.6468678038773545	0.5330213941671550	T	T	T

CONTCAR(2) -co+oh-pd3pt

1.0000000000000000

10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9857006073000001

O	In	Pd	Pt	C	H
50	32	3	1	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6798498395080941	0.0277987393988894	0.2540655932038973	T	T	T
0.1797087934949246	0.5178559073861919	0.2619800424630725	T	T	T
0.9179626080596108	0.3782252708988025	0.3590277586157384	T	T	T
0.4093165224449180	0.8829893026338169	0.3581284081574125	T	T	T
0.4219059563050038	0.6736541977280908	0.3489187135267002	T	T	T
0.9174708825762750	0.1629070503480179	0.3497633715406110	T	T	T
0.9545099696828743	0.3957999996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6416923358373410	0.7851325297014000	0.2652407375760930	T	T	T
0.1454058690504638	0.2863217742711299	0.2733825062801074	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F
0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6898568949717259	0.2650099333511093	0.2531028441654399	T	T	T
0.1865546314091446	0.7618179828700917	0.2528491565809290	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F

0.9164757533130512	0.7659127224776157	0.2852907616201321	T	T	T
0.4185409946729663	0.2668123860639184	0.2830790153698288	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6475048728576738	0.3922153352714943	0.3486625559208605	T	T	T
0.1368907280400080	0.8963396749798989	0.3516853961022193	T	T	T
0.9564970106035418	0.0115964213093349	0.2706975476178854	T	T	T
0.4570238318900266	0.5139616264108398	0.2716641593753479	T	T	T
0.1488408129250658	0.6512085194110000	0.3630502644627924	T	T	T
0.6451509444846337	0.1504421079117506	0.3630152168854721	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7140713082677337	0.9160702470538880	0.3674622399671108	T	T	T
0.3146430804386000	0.3916111947559031	0.3978914252023955	T	T	T
0.1999704739114350	0.1304011175031192	0.3576209696983241	T	T	T
0.6925338604369102	0.6426245092477672	0.3620349538860026	T	T	T
0.8977807514092504	0.5388385803953568	0.2825210805016312	T	T	T
0.4065765437966604	0.0386948744303837	0.2782018996247686	T	T	T
0.3758579864341414	0.6324467980216895	0.4929190801346692	T	T	T
0.7063458536038709	0.6599653760661468	0.5436944648195166	T	T	T
0.799999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7739579897756386	0.2673540711980849	0.3494596779865873	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2641218822136153	0.7749815578072585	0.3503006808500970	T	T	T
0.5448532581845811	0.9164448931439395	0.2812143179386410	T	T	T
0.5500000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0336821781470675	0.4119447928375592	0.2784481721702647	T	T	T
0.0499999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7948558140171897	0.0442501565101807	0.3416549828872775	T	T	T
0.2814824516825354	0.9997483088090249	0.3535162663570546	T	T	T
0.3024907244349322	0.5480342671522394	0.3439421093509836	T	T	T
0.7946397508438849	0.5012229960632624	0.3678049923419522	T	T	T
0.7610975032133922	0.7809549919897449	0.3496688640813232	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2731370922514031	0.2646414784647604	0.3539196480563334	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F

0.0485407862888607	0.8813057669169240	0.2581334200095213	T	T	T
0.0499999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5493082411746713	0.3817003650466120	0.2565664022819547	T	T	T
0.5500000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.5500000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0481314665411219	0.1475451632437483	0.2713034040007898	T	T	T
0.5500000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0484809868200387	0.6471333944031059	0.2720449998850469	T	T	T
0.0499999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.0499999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5486686424954073	0.6504299654765404	0.2672480267337463	T	T	T
0.5525309269716061	0.1491866615589572	0.2693238338073130	T	T	T
0.3139867954136477	0.5033730919122732	0.4643570161268542	T	T	T
0.5121699353644900	0.4295325700050370	0.4181933438291310	T	T	T
0.5407445883384483	0.6443272177866746	0.4310701175401235	T	T	T
0.7042342866084113	0.4872881146419488	0.4856723815152080	T	T	T
0.6609884994226363	0.6179871682878684	0.4994310115655267	T	T	T
0.4062053197807174	0.6315766733119048	0.5370275832975508	T	T	T

CONTCAR(3) -co+oh-pd4

1.0000000000000000

10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9857006073000001

O	In	Pd	C	H
50	32	4	1	1

Selective dynamics

Direct

0.1819400070339938	0.5179200200303384	0.1152000000018631	F	F	F
0.6819400070927131	0.0179200014037875	0.1152000000018631	F	F	F
0.6792557781462492	0.0276539980587600	0.2541054125377329	T	T	T
0.1795660422558569	0.5175370091105336	0.2619783449035964	T	T	T
0.9188757253969513	0.3782333398551430	0.3598107739129617	T	T	T
0.4088039703596706	0.8826009622580173	0.3582552115423780	T	T	T
0.4223217148421199	0.6726164062418292	0.3501371054056435	T	T	T
0.9173743079053693	0.1627686578882361	0.3496742166179843	T	T	T
0.9545099696828743	0.3957999996524748	0.1866900003632566	F	F	F
0.4545100164061751	0.8957999666520209	0.1866900003632566	F	F	F
0.6413732303826905	0.7851191613391606	0.2653014279921777	T	T	T
0.1449515759363891	0.2862234722175572	0.2732175677150934	T	T	T
0.4545100164061751	0.1542000069403500	0.1726800107755011	F	F	F
0.9545099696828743	0.6542000234215450	0.1726800107755011	F	F	F
0.1454900069574379	0.7638599674827660	0.1037499962351802	F	F	F

0.6454899836251471	0.2638599840124058	0.1037499962351802	F	F	F
0.1903399943208370	0.2862900056299651	0.1125700076069052	F	F	F
0.6903399592441062	0.7862899726295041	0.1125700076069052	F	F	F
0.9096599473797582	0.8817800337476598	0.1725899975309915	F	F	F
0.4096599940051888	0.3817800007264367	0.1725899975309915	F	F	F
0.4096599940051888	0.6682199563951130	0.1867800022190593	F	F	F
0.9096599473797582	0.1682200058663881	0.1867800022190593	F	F	F
0.6895352543865272	0.2646087616988879	0.2529184987910114	T	T	T
0.1869125735424575	0.7616736051941686	0.2529597073801781	T	T	T
0.4180599929386020	0.7820899854364924	0.0870100033908230	F	F	F
0.9180600395836080	0.2820900184369464	0.0870100033908230	F	F	F
0.9166969813577595	0.7659522099113332	0.2848676710971816	T	T	T
0.4180371506814851	0.2669335551873431	0.2831773438544261	T	T	T
0.6819400070927131	0.4224300249338668	0.1752299989317905	F	F	F
0.1819400070339938	0.9224299589225708	0.1752299989317905	F	F	F
0.1819400070339938	0.1275800053274239	0.1841400008182603	F	F	F
0.6819400070927131	0.6275799970331946	0.1841400008182603	F	F	F
0.6500480396377526	0.3925897382373051	0.3471797140622925	T	T	T
0.1362707932271761	0.8960194061362188	0.3517851977946265	T	T	T
0.9564441310388858	0.0114584587168167	0.2706788836658589	T	T	T
0.4567935464518058	0.5142241715729341	0.2715632735788560	T	T	T
0.1488000445679347	0.6509056904180568	0.3628572375178791	T	T	T
0.6451311582094803	0.1507494050146292	0.3630704645619360	T	T	T
0.4545100164061751	0.5361400390910305	0.0984700048222891	F	F	F
0.9545099696828743	0.0361399978344039	0.0984700048222891	F	F	F
0.4096599940051888	0.0137099999541945	0.0896599967858833	F	F	F
0.9096599473797582	0.5137100339442853	0.0896599967858833	F	F	F
0.7138489697473531	0.9163294139088975	0.3677611346509408	T	T	T
0.3128919609697718	0.3922528171690161	0.3978654909782833	T	T	T
0.2000271076842779	0.1305482306945436	0.3575874484548862	T	T	T
0.6924179296979887	0.6446571435229131	0.3636895852443800	T	T	T
0.8974907386119853	0.5386939955140946	0.2825695592111472	T	T	T
0.4060474752561376	0.0384211523812752	0.2783332079945637	T	T	T
0.7084218510628375	0.6609917081119860	0.5447035870938848	T	T	T
0.3726305627330504	0.6325881414190562	0.4934725145786487	T	T	T
0.799999999960821	0.7581899815576136	0.1902599906343454	F	F	F
0.3000000233283728	0.7918100085159523	0.1691199954394378	F	F	F
0.3000000233283728	0.2581899980872535	0.1902599906343454	F	F	F
0.799999999960821	0.2918100085747710	0.1691199954394378	F	F	F
0.8336300498524380	0.0250000012150693	0.1796899987074170	F	F	F
0.7743584054186528	0.2674340048060486	0.3492121051359689	T	T	T
0.3336300032074320	0.5249999785261750	0.1796899987074170	F	F	F
0.2638487034088683	0.7745404571855659	0.3504761408721251	T	T	T
0.5441380104294140	0.9162781224305192	0.2812596723727054	T	T	T

0.550000000156575	0.1331900063373723	0.0905399972845800	F	F	F
0.0330411083036992	0.4118345470505957	0.2786657482918073	T	T	T
0.049999999569383	0.6331899898077324	0.0905399972845800	F	F	F
0.7944646993578246	0.0443426187808456	0.3415702915810428	T	T	T
0.2808662568822058	0.9989101300176202	0.3539299292641971	T	T	T
0.3012856824419501	0.5465168478193903	0.3443315670270835	T	T	T
0.7948125137551258	0.5017097325707525	0.3685795843140269	T	T	T
0.7622012698859137	0.7817858123901260	0.3493826273186542	T	T	T
0.8336300498524380	0.5249999785261750	0.1796899987074170	F	F	F
0.2721545275187864	0.2653498520139124	0.3540003853336060	T	T	T
0.3336300032074320	0.0250000012150693	0.1796899987074170	F	F	F
0.0488518396290445	0.8812292300537123	0.2579468571142272	T	T	T
0.049999999569383	0.1668100002848689	0.1116700004375772	F	F	F
0.5491926851421098	0.3816532932021914	0.2563397630334379	T	T	T
0.550000000156575	0.6668099508135938	0.1116700004375772	F	F	F
0.550000000156575	0.4000000197871287	0.1011099948343812	F	F	F
0.0482592990405664	0.1474044180469392	0.2713390691503790	T	T	T
0.550000000156575	0.8999999537758328	0.1011099948343812	F	F	F
0.0483687017333807	0.6468396822079185	0.2719084753522623	T	T	T
0.049999999569383	0.4000000197871287	0.1011099948343812	F	F	F
0.049999999569383	0.8999999537758328	0.1011099948343812	F	F	F
0.5484850342862657	0.6504138322307753	0.2674846694736033	T	T	T
0.5517541663052370	0.1491415545973425	0.2695659423043111	T	T	T
0.3157103103464536	0.5026321135059320	0.4645749242041717	T	T	T
0.5161280483303159	0.4341206032730227	0.4154429621917046	T	T	T
0.7045559482897374	0.4917360988092767	0.4877372342044382	T	T	T
0.5388551674887836	0.6446523028503321	0.4319701959031192	T	T	T
0.6587323374750511	0.6232483335147521	0.5001929485843064	T	T	T
0.4021047202774994	0.6323191376046609	0.5376849214340709	T	T	T

