

PdnPt(4-n)/In₂O₃ catalysts models

Pt4/In2O3

1.000000000000000		
10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.9857006073000001

O	In	Pt
48	32	4

Selective dynamics

Direct

0.1819400070000015	0.5179200199999983	0.1472299930000034	F	F	F
0.6819400070000015	0.0179200010000002	0.1472299930000034	F	F	F
0.6799630430074957	0.0271345123959957	0.3142087952073199	T	T	T
0.1817179092379596	0.5175432562429229	0.3274973734267047	T	T	T
0.9130420671722591	0.3758284822438426	0.4371471828891474	T	T	T
0.4079660861120107	0.8837175374501078	0.4378008402517349	T	T	T
0.4267539097423516	0.6785574006262343	0.4241215586548748	T	T	T
0.9156860225165383	0.1629943135551819	0.4267118766624952	T	T	T
0.9545099699999966	0.3958000000000013	0.2385899980000019	F	F	F
0.4545100160000004	0.8957999670000021	0.2385899980000019	F	F	F
0.6433245737306827	0.7884018062734054	0.3267416962150896	T	T	T
0.1455048541621339	0.2859555646114896	0.3373060963828153	T	T	T
0.4545100160000004	0.1542000070000000	0.2206899999999976	F	F	F
0.9545099699999966	0.6542000230000014	0.2206899999999976	F	F	F
0.1454900069999994	0.7638599679999984	0.1325899919999998	F	F	F
0.6454899840000010	0.2638599839999998	0.1325899919999998	F	F	F
0.1903399939999986	0.2862900060000015	0.1438599980000035	F	F	F
0.6903399589999992	0.7862899730000024	0.1438599980000035	F	F	F
0.9096599470000015	0.8817800340000019	0.2205699929999980	F	F	F
0.4096599940000019	0.3817800010000028	0.2205699929999980	F	F	F
0.4096599940000019	0.6682199560000015	0.2387099910000003	F	F	F
0.9096599470000015	0.1682200059999985	0.2387099910000003	F	F	F
0.6898021112970583	0.2664370437242382	0.3141022652859193	T	T	T
0.1865782501176249	0.7612044279453878	0.3130984983903706	T	T	T
0.4180599930000000	0.7820899849999989	0.1111999929999996	F	F	F
0.9180600400000003	0.2820900179999981	0.1111999929999996	F	F	F
0.9190479466142425	0.7659324465881210	0.3522734327950481	T	T	T
0.4208279871720652	0.2649356458392920	0.3470450160519634	T	T	T
0.6819400070000015	0.4224300249999970	0.2239500100000029	F	F	F
0.1819400070000015	0.9224299589999987	0.2239500100000029	F	F	F
0.1819400070000015	0.1275800049999987	0.2353300010000012	F	F	F

0.6819400070000015	0.6275799969999980	0.2353300010000012	F	F	F
0.6358335049046191	0.3883114654144719	0.4315713139701490	T	T	T
0.1358285574283958	0.8966302133530600	0.4281015322283028	T	T	T
0.9564894776754931	0.0117615513343107	0.3346056679283121	T	T	T
0.4562912672537340	0.5153629524215363	0.3361356642788154	T	T	T
0.1520773141999759	0.6517782818989797	0.4430731528726422	T	T	T
0.6429369125466601	0.1485747894028545	0.4413387462022308	T	T	T
0.4545100160000004	0.5361400390000028	0.1258399929999996	F	F	F
0.9545099699999966	0.0361399980000030	0.1258399929999996	F	F	F
0.4096599940000019	0.0137100000000032	0.1145799960000033	F	F	F
0.9096599470000015	0.5137100339999989	0.1145799960000033	F	F	F
0.7128357032142475	0.9172468678394415	0.4489286757329503	T	T	T
0.3153999698666230	0.3919848900924185	0.4734306463002370	T	T	T
0.1998020458911306	0.1309098756774807	0.4364932962180707	T	T	T
0.6983844006555792	0.6443893948461041	0.4304446034633871	T	T	T
0.8992358828559286	0.5369859647286525	0.3508717773477686	T	T	T
0.4067239331326433	0.0387299212661887	0.3443131030716447	T	T	T
0.7999999999999972	0.7581899819999975	0.2431499850000023	F	F	F
0.3000000230000026	0.7918100090000024	0.2161299999999997	F	F	F
0.3000000230000026	0.2581899979999989	0.2431499850000023	F	F	F
0.7999999999999972	0.2918100090000024	0.2161299999999997	F	F	F
0.8336300499999965	0.0250000010000022	0.2296400190000014	F	F	F
0.7693041280331768	0.2664018118906111	0.4273815431123077	T	T	T
0.3336300030000032	0.5249999790000004	0.2296400190000014	F	F	F
0.2640229606595474	0.7754448384573295	0.4269726263441370	T	T	T
0.5434866252733154	0.9168778465593328	0.3477720274257531	T	T	T
0.5499999999999972	0.1331900059999995	0.1157099910000028	F	F	F
0.0341958756681161	0.4118121309204192	0.3452176090259954	T	T	T
0.0499999999999972	0.6331899899999982	0.1157099910000028	F	F	F
0.7945440251849238	0.0443358630045239	0.4173209999318528	T	T	T
0.2802676917458526	0.9994921869704492	0.4319148334514858	T	T	T
0.3020628639153330	0.5436755777458311	0.4300281066773329	T	T	T
0.7924345327257580	0.4975549058689678	0.4510293180996903	T	T	T
0.7622675166112192	0.7835698736282636	0.4256562078684900	T	T	T
0.8336300499999965	0.5249999790000004	0.2296400190000014	F	F	F
0.2773515046400993	0.2633870957694945	0.4300785919092469	T	T	T
0.3336300030000032	0.0250000010000022	0.2296400190000014	F	F	F
0.0489791486232984	0.8813421821089934	0.3185138875274899	T	T	T
0.0499999999999972	0.1668099999999981	0.1427199939999966	F	F	F
0.5479959597162783	0.3831982886792503	0.3192190811946757	T	T	T
0.5499999999999972	0.6668099509999976	0.1427199939999966	F	F	F
0.5499999999999972	0.4000000200000002	0.1292199969999999	F	F	F
0.0478647912171081	0.1481435851154588	0.3355460650665034	T	T	T
0.5499999999999972	0.8999999540000019	0.1292199969999999	F	F	F

0.0505195536661425	0.6454255314258321	0.3364783323017322	T	T	T
0.0499999999999972	0.4000000200000002	0.1292199969999999	F	F	F
0.0499999999999972	0.8999999540000019	0.1292199969999999	F	F	F
0.5502634457101748	0.6507798510763371	0.3288966320602602	T	T	T
0.5535877330157322	0.1487727388096571	0.3310199653936947	T	T	T
0.5463487090982956	0.6202003640375777	0.5058162718353764	T	T	T
0.3600279918490961	0.5539360609242127	0.5814392025059100	T	T	T
0.6878474702606853	0.5132971162795869	0.5826549574406789	T	T	T
0.4986171402265359	0.4373074616020720	0.5127579978053926	T	T	T

PdPt3/In2O3

1.0000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.9857006073000001

O	In	Pd	Pt
48	32	1	3

Selective dynamics

Direct

0.1819400070000015	0.5179200199999983	0.1472299930000034	F	F	F
0.6819400070000015	0.0179200010000002	0.1472299930000034	F	F	F
0.6799822452147029	0.0271267616899955	0.3142145505868038	T	T	T
0.1817786035472239	0.5179013519340520	0.3276602117804445	T	T	T
0.9116469370323682	0.3764378642650728	0.4371653939613049	T	T	T
0.4090574246000860	0.8839798197779352	0.4383367925034292	T	T	T
0.4236505131148900	0.6777130494210254	0.4229387030449652	T	T	T
0.9153943683824034	0.1632846111238904	0.4264802162695567	T	T	T
0.9545099699999966	0.3958000000000013	0.2385899980000019	F	F	F
0.4545100160000004	0.8957999670000021	0.2385899980000019	F	F	F
0.6431425236889703	0.7882321305643276	0.3266265044107674	T	T	T
0.1445420941492553	0.2859488108726418	0.3368365931411543	T	T	T
0.4545100160000004	0.1542000070000000	0.2206899999999976	F	F	F
0.9545099699999966	0.6542000230000014	0.2206899999999976	F	F	F
0.1454900069999994	0.7638599679999984	0.1325899919999998	F	F	F
0.6454899840000010	0.2638599839999998	0.1325899919999998	F	F	F
0.1903399939999986	0.2862900060000015	0.1438599980000035	F	F	F
0.6903399589999992	0.7862899730000024	0.1438599980000035	F	F	F
0.9096599470000015	0.8817800340000019	0.2205699929999980	F	F	F
0.4096599940000019	0.3817800010000028	0.2205699929999980	F	F	F
0.4096599940000019	0.6682199560000015	0.2387099910000003	F	F	F
0.9096599470000015	0.1682200059999985	0.2387099910000003	F	F	F
0.6893246895966345	0.2663197393342465	0.3138872789442181	T	T	T
0.1862736699064413	0.7612468807672960	0.3128992693281579	T	T	T

0.4180599930000000	0.7820899849999989	0.1111999929999996	F	F	F
0.9180600400000003	0.2820900179999981	0.1111999929999996	F	F	F
0.9192297193612358	0.7661228563588135	0.3519693604041303	T	T	T
0.4200256958832930	0.2646604602655216	0.3471410658756846	T	T	T
0.6819400070000015	0.4224300249999970	0.2239500100000029	F	F	F
0.1819400070000015	0.9224299589999987	0.2239500100000029	F	F	F
0.1819400070000015	0.1275800049999987	0.2353300010000012	F	F	F
0.6819400070000015	0.6275799969999980	0.2353300010000012	F	F	F
0.6342982780787819	0.3882452522534414	0.4311220057319034	T	T	T
0.1368974294252182	0.8968089632542433	0.4278054671747519	T	T	T
0.9564595369178774	0.0117487949753047	0.3344686872278291	T	T	T
0.4567946710481705	0.5151124046048681	0.3355200493966379	T	T	T
0.1504597924665502	0.6522092764530510	0.4436146321413180	T	T	T
0.6430150034425277	0.1486647869461184	0.4412225292583208	T	T	T
0.4545100160000004	0.5361400390000028	0.1258399929999996	F	F	F
0.9545099699999966	0.0361399980000030	0.1258399929999996	F	F	F
0.4096599940000019	0.0137100000000032	0.1145799960000033	F	F	F
0.9096599470000015	0.5137100339999989	0.1145799960000033	F	F	F
0.7143268226930437	0.9167001762226916	0.4486044250680195	T	T	T
0.3130776177467995	0.3923436338934570	0.4718535936507379	T	T	T
0.1990804614089981	0.1305412374642926	0.4364449714962524	T	T	T
0.6988944215295120	0.6439844552267312	0.4300070069161502	T	T	T
0.8990968262369894	0.5369738534703876	0.3507736624041062	T	T	T
0.4067129913743905	0.0386893601305372	0.3442798519722175	T	T	T
0.7999999999999972	0.7581899819999975	0.2431499850000023	F	F	F
0.3000000230000026	0.7918100090000024	0.2161299999999997	F	F	F
0.3000000230000026	0.2581899979999989	0.2431499850000023	F	F	F
0.7999999999999972	0.2918100090000024	0.2161299999999997	F	F	F
0.8336300499999965	0.0250000010000022	0.2296400190000014	F	F	F
0.7689375052794885	0.2667157652726896	0.4271485926792754	T	T	T
0.3336300030000032	0.5249999790000004	0.2296400190000014	F	F	F
0.2644157832207315	0.7754802615938308	0.4265959014616753	T	T	T
0.5437969666359115	0.9167591925782278	0.3478125747315016	T	T	T
0.5499999999999972	0.1331900059999995	0.1157099910000028	F	F	F
0.0338921082399575	0.4122308399316740	0.3454125623987802	T	T	T
0.0499999999999972	0.6331899899999982	0.1157099910000028	F	F	F
0.7946793728274142	0.0443125382082857	0.4173025369155515	T	T	T
0.2812300082015425	0.9995749627533996	0.4322452464840540	T	T	T
0.3027316706903339	0.5453362122909238	0.4298968479363142	T	T	T
0.7915237882714552	0.4988278975251500	0.4512256548245576	T	T	T
0.7624349698366396	0.7827116748157958	0.4253798211895637	T	T	T
0.8336300499999965	0.5249999790000004	0.2296400190000014	F	F	F
0.2756400499625817	0.2630849515333339	0.4297451868090467	T	T	T
0.3336300030000032	0.0250000010000022	0.2296400190000014	F	F	F

0.0491661599963035	0.8813710620625086	0.3185382172667977	T	T	T
0.049999999999972	0.166809999999981	0.142719993999966	F	F	F
0.5474771902771008	0.3829570919810986	0.3188575512072691	T	T	T
0.549999999999972	0.666809950999976	0.142719993999966	F	F	F
0.549999999999972	0.4000000200000002	0.129219996999999	F	F	F
0.0475275025158970	0.1480834560640158	0.3353702409719702	T	T	T
0.549999999999972	0.8999999540000019	0.129219996999999	F	F	F
0.0502941911730243	0.6454661885866545	0.3367571487095296	T	T	T
0.049999999999972	0.4000000200000002	0.129219996999999	F	F	F
0.049999999999972	0.8999999540000019	0.129219996999999	F	F	F
0.5503408796313458	0.6504859267804532	0.3293821535005614	T	T	T
0.5533206501061287	0.1487358769024716	0.3310731767683795	T	T	T
0.5469062349618392	0.6245186519511958	0.5062852194215237	T	T	T
0.3642512107629959	0.5529326170791660	0.5813875385290732	T	T	T
0.4959994675220363	0.4355509966130246	0.5108967227041989	T	T	T
0.6819346536007262	0.5118939741230767	0.5815733945069378	T	T	T

Pd2Pt2/In2O3

1.000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.9857006073000001

O In Pd Pt
48 32 2 2

Selective dynamics

Direct

0.1819400070000015	0.5179200199999983	0.1472299930000034	F	F	F
0.6819400070000015	0.0179200010000002	0.1472299930000034	F	F	F
0.6798136340267052	0.0272362360224550	0.3141224179211281	T	T	T
0.1816287550486098	0.5180394388532623	0.3270579588575125	T	T	T
0.9137394751596239	0.3764946026369843	0.4376396286109546	T	T	T
0.4083138359187687	0.8839864775308148	0.4381082975490499	T	T	T
0.4236593856874937	0.6770014334425350	0.4230722921984305	T	T	T
0.9151727254868484	0.1635017194236316	0.4263994360464323	T	T	T
0.9545099699999966	0.3958000000000013	0.2385899980000019	F	F	F
0.4545100160000004	0.8957999670000021	0.2385899980000019	F	F	F
0.6429275199125760	0.7883367311550590	0.3265627072817422	T	T	T
0.1443654635976667	0.2860679513795811	0.3361735712968356	T	T	T
0.4545100160000004	0.1542000070000000	0.2206899999999976	F	F	F
0.9545099699999966	0.6542000230000014	0.2206899999999976	F	F	F
0.1454900069999994	0.7638599679999984	0.1325899919999998	F	F	F
0.6454899840000010	0.2638599839999998	0.1325899919999998	F	F	F
0.1903399939999986	0.2862900060000015	0.1438599980000035	F	F	F

0.6903399589999992	0.7862899730000024	0.1438599980000035	F	F	F
0.9096599470000015	0.8817800340000019	0.2205699929999980	F	F	F
0.4096599940000019	0.3817800010000028	0.2205699929999980	F	F	F
0.4096599940000019	0.6682199560000015	0.2387099910000003	F	F	F
0.9096599470000015	0.1682200059999985	0.2387099910000003	F	F	F
0.6889575363563011	0.2656065531870752	0.3134322558405312	T	T	T
0.1860502988895764	0.7612553508136152	0.3128914622354023	T	T	T
0.4180599930000000	0.7820899849999989	0.1111999929999996	F	F	F
0.9180600400000003	0.2820900179999981	0.1111999929999996	F	F	F
0.9189907784668117	0.7661107996855983	0.3518270622573536	T	T	T
0.4199039162492278	0.2649510644891317	0.3473907368090867	T	T	T
0.6819400070000015	0.4224300249999970	0.2239500100000029	F	F	F
0.1819400070000015	0.9224299589999987	0.2239500100000029	F	F	F
0.1819400070000015	0.1275800049999987	0.2353300010000012	F	F	F
0.6819400070000015	0.6275799969999980	0.2353300010000012	F	F	F
0.6375814264190602	0.3891465293225719	0.4301577818147030	T	T	T
0.1366768408517283	0.8965694840625121	0.4279312510292060	T	T	T
0.9564927150152578	0.0118126542573292	0.3344746543994555	T	T	T
0.4564773072053402	0.5148625113879379	0.3359982349771131	T	T	T
0.1509019075911440	0.6515118662692699	0.4434534100100821	T	T	T
0.6429800900493085	0.1491058064093058	0.4413749324254647	T	T	T
0.4545100160000004	0.5361400390000028	0.1258399929999996	F	F	F
0.9545099699999966	0.0361399980000030	0.1258399929999996	F	F	F
0.4096599940000019	0.0137100000000032	0.1145799960000033	F	F	F
0.9096599470000015	0.5137100339999989	0.1145799960000033	F	F	F
0.7139425111260198	0.9169409838012459	0.4486876003241185	T	T	T
0.3103249459818194	0.3941832727093849	0.4722462475169373	T	T	T
0.1997880128700975	0.1315108583960370	0.4359177145415391	T	T	T
0.6989729062641695	0.6441135465570101	0.4300305749298690	T	T	T
0.8987697691367149	0.5369128461415471	0.3506820789544926	T	T	T
0.4067416067130710	0.0386011941886378	0.3442893240329730	T	T	T
0.7999999999999972	0.7581899819999975	0.2431499850000023	F	F	F
0.3000000230000026	0.7918100090000024	0.2161299999999997	F	F	F
0.3000000230000026	0.2581899979999989	0.2431499850000023	F	F	F
0.7999999999999972	0.2918100090000024	0.2161299999999997	F	F	F
0.8336300499999965	0.0250000010000022	0.2296400190000014	F	F	F
0.7693249122343958	0.2673321355090039	0.4266920712941662	T	T	T
0.3336300030000032	0.5249999790000004	0.2296400190000014	F	F	F
0.2644149791154757	0.7749286193909477	0.4265593010859615	T	T	T
0.5436602425941309	0.9168732896634573	0.3479704647288433	T	T	T
0.5499999999999972	0.1331900059999995	0.1157099910000028	F	F	F
0.0340382320042014	0.4124582566985799	0.3454123960840813	T	T	T
0.0499999999999972	0.6331899899999982	0.1157099910000028	F	F	F
0.7941957084041663	0.0447344953830771	0.4171406756279228	T	T	T

0.2804775642760686	0.9998337537539689	0.4320473423937080	T	T	T
0.3020457007825064	0.5434825047699281	0.4301026444268520	T	T	T
0.7909637151507710	0.4979768587677434	0.4512343258550296	T	T	T
0.7622081568312851	0.7829352053468842	0.4252209528917059	T	T	T
0.8336300499999965	0.5249999790000004	0.2296400190000014	F	F	F
0.2745497732393648	0.2653291904795561	0.4296962829105234	T	T	T
0.3336300030000032	0.0250000010000022	0.2296400190000014	F	F	F
0.0490194996813966	0.8813612390147089	0.3186239114069389	T	T	T
0.049999999999972	0.166809999999981	0.1427199939999966	F	F	F
0.5478604881843704	0.3829203910109475	0.3193159792379144	T	T	T
0.549999999999972	0.6668099509999976	0.1427199939999966	F	F	F
0.549999999999972	0.4000000200000002	0.1292199969999999	F	F	F
0.0479584357808157	0.1481405417110664	0.3355965815975135	T	T	T
0.549999999999972	0.8999999540000019	0.1292199969999999	F	F	F
0.0501946226892019	0.6452245885704802	0.3367492600707482	T	T	T
0.049999999999972	0.4000000200000002	0.1292199969999999	F	F	F
0.049999999999972	0.8999999540000019	0.1292199969999999	F	F	F
0.5502535050651738	0.6503419897518271	0.3294516676341170	T	T	T
0.5528553956254957	0.1487960201399306	0.3313074144942718	T	T	T
0.5466826448356351	0.6228549406281700	0.5056720035719355	T	T	T
0.4982802601540444	0.4332908680618459	0.5121527178690863	T	T	T
0.6828001753694652	0.5133313531818893	0.5822535045096805	T	T	T
0.3657727606419058	0.5514934821656284	0.5808456303780546	T	T	T

Pd3Pt/In2O3

1.0000000000000000

10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.9857006073000001

O	In	Pt	Pd
48	32	3	1

Selective dynamics

Direct

0.1807543798434423	0.5162538237694605	0.1512043039725839	F	F	F
0.6867331648872721	0.0158818785048425	0.1357593882947938	F	F	F
0.6766414812704771	0.0270437600982412	0.3054048712483423	T	T	T
0.1769443161836889	0.5156439621160462	0.3308543051855865	T	T	T
0.9068380994306082	0.3722286138436259	0.4391790459717245	T	T	T
0.4082978548815677	0.8839366314131066	0.4358676264939107	T	T	T
0.4242314798825191	0.6792236350912909	0.4187100641701125	T	T	T
0.9108378282596629	0.1603304345396132	0.4238000732168768	T	T	T
0.9450799309904454	0.3949137382621473	0.2406382233922884	F	F	F
0.4498348853838863	0.8944098537147553	0.2378850734373970	F	F	F

0.6400712314414848	0.7873304615432115	0.3199890319741257	T	T	T
0.1389002863147525	0.2858323213085521	0.3362015667251699	T	T	T
0.4506829856441144	0.1562864535042010	0.2199716243710412	F	F	F
0.9531867801323415	0.6508200817200276	0.2315927730873852	F	F	F
0.1235194602030347	0.7633182738237210	0.1192328848650419	F	F	F
0.6220816049528040	0.2662430303350263	0.1167990547483697	F	F	F
0.1847204470617640	0.2834701942544982	0.1421490377690660	F	F	F
0.6863511734632226	0.7794004407303419	0.1356497127132670	F	F	F
0.9048060281166812	0.8786951925684647	0.2178137984176516	F	F	F
0.4028361214298215	0.3825364446881210	0.2206066545489023	F	F	F
0.4007667692523285	0.6606687395001529	0.2333385266651575	F	F	F
0.9019097346236151	0.1644847735247978	0.2361565933850613	F	F	F
0.6866148040929382	0.2638976853044752	0.3066967395351630	T	T	T
0.1852684187712386	0.7586656995687125	0.3075106233685315	T	T	T
0.4197002433186228	0.7828804674168026	0.1072047259510924	F	F	F
0.9204640714685439	0.2842971093496018	0.1082328699634658	F	F	F
0.9172180225613176	0.7672207736344840	0.3524173692933192	T	T	T
0.4153862927899249	0.2650271803344957	0.3451721959097359	T	T	T
0.6792027412891244	0.4193365147432928	0.2199050104824849	F	F	F
0.1829787504853755	0.9181241793272505	0.2193989454229737	F	F	F
0.1787785573954537	0.1273573764215428	0.2409161868268015	F	F	F
0.6793035704335466	0.6256299155370684	0.2335465721899439	F	F	F
0.6310076778478789	0.3850329921743287	0.4288665520217549	T	T	T
0.1364820978465441	0.8969566882009123	0.4242474314393345	T	T	T
0.9533634413494911	0.0092395859465279	0.3287941895645946	T	T	T
0.4543781826627785	0.5134367139379619	0.3345742300234760	T	T	T
0.1536129798355734	0.6534467880805042	0.4450305672760568	T	T	T
0.6392358192964971	0.1461306899741757	0.4365204352728627	T	T	T
0.4821831014900013	0.5327713444985207	0.1126132989927768	F	F	F
0.9840656240798111	0.0333763322357683	0.1205712731739439	F	F	F
0.4183975654083980	0.0177015755663987	0.1083088574149187	F	F	F
0.9181600780561610	0.5195208245786844	0.1128711899190691	F	F	F
0.7049793214756559	0.9170201767819627	0.4412672199224302	T	T	T
0.3053579954478843	0.3906326091819288	0.4762349655173731	T	T	T
0.1979831205284946	0.1299854809763661	0.4351403770601029	T	T	T
0.6923361964042762	0.6437707856146353	0.4266738163161791	T	T	T
0.8938500204569961	0.5343506246160984	0.3538022503106732	T	T	T
0.4035871928709671	0.0371115498261960	0.3392698620921643	T	T	T
0.7941335826688771	0.7558469454495054	0.2363368113538584	F	F	F
0.2970848907517407	0.7884673272029303	0.2051338737269148	F	F	F
0.2927772407109543	0.2571588202315169	0.2412161475842041	F	F	F
0.7919741836641592	0.2884247962807223	0.2033595043939727	F	F	F
0.8325523384839428	0.0232203766249484	0.2204340848359010	F	F	F
0.7646723875335290	0.2643031509220595	0.4221768465408183	T	T	T

0.3246404835850853	0.5212303917651866	0.2338612095294366	F	F	F
0.2643975592814947	0.7764885646567491	0.4218680978959834	T	T	T
0.5423123381003170	0.9170000577401904	0.3452856896274252	T	T	T
0.5554632793807883	0.1273601989640341	0.1218561316796425	F	F	F
0.0263922731475883	0.4104908904767378	0.3475723684031996	T	T	T
0.0533799802195176	0.6280077327186717	0.1298751863179675	F	F	F
0.7904741490364413	0.0425547369727384	0.4094172816901205	T	T	T
0.2812654676021449	0.9996901551856511	0.4290119650937528	T	T	T
0.3021090653202964	0.5433956904462247	0.4306506548124601	T	T	T
0.7837126928132818	0.4940741970814044	0.4516233987295595	T	T	T
0.7554906591850409	0.7822687203722074	0.4209733149119230	T	T	T
0.8301862885156268	0.5232948929866339	0.2274043651788205	F	F	F
0.2723365419765877	0.2637013684375816	0.4285880502023157	T	T	T
0.3331054255992214	0.0242575550271624	0.2216880139098762	F	F	F
0.0478629573219046	0.8788598543403368	0.3164478990839609	T	T	T
0.0449977269881643	0.1710424189286712	0.1452445867000662	F	F	F
0.5466505082621226	0.3808626976455577	0.3174273136445025	T	T	T
0.5429923449161720	0.6677726747146693	0.1378465744492203	F	F	F
0.5425068565244828	0.4004511714331684	0.1318192897994521	F	F	F
0.0461858951412929	0.1450344777817985	0.3361989634012268	T	T	T
0.5516039013307648	0.8971695595514362	0.1311604450889021	F	F	F
0.0447765932967883	0.6447793909243080	0.3426551222344357	T	T	T
0.0481446970045738	0.3986436433700646	0.1342522577617586	F	F	F
0.0468560485094400	0.8981606690356401	0.1317025983878750	F	F	F
0.5469320111434135	0.6491402760851449	0.3247924308084903	T	T	T
0.5480860701792486	0.1480818589131251	0.3286143570655139	T	T	T
0.4891129711973728	0.4361858809247048	0.5120628785715183	T	T	T
0.5391918303721944	0.6190260093910844	0.5018893253262957	T	T	T
0.6764399847759505	0.5138485980520405	0.5818289605224379	T	T	T
0.3569496731145727	0.5548036847615917	0.5836291261793026	T	T	T

Pd4/In2O3

1.00000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.9857006073000001

O In Pd

48 32 4

Selective dynamics

Direct

0.1819400070000015	0.5179200199999983	0.1472299930000034	F	F	F
0.6819400070000015	0.0179200010000002	0.1472299930000034	F	F	F
0.6799139495799047	0.0265534961592835	0.3144838440250898	T	T	T

0.1814281119526207	0.5171690356592527	0.3272654304625494	T	T	T
0.9101421134592109	0.3771158859058309	0.4383322463386569	T	T	T
0.4081853549019622	0.8830752675657477	0.4379309262728165	T	T	T
0.4239665732519315	0.6769701380708927	0.4235002946254279	T	T	T
0.9155302905381623	0.1627028858646431	0.4268439348755736	T	T	T
0.9545099699999966	0.3958000000000013	0.2385899980000019	F	F	F
0.4545100160000004	0.8957999670000021	0.2385899980000019	F	F	F
0.6432654461705845	0.7880938952608071	0.3269566045056125	T	T	T
0.1443424609100290	0.2861339855780829	0.3377332567591099	T	T	T
0.4545100160000004	0.1542000070000000	0.2206899999999976	F	F	F
0.9545099699999966	0.6542000230000014	0.2206899999999976	F	F	F
0.1454900069999994	0.7638599679999984	0.1325899919999998	F	F	F
0.6454899840000010	0.2638599839999998	0.1325899919999998	F	F	F
0.1903399939999986	0.2862900060000015	0.1438599980000035	F	F	F
0.6903399589999992	0.7862899730000024	0.1438599980000035	F	F	F
0.9096599470000015	0.8817800340000019	0.2205699929999980	F	F	F
0.4096599940000019	0.3817800010000028	0.2205699929999980	F	F	F
0.4096599940000019	0.6682199560000015	0.2387099910000003	F	F	F
0.9096599470000015	0.1682200059999985	0.2387099910000003	F	F	F
0.6895684577289606	0.2655490601178056	0.3137981149920784	T	T	T
0.1858304134502363	0.7604517931720962	0.3128859909420850	T	T	T
0.4180599930000000	0.7820899849999989	0.1111999929999996	F	F	F
0.9180600400000003	0.2820900179999981	0.1111999929999996	F	F	F
0.9192689673041924	0.7657065654836304	0.3521189891582484	T	T	T
0.4199401839711034	0.2649295447346222	0.3474222399208796	T	T	T
0.6819400070000015	0.4224300249999970	0.2239500100000029	F	F	F
0.1819400070000015	0.9224299589999987	0.2239500100000029	F	F	F
0.1819400070000015	0.1275800049999987	0.2353300010000012	F	F	F
0.6819400070000015	0.6275799969999980	0.2353300010000012	F	F	F
0.6346105752957260	0.3877961952421629	0.4300605400784177	T	T	T
0.1359317856721544	0.8956787111280928	0.4281181161908473	T	T	T
0.9564313017281344	0.0114695614317495	0.3347034218706346	T	T	T
0.4571206204024242	0.5147182153782043	0.3352990868940673	T	T	T
0.1512598757180456	0.6503786861701348	0.4439941803216865	T	T	T
0.6428950242866257	0.1482765253346355	0.4414581007298068	T	T	T
0.4545100160000004	0.5361400390000028	0.1258399929999996	F	F	F
0.9545099699999966	0.0361399980000030	0.1258399929999996	F	F	F
0.4096599940000019	0.0137100000000032	0.1145799960000033	F	F	F
0.9096599470000015	0.5137100339999989	0.1145799960000033	F	F	F
0.7139325806262167	0.9162952438007641	0.4494101261396672	T	T	T
0.3112752040451278	0.3913807363389168	0.4766063994478466	T	T	T
0.1994047180269375	0.1301556011696597	0.4362038740629255	T	T	T
0.6998966495272946	0.6438639823389524	0.4304896825900049	T	T	T
0.8981443441237796	0.5364211845962700	0.3508060084063238	T	T	T

0.4066328431767460	0.0383497645425872	0.3444229979597260	T	T	T
0.7999999999999972	0.7581899819999975	0.2431499850000023	F	F	F
0.3000000230000026	0.7918100090000024	0.2161299999999997	F	F	F
0.3000000230000026	0.2581899979999989	0.2431499850000023	F	F	F
0.7999999999999972	0.2918100090000024	0.2161299999999997	F	F	F
0.8336300499999965	0.0250000010000022	0.2296400190000014	F	F	F
0.7692062032103506	0.2660745944955170	0.4270574239626160	T	T	T
0.3336300030000032	0.5249999790000004	0.2296400190000014	F	F	F
0.2640082896973868	0.7743819391998273	0.4263349615563685	T	T	T
0.5431823291467240	0.9164188685944329	0.3478381963292066	T	T	T
0.5499999999999972	0.1331900059999995	0.1157099910000028	F	F	F
0.0325401412279606	0.4119852341391742	0.3458937352561088	T	T	T
0.0499999999999972	0.6331899899999982	0.1157099910000028	F	F	F
0.7945958928980585	0.0437009353950222	0.4174558736561097	T	T	T
0.2801240957303251	0.9987756673608622	0.4318939286409020	T	T	T
0.3044553931930556	0.5442940540264214	0.4278381215500786	T	T	T
0.7866863743653980	0.4988417491667765	0.4511402866986956	T	T	T
0.7630139310778682	0.7826440523580871	0.4255495928097625	T	T	T
0.8336300499999965	0.5249999790000004	0.2296400190000014	F	F	F
0.2758188294921346	0.2631108630725184	0.4303550165002169	T	T	T
0.3336300030000032	0.0250000010000022	0.2296400190000014	F	F	F
0.0487973072174477	0.8810108155085737	0.3184270211558447	T	T	T
0.0499999999999972	0.1668099999999981	0.1427199939999966	F	F	F
0.5481703297125990	0.3823815470432783	0.3178750574964749	T	T	T
0.5499999999999972	0.6668099509999976	0.1427199939999966	F	F	F
0.5499999999999972	0.4000000200000002	0.1292199969999999	F	F	F
0.0476041986518986	0.1479937007329376	0.3354001521079961	T	T	T
0.5499999999999972	0.8999999540000019	0.1292199969999999	F	F	F
0.0496859943689566	0.6446693158654011	0.3368146516228913	T	T	T
0.0499999999999972	0.4000000200000002	0.1292199969999999	F	F	F
0.0499999999999972	0.8999999540000019	0.1292199969999999	F	F	F
0.5506249653949427	0.6507251805968730	0.3295397309175270	T	T	T
0.5530742774632527	0.1483645501151034	0.3312516085744615	T	T	T
0.3560608293226237	0.5506920933930439	0.5811298999748893	T	T	T
0.6838754207356440	0.5087119672984995	0.5849860750323098	T	T	T
0.5458598117468726	0.6183938605084268	0.5066454716101114	T	T	T
0.4958683296952500	0.4371565530203027	0.5100197030524313	T	T	T

CO₂ adsorption on Pd_nPt(4-n)/In₂O₃ catalysts

Pt4/In₂O₃

1.000000000000000		
10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9857006073000001

O	In	Pt	C
50	32	4	1

Selective dynamics

Direct

0.1819400070000015	0.5179200199999983	0.1152000000000015	F	F	F
0.6819400070000015	0.0179200010000002	0.1152000000000015	F	F	F
0.6798458645008909	0.0324191792156943	0.2510948292134095	T	T	T
0.1797853885985107	0.5177982686142327	0.2653852585926430	T	T	T
0.9104927654140789	0.3772637029174626	0.3582005340548794	T	T	T
0.4087596731407810	0.8825238365716762	0.3575342370615927	T	T	T
0.4245982567721349	0.6751973106292741	0.3494452744610927	T	T	T
0.9149897415235411	0.1635859001903566	0.3491757137211348	T	T	T
0.9545099699999966	0.3958000000000013	0.1866899999999987	F	F	F
0.4545100160000004	0.8957999670000021	0.1866899999999987	F	F	F
0.6430194001779355	0.7849186914534728	0.2648403503973890	T	T	T
0.1428716972025872	0.2856458952018435	0.2725608647366454	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
0.6894797118403487	0.2682929661525317	0.2535344549457061	T	T	T
0.1862329492272554	0.7612268410384412	0.2529519316597843	T	T	T
0.4180599930000000	0.7820899849999989	0.0870100030000032	F	F	F
0.9180600400000003	0.2820900179999981	0.0870100030000032	F	F	F
0.9164147674612297	0.7651671397810649	0.2863703958718902	T	T	T
0.4184030202286087	0.2650524110011228	0.2801145085134773	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

0.6326296240372693	0.3880880504662754	0.3540034592945757	T	T	T
0.1365503634496721	0.8966851615245791	0.3514650072227702	T	T	T
0.9573903652026137	0.0117980413783137	0.2699096609702747	T	T	T
0.4541266899584229	0.5147729551177248	0.2713876966948341	T	T	T
0.1507923012161198	0.6519320806252219	0.3647320492782940	T	T	T
0.6414784056399181	0.1507970672022608	0.3625145050535687	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
0.7089643302564317	0.9196678516363299	0.3587297965633434	T	T	T
0.3121588721087022	0.3922788933606469	0.3877509826669458	T	T	T
0.1998750645458960	0.1299590336760619	0.3567067601630813	T	T	T
0.6926382171559984	0.6350711903868156	0.3489546375887891	T	T	T
0.8990654312409531	0.5364837281810079	0.2826677901346553	T	T	T
0.4073239251523676	0.0383215025400737	0.2778679031200773	T	T	T
0.7248693181539940	0.7682770091479469	0.4536171491315106	T	T	T
0.5422068625459632	0.7587437783840736	0.5158937207140553	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
0.7686613827338643	0.2669801830214552	0.3505092071594790	T	T	T
0.3336300030000032	0.5249999790000004	0.1796899989999972	F	F	F
0.2643781067514547	0.7753671963574029	0.3505439486157546	T	T	T
0.5487945273881796	0.9169811958719816	0.2815148871708044	T	T	T
0.5499999999999972	0.1331900059999995	0.0905399970000005	F	F	F
0.0326420112663109	0.4118961639785695	0.2791459728731949	T	T	T
0.0499999999999972	0.6331899899999982	0.0905399970000005	F	F	F
0.7929552967633543	0.0459839690350530	0.3401291501683538	T	T	T
0.2825756211795792	0.9987039987462507	0.3533331022353616	T	T	T
0.2989653117595266	0.5433126449850200	0.3524281331377918	T	T	T
0.7887065146663905	0.4983686345510941	0.3683526014395436	T	T	T
0.7613146154317197	0.7803908485133465	0.3518938527562586	T	T	T
0.8336300499999965	0.5249999790000004	0.1796899989999972	F	F	F
0.2752221366495474	0.2627059332619644	0.3513092873260845	T	T	T
0.3336300030000032	0.0250000010000022	0.1796899989999972	F	F	F
0.0469930727891879	0.8804204024967461	0.2588085657403263	T	T	T
0.0499999999999972	0.1668099999999981	0.1116699999999966	F	F	F
0.5464344058612796	0.3831899028179984	0.2579919097232751	T	T	T
0.5499999999999972	0.6668099509999976	0.1116699999999966	F	F	F
0.5499999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0471942457932920	0.1475859503496515	0.2713911287976278	T	T	T

0.549999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.0488643392784587	0.6459167072871798	0.2737182777437568	T	T	T
0.049999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.049999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.5492443521443204	0.6497810824523187	0.2661197244489165	T	T	T
0.5527424027367022	0.1497602039060689	0.2681146739041782	T	T	T
0.3623024245404669	0.5519399817740841	0.4832717650514059	T	T	T
0.4941139767811382	0.4342217632596560	0.4223313525434992	T	T	T
0.6837711843108728	0.5075369092608756	0.4825701809142839	T	T	T
0.5485164719854571	0.6229142506152763	0.4212159667507046	T	T	T
0.6133191447963587	0.7368961664282077	0.4718416509778564	T	T	T

PdPt3/In2O3

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
50	32	1	3	1

Selective dynamics

Direct

0.1819400070000015	0.5179200199999983	0.1152000000000015	F	F	F
0.6819400070000015	0.0179200010000002	0.1152000000000015	F	F	F
0.6797761470110046	0.0328084333482579	0.2511787019799954	T	T	T
0.1801715319451418	0.5177773667383931	0.2650679539301777	T	T	T
0.9101251654527758	0.3773506936558348	0.3584173520729337	T	T	T
0.4089817641113385	0.8828445160402438	0.3575664713103919	T	T	T
0.4252202248168970	0.6757716291709741	0.3488389045290674	T	T	T
0.9142571205317438	0.1639345493964512	0.3491547352637028	T	T	T
0.9545099699999966	0.3958000000000013	0.1866899999999987	F	F	F
0.4545100160000004	0.8957999670000021	0.1866899999999987	F	F	F
0.6431310281259357	0.7852082200380366	0.2647690422638505	T	T	T
0.1427236408881782	0.2857879113873949	0.2727344581546447	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

0.6892692903951598	0.2678980012611234	0.2533925669020718	T	T	T
0.1860441840844800	0.7610148889263542	0.2530755299295535	T	T	T
0.4180599930000000	0.7820899849999989	0.0870100030000032	F	F	F
0.9180600400000003	0.2820900179999981	0.0870100030000032	F	F	F
0.9164838735389722	0.7647887049519682	0.2868935652452649	T	T	T
0.4177975472461739	0.2658205608747366	0.2805358447559598	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
0.6323318220766154	0.3887753725514003	0.3534364848737042	T	T	T
0.1365377018053593	0.8965010639703479	0.3515630770238829	T	T	T
0.9572358704965964	0.0118108366598406	0.2699803422088536	T	T	T
0.4545269028107981	0.5147665397115802	0.2710169729460006	T	T	T
0.1532167579230759	0.6509511300811823	0.3652429636508572	T	T	T
0.6407377353198882	0.1509814898511266	0.3627435512347787	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
0.7093535462801484	0.9196173423323515	0.3586774985218710	T	T	T
0.3062398299338511	0.3927495558500596	0.3906658260978020	T	T	T
0.1995732870767171	0.1300199336307557	0.3564923597508525	T	T	T
0.6931820078752864	0.6341775038410304	0.3480004639065513	T	T	T
0.8998373593940627	0.5362965448821839	0.2826867429744624	T	T	T
0.4073255490718140	0.0384408170513382	0.2778179430991514	T	T	T
0.7179213331332122	0.7687358596225948	0.4536156539668994	T	T	T
0.5354135302030372	0.7539812698790342	0.5154940989133934	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
0.7677334359946073	0.2672192439833907	0.3505465135954253	T	T	T
0.3336300030000032	0.5249999790000004	0.1796899989999972	F	F	F
0.2648408408908409	0.7754773178072654	0.3505657235878274	T	T	T
0.5490535442486930	0.9172143306513050	0.2814725857891531	T	T	T
0.5499999999999972	0.1331900059999995	0.0905399970000005	F	F	F
0.0324885455194988	0.4119073671173155	0.2792749893368125	T	T	T
0.0499999999999972	0.6331899899999982	0.0905399970000005	F	F	F
0.7925697646950383	0.0462936461270118	0.3401664029731748	T	T	T
0.2822901692845505	0.9987254518088804	0.3531615733640265	T	T	T
0.3017607840217877	0.5430706145750364	0.3510544671729576	T	T	T
0.7872448756698702	0.4978368319059712	0.3679465765701480	T	T	T

0.7603294221378718	0.7800352564423179	0.3521607405633489	T	T	T
0.8336300499999965	0.5249999790000004	0.1796899989999972	F	F	F
0.2745255482852613	0.2631525742077727	0.3517506732075475	T	T	T
0.3336300030000032	0.0250000010000022	0.1796899989999972	F	F	F
0.0465798643806963	0.8801768360962399	0.2590132190581471	T	T	T
0.0499999999999972	0.1668099999999981	0.1116699999999966	F	F	F
0.5471378972175103	0.3832346012955057	0.2577286845408366	T	T	T
0.5499999999999972	0.6668099509999976	0.1116699999999966	F	F	F
0.5499999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0468270264992867	0.1476685222895071	0.2714849345120456	T	T	T
0.5499999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.0490724036106727	0.6458044164849142	0.2739938920777689	T	T	T
0.0499999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0499999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.5499257961854482	0.6499009140514360	0.2658285222631491	T	T	T
0.5519826799029133	0.1500373768543852	0.2683803071440636	T	T	T
0.3592006048496188	0.5550003046874110	0.4850639999530202	T	T	T
0.4887531173922355	0.4350010135927036	0.4223654306818148	T	T	T
0.5468386843387520	0.6206894051722855	0.4204711755692614	T	T	T
0.6812930050207839	0.5057508885670003	0.4823288054758308	T	T	T
0.6077528970427153	0.7343165567018701	0.4711743801507140	T	T	T

Pd2Pt2/In2O3

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
50	32	2	2	1

Selective dynamics

Direct

0.1819400070000015	0.5179200199999983	0.1152000000000015	F	F	F
0.6819400070000015	0.0179200010000002	0.1152000000000015	F	F	F
0.6795518418028000	0.0324002837743711	0.2512472560914356	T	T	T
0.1803441622171521	0.5184025759713751	0.2643459167291155	T	T	T
0.9132258782697065	0.3777145210404594	0.3585503069563649	T	T	T
0.4083762267621328	0.8829373973331244	0.3575575927033073	T	T	T
0.4254306045042985	0.6752737877455384	0.3488195095877480	T	T	T
0.9146040024879000	0.1641455435378785	0.3489677470268210	T	T	T
0.9545099699999966	0.3958000000000013	0.1866899999999987	F	F	F
0.4545100160000004	0.8957999670000021	0.1866899999999987	F	F	F
0.6426901572405407	0.7851970886339684	0.2646866176555515	T	T	T
0.1426306402665413	0.2859903850191282	0.2718109233898209	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
0.6888839674249376	0.2668375152904021	0.2527249201996447	T	T	T
0.1860243862009200	0.7611879425635460	0.2531603061670128	T	T	T
0.4180599930000000	0.7820899849999989	0.0870100030000032	F	F	F
0.9180600400000003	0.2820900179999981	0.0870100030000032	F	F	F
0.9162294735967268	0.7649193597006695	0.2869192026895097	T	T	T
0.4173353943556399	0.2657666351937661	0.2807463544600413	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
0.6361097507609598	0.3895585394400305	0.3518263133446314	T	T	T
0.1362720746791438	0.8965361188742134	0.3517120584277911	T	T	T
0.9572907698006012	0.0117644652977046	0.2699959323868136	T	T	T
0.4545363039902556	0.5145773694272420	0.2712942677465621	T	T	T
0.1533245220328087	0.6507278305116996	0.3651163586859792	T	T	T
0.6416800752041585	0.1515309109359603	0.3625807673470417	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
0.7095035294771759	0.9195079267086949	0.3589638171506690	T	T	T
0.3032774999212812	0.3944232731002417	0.3904837208621464	T	T	T
0.1999720525025430	0.1309144010465751	0.3559252700336442	T	T	T
0.6935586443592179	0.6341905389905498	0.3482243280281736	T	T	T
0.8998644814500536	0.5367248696753730	0.2825795175182877	T	T	T
0.4072579488397942	0.0382695290561251	0.2777700488313652	T	T	T
0.7144888982743347	0.7678478055124428	0.4538549111249251	T	T	T
0.5338522935820083	0.7485170548726601	0.5165916102356233	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
0.7690595544562482	0.2681425666436391	0.3496120810911489	T	T	T

0.3336300030000032	0.5249999790000004	0.1796899989999972	F	F	F
0.2649783310699018	0.7751874639616053	0.3506961782232683	T	T	T
0.5487275012457369	0.9172021808189481	0.2816038418413744	T	T	T
0.5499999999999972	0.1331900059999995	0.0905399970000005	F	F	F
0.0334374143208143	0.4125025997268945	0.2790521684553606	T	T	T
0.0499999999999972	0.6331899899999982	0.0905399970000005	F	F	F
0.7926232808207277	0.0464430000140285	0.3401544232295587	T	T	T
0.2816225783224702	0.9991322973107448	0.3529913965704283	T	T	T
0.3007852802996548	0.5416604356785698	0.3510573100652206	T	T	T
0.7874055408097600	0.4971859363643076	0.3677955082109590	T	T	T
0.7593035330296202	0.7798630759644907	0.3520326517726821	T	T	T
0.8336300499999965	0.5249999790000004	0.1796899989999972	F	F	F
0.2722820694091386	0.2653411580913252	0.3516844988792435	T	T	T
0.3336300030000032	0.0250000010000022	0.1796899989999972	F	F	F
0.0464462451929605	0.8801627485166238	0.2591616548330321	T	T	T
0.0499999999999972	0.1668099999999981	0.1116699999999966	F	F	F
0.5473652046364630	0.3829414779414153	0.2579393046103035	T	T	T
0.5499999999999972	0.6668099509999976	0.1116699999999966	F	F	F
0.5499999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0473539663105098	0.1476388719484634	0.2714469870958786	T	T	T
0.5499999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.0488895977887409	0.6458583117335948	0.2740208001565571	T	T	T
0.0499999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0499999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.5498577496585870	0.6496231416413702	0.2658113204580989	T	T	T
0.5516364000264043	0.1499605414617418	0.2686264596905647	T	T	T
0.3585858181392738	0.5525070816491923	0.4835032204441607	T	T	T
0.4905966785962588	0.4314897509913349	0.4229207192513647	T	T	T
0.5464467272323479	0.6186856767497094	0.4198271345082780	T	T	T
0.6818162794079407	0.5055764950962315	0.4825994078815870	T	T	T
0.6065221298162894	0.7314877843245773	0.4719430066441556	T	T	T

Pd3Pt/In2O3

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
50	32	3	1	1

Selective dynamics

Direct

0.1819400070000015	0.5179200199999983	0.1152000000000015	F	F	F
0.6819400070000015	0.0179200010000002	0.1152000000000015	F	F	F

0.6793677190463588	0.0318595991552185	0.2516250850322085	T	T	T
0.1809024531410271	0.5185578644826098	0.2644273832011579	T	T	T
0.9124820879691082	0.3782565276111926	0.3584279652209121	T	T	T
0.4089782811883769	0.8834912083408858	0.3583651649658777	T	T	T
0.4237113422739276	0.6757620072174181	0.3484471421287575	T	T	T
0.9145424800032019	0.1641887064203758	0.3489865310769501	T	T	T
0.9545099699999966	0.3958000000000013	0.1866899999999987	F	F	F
0.4545100160000004	0.8957999670000021	0.1866899999999987	F	F	F
0.6426079187475220	0.7857381847725933	0.2644980789610443	T	T	T
0.1427609177370944	0.2861572956238280	0.2719693748812629	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
0.6889426894070717	0.2669037740987827	0.2528100579765868	T	T	T
0.1860528002277303	0.7613757267847299	0.2529990380333552	T	T	T
0.4180599930000000	0.7820899849999989	0.0870100030000032	F	F	F
0.9180600400000003	0.2820900179999981	0.0870100030000032	F	F	F
0.9171099346284766	0.7653447929910197	0.2863636448212892	T	T	T
0.4175604453991553	0.2658968435819392	0.2807830235357323	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
0.6360472575557485	0.3901132610108222	0.3520414926169514	T	T	T
0.1368905740924315	0.8968234775403848	0.3515030701429809	T	T	T
0.9571225995778110	0.0119953284908800	0.2700346781765611	T	T	T
0.4551323733505365	0.5146694434990169	0.2712952400159171	T	T	T
0.1521898413803816	0.6511044132367704	0.3652280764603597	T	T	T
0.6418817662583203	0.1513739367135686	0.3625994223883021	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
0.7104405744223610	0.9186764526560549	0.3602278430074394	T	T	T
0.3049349155576695	0.3948793359048493	0.3905615769812379	T	T	T
0.2003635559239059	0.1313354028918461	0.3562619228257177	T	T	T
0.6954543618212530	0.6357960458929114	0.3479168411891750	T	T	T

0.9001898736206592	0.5366526107559900	0.2823189680469496	T	T	T
0.4070236073326594	0.0382657771617322	0.2778517072422928	T	T	T
0.5379464730650003	0.7461818602641488	0.5186978982548954	T	T	T
0.7214180675387563	0.7652841718201482	0.4561277935388600	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
0.7691668677801438	0.2683749690303641	0.3496578361721141	T	T	T
0.3336300030000032	0.5249999790000004	0.1796899989999972	F	F	F
0.2649848835951180	0.7753486574406239	0.3503695881586726	T	T	T
0.5481583990767720	0.9172057126542895	0.2818071247147541	T	T	T
0.5499999999999972	0.1331900059999995	0.0905399970000005	F	F	F
0.0335159847924773	0.4127376206726284	0.2790554910527727	T	T	T
0.0499999999999972	0.6331899899999982	0.0905399970000005	F	F	F
0.7926815654715524	0.0462837810258538	0.3402462627140513	T	T	T
0.2818363580692169	-0.0004522891369554	0.3533548481602024	T	T	T
0.3021414609524999	0.5428438364813327	0.3509287913165543	T	T	T
0.7873291498628062	0.4985384540284150	0.3676719442056451	T	T	T
0.7606708947485683	0.7797980217870386	0.3510967401800147	T	T	T
0.8336300499999965	0.5249999790000004	0.1796899989999972	F	F	F
0.2730624684532605	0.2658603184235008	0.3518350240880758	T	T	T
0.3336300030000032	0.0250000010000022	0.1796899989999972	F	F	F
0.0470959285493646	0.8806867691356617	0.2588368711108786	T	T	T
0.0499999999999972	0.1668099999999981	0.1116699999999966	F	F	F
0.5475077131580164	0.3830743023748491	0.2579180584204117	T	T	T
0.5499999999999972	0.6668099509999976	0.1116699999999966	F	F	F
0.5499999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0474422116056642	0.1479523887110801	0.2715432832887693	T	T	T
0.5499999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.0492868468245386	0.6458991563905102	0.2739045911883662	T	T	T
0.0499999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0499999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.5497268017325165	0.6499585186976129	0.2663666937251125	T	T	T
0.5516085962776818	0.1500064330502526	0.2686496872692812	T	T	T
0.3598161433820093	0.5535450880214012	0.4822883101072009	T	T	T
0.4917951117041703	0.4328333352678273	0.4223591072826764	T	T	T
0.5480195167345500	0.6229027835075042	0.4198683474742506	T	T	T
0.6813707086714607	0.5077342521963816	0.4821623614071284	T	T	T
0.6141021155616925	0.7327979887104942	0.4753550835243739	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 C
 50 32 4 1

Selective dynamics

Direct

0.1819400070000015	0.5179200199999983	0.1152000000000015	F	F	F
0.6819400070000015	0.0179200010000002	0.1152000000000015	F	F	F
0.6795335676902915	0.0317917441707744	0.2516551713510481	T	T	T
0.1806792823848432	0.5183772630473064	0.2644218125237449	T	T	T
0.9116970867977809	0.3786606660695459	0.3590858618601828	T	T	T
0.4090427840425114	0.8836068807012981	0.3583095509677714	T	T	T
0.4234352935785431	0.6757415084947483	0.3482553698013556	T	T	T
0.9148188928727016	0.1639643714461942	0.3489916193297786	T	T	T
0.9545099699999966	0.3958000000000013	0.1866899999999987	F	F	F
0.4545100160000004	0.8957999670000021	0.1866899999999987	F	F	F
0.6427609372528904	0.7858381711553357	0.2644987766738416	T	T	T
0.1424406776478226	0.2863812984435769	0.2721097499137226	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
0.6889829688145211	0.2668826293713527	0.2528676075464436	T	T	T
0.1858673231574846	0.7613392701389284	0.2528180975407402	T	T	T
0.4180599930000000	0.7820899849999989	0.0870100030000032	F	F	F
0.9180600400000003	0.2820900179999981	0.0870100030000032	F	F	F
0.9170163538716711	0.7653190319957686	0.2862068004139039	T	T	T
0.4174231061635350	0.2658862399286659	0.2807963337116017	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
0.6360604629833071	0.3895669026231421	0.3521155548686958	T	T	T
0.1370553988797484	0.8967471453851508	0.3514674819313915	T	T	T
0.9571127464537138	0.0119259194591623	0.2700293924244230	T	T	T
0.4553216735957368	0.5144839852878663	0.2712236095088602	T	T	T

0.1516675492883297	0.6510776075624768	0.3650585244251247	T	T	T
0.6420736461943753	0.1512146487599682	0.3626380781351543	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
0.7101075320658182	0.9186973321444336	0.3604952026207183	T	T	T
0.3060683436823005	0.3949568780193204	0.3912138576737897	T	T	T
0.2004888514918241	0.1314452575969385	0.3561062332852238	T	T	T
0.6956383688482712	0.6357860646825747	0.3474302817711215	T	T	T
0.8996862031480937	0.5363734567117244	0.2822619350485290	T	T	T
0.4070690812624118	0.0383603091757896	0.2777794281262430	T	T	T
0.7282856486768579	0.7624030761929743	0.4559006808607594	T	T	T
0.5548427616310927	0.7360996370277839	0.5234437918674687	T	T	T
0.799999999999972	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
0.799999999999972	0.2918100090000024	0.1691199950000026	F	F	F
0.8336300499999965	0.0250000010000022	0.1796899989999972	F	F	F
0.7694392694067030	0.2681643042891715	0.3496862931526532	T	T	T
0.3336300030000032	0.5249999790000004	0.1796899989999972	F	F	F
0.2652278545073987	0.7751841669935782	0.3500503018700377	T	T	T
0.5481652705276217	0.9171854554058231	0.2818604118955190	T	T	T
0.549999999999972	0.1331900059999995	0.0905399970000005	F	F	F
0.0328391423641434	0.4128121497746493	0.2792946007846946	T	T	T
0.049999999999972	0.6331899899999982	0.0905399970000005	F	F	F
0.7926628495358737	0.0459633166770686	0.3403059567357500	T	T	T
0.2818908600114715	0.9995283672663324	0.3533146262189676	T	T	T
0.3020988353707398	0.5431823526432660	0.3507981681732663	T	T	T
0.7854217746647169	0.4989427295547466	0.3677860196472180	T	T	T
0.7609166389750954	0.7798564527218558	0.3511127443512069	T	T	T
0.8336300499999965	0.5249999790000004	0.1796899989999972	F	F	F
0.2728583312801173	0.2662260848138417	0.3519651799169859	T	T	T
0.3336300030000032	0.0250000010000022	0.1796899989999972	F	F	F
0.0471142254367689	0.8805748591467534	0.2588503824440302	T	T	T
0.049999999999972	0.1668099999999981	0.1116699999999966	F	F	F
0.5473513337433520	0.3829413477244467	0.2577609041386983	T	T	T
0.549999999999972	0.6668099509999976	0.1116699999999966	F	F	F
0.549999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0476877041265729	0.1478528023768778	0.2715548718875954	T	T	T
0.549999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.0489912067448717	0.6457574936484551	0.2739032784359595	T	T	T
0.049999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.049999999999972	0.8999999540000019	0.1011099950000016	F	F	F

0.5493784402624030	0.6501340031841222	0.2663368695878040	T	T	T
0.5516152016005992	0.1499552720736156	0.2687115841711179	T	T	T
0.3596494659802855	0.5532187420703197	0.4815711642909937	T	T	T
0.4941259081872543	0.4344436368811784	0.4213776541713983	T	T	T
0.6838472516813596	0.5071257466328462	0.4842395541100109	T	T	T
0.5503093544720559	0.6218004362689319	0.4200331969849447	T	T	T
0.6244160385139175	0.7263552259279249	0.4769696585357660	T	T	T

CO₂ dissociation transition states on Pd_nPt(4-n)/In₂O₃

Pd₂Pt₂/In₂O₃

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
50 32 2 2 1

Selective dynamics

Direct

0.1819400070000015	0.5179200199999985	0.1152000000000015	F	F	F
0.6819400070000015	0.0179200010000003	0.1152000000000015	F	F	F
0.6797144446296800	0.0282397213738402	0.2539902736326777	F	F	F
0.1808263503529819	0.5179045771426835	0.2630751536376932	F	F	F
0.9197215014045517	0.3771680785080812	0.3596455055173240	F	F	F
0.4091997692147882	0.8833640543960446	0.3580722797775387	F	F	F
0.4267277314945125	0.6750872302868339	0.3496491504940610	F	F	F
0.9174310872411100	0.1628369616506604	0.3496361336342715	F	F	F
0.9545099699999966	0.3958000000000880	0.1866899999999987	F	F	F
0.4545100160000004	0.8957999670001882	0.1866899999999987	F	F	F
0.6419903506687300	0.7865246580453913	0.2642784756085626	F	F	F
0.1448009161037753	0.2860665996648728	0.2723790642615227	F	F	F
0.4545100160000004	0.1542000070000000	0.1726800109999971	F	F	F
0.9545099699999966	0.6542000230000017	0.1726800109999971	F	F	F
0.1454900069999994	0.7638599680001649	0.1037499959999977	F	F	F
0.6454899840000010	0.2638599840000011	0.1037499959999977	F	F	F
0.1903399939999985	0.2862900060000015	0.1125700079999987	F	F	F
0.6903399589999992	0.7862899730001688	0.1125700079999987	F	F	F
0.9096599470000013	0.8817800340001873	0.1725899979999994	F	F	F
0.4096599940000019	0.3817800010000895	0.1725899979999994	F	F	F
0.4096599940000019	0.6682199560000017	0.1867800019999990	F	F	F
0.9096599470000013	0.1682200059999988	0.1867800019999990	F	F	F
0.6897363071797936	0.2647491299287696	0.2528880001883563	F	F	F
0.1872818863791097	0.7616219594534800	0.2532182175863960	F	F	F
0.4180599929999999	0.7820899850001652	0.0870100030000032	F	F	F
0.9180600400000002	0.2820900179999983	0.0870100030000032	F	F	F
0.9174638250221685	0.7654090504095706	0.2856321975974095	F	F	F
0.4182217468223877	0.2670659852699725	0.2829717837451884	F	F	F
0.6819400070000015	0.4224300250000848	0.1752299990000026	F	F	F
0.1819400070000015	0.9224299590001848	0.1752299990000026	F	F	F
0.1819400070000015	0.1275800049999987	0.1841400010000029	F	F	F
0.6819400070000015	0.6275799969999982	0.1841400010000029	F	F	F

0.6490350117216319	0.3924538311671810	0.3477789727050045	F	F	F
0.1368658764002675	0.8966410635045490	0.3516673128802681	F	F	F
0.9564859347688802	0.0114015036669086	0.2706338377087313	F	F	F
0.4566120780556526	0.5147707253213141	0.2717077966091584	F	F	F
0.1539564148503793	0.6509129575938242	0.3637205273345657	F	F	F
0.6449427783346177	0.1505963261135078	0.3629917344949533	F	F	F
0.4545100160000004	0.5361400390000048	0.0984700050000029	F	F	F
0.9545099699999966	0.0361399980000030	0.0984700050000029	F	F	F
0.4096599940000019	0.0137100000000040	0.0896599969999983	F	F	F
0.9096599470000013	0.5137100339999991	0.0896599969999983	F	F	F
0.7130424263593530	0.9170180944388726	0.3675910670761272	F	F	F
0.3071766731666210	0.3940066822090023	0.3962316374395867	F	F	F
0.2000841351324248	0.1310101849145499	0.3571376223973998	F	F	F
0.6911459421844089	0.6437391357136968	0.3578817522151078	F	F	F
0.8987826000295253	0.5384922589735117	0.2832438750290637	F	F	F
0.4063439187341527	0.0388322199161758	0.2781640564986392	F	F	F
0.6243526171643664	0.6583948546535552	0.5676603762673675	T	T	T
0.4190164738606999	0.6179827211948004	0.5018256109070255	T	T	T
0.799999999999972	0.7581899820001639	0.1902599909999978	F	F	F
0.3000000230000026	0.7918100090001688	0.1691199950000026	F	F	F
0.3000000230000026	0.2581899979999991	0.1902599909999978	F	F	F
0.799999999999972	0.2918100090000028	0.1691199950000026	F	F	F
0.8336300499999965	0.0250000010000107	0.1796899989999972	F	F	F
0.7738819567872911	0.2673957395298164	0.3495291520634461	F	F	F
0.3336300030000032	0.5249999790000024	0.1796899989999972	F	F	F
0.2648263504588570	0.7756724984468788	0.3505557894839516	F	F	F
0.5446671071309510	0.9172590352630425	0.2811167077574487	F	F	F
0.549999999999972	0.1331900059999997	0.0905399970000005	F	F	F
0.0338512024200501	0.4120738173086115	0.2785990590438792	F	F	F
0.049999999999972	0.6331899899999991	0.0905399970000005	F	F	F
0.7947647610634972	0.0446969109258581	0.3416807963985304	F	F	F
0.2813865969755767	-0.0003266126461643	0.3538407192692112	F	F	F
0.3040474795689352	0.5449802850150255	0.3465967462951504	F	F	F
0.7968063435530520	0.4996734553533432	0.3699177304635563	F	F	F
0.7607438652690912	0.7827407912861895	0.3488433508307229	F	F	F
0.8336300499999965	0.5249999790000024	0.1796899989999972	F	F	F
0.2714589312493959	0.2658868307735356	0.3534479087819954	F	F	F
0.3336300030000032	0.0250000010000107	0.1796899989999972	F	F	F
0.0487863127619821	0.8811810490748979	0.2581188959078636	F	F	F
0.049999999999972	0.1668099999999982	0.1116699999999966	F	F	F
0.5494558725093482	0.3820153377557983	0.2566726114126643	F	F	F
0.549999999999972	0.6668099509999977	0.1116699999999966	F	F	F
0.549999999999972	0.4000000200000870	0.1011099950000016	F	F	F
0.0481369300645224	0.1475062922783915	0.2712801045279670	F	F	F

0.549999999999972	0.8999999540001878	0.1011099950000016	F	F	F
0.0502257922260456	0.6463420161018723	0.2726038334552804	F	F	F
0.049999999999972	0.4000000200000870	0.1011099950000016	F	F	F
0.049999999999972	0.8999999540001878	0.1011099950000016	F	F	F
0.5492771546613234	0.6507933726390692	0.2659644062009496	F	F	F
0.5521514187550481	0.1495306632649821	0.2694968730903901	F	F	F
0.3252023283034760	0.5048062064473184	0.4703544979703678	F	F	F
0.5089138332823495	0.4295700503170740	0.4160596531492343	F	F	F
0.5473127273722265	0.6405846303544378	0.4274247227518099	F	F	F
0.6845278031343280	0.5051190952501400	0.4854644823230820	F	F	F
0.5914297678080689	0.6237047414711511	0.5184788733468482	T	T	T

Pd3Pt/In2O3

1.000000000000000

10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9857006073000001

O	In	Pd	C
50	32	4	1

Selective dynamics

Direct

0.1819400070000015	0.5179200199999985	0.1152000000000015	F	F	F
0.6819400070000015	0.0179200010000003	0.1152000000000015	F	F	F
0.6796741836006431	0.0282300606787275	0.2540252066742101	F	F	F
0.1802952365098858	0.5181830328817369	0.2629593164314049	F	F	F
0.9190464200958827	0.3791751396519774	0.3606061343168728	F	F	F
0.4097373681328793	0.8836525458104750	0.3582106426647080	F	F	F
0.4229146585424923	0.6740303363283386	0.3482857055778463	F	F	F
0.9178931430140396	0.1632869982255301	0.3495695730843786	F	F	F
0.9545099699999966	0.3958000000000480	0.1866899999999987	F	F	F
0.4545100160000004	0.8957999670001067	0.1866899999999987	F	F	F
0.6419719208041736	0.7862256046631461	0.2643905082380861	F	F	F
0.1441728979116290	0.2866254290536893	0.2724788044851401	F	F	F
0.4545100160000004	0.1542000070000000	0.1726800109999971	F	F	F
0.9545099699999966	0.6542000230000017	0.1726800109999971	F	F	F
0.1454900069999994	0.7638599680000918	0.1037499959999977	F	F	F
0.6454899840000010	0.2638599840000011	0.1037499959999977	F	F	F
0.1903399939999985	0.2862900060000015	0.1125700079999987	F	F	F
0.6903399589999992	0.7862899730000957	0.1125700079999987	F	F	F
0.9096599470000013	0.8817800340001049	0.1725899979999994	F	F	F
0.4096599940000019	0.3817800010000494	0.1725899979999994	F	F	F
0.4096599940000019	0.6682199560000017	0.1867800019999990	F	F	F
0.9096599470000013	0.1682200059999988	0.1867800019999990	F	F	F

0.6894732841851822	0.2642157285914255	0.2525558201556565	F	F	F
0.1866839867487988	0.7619220178662579	0.2527946748894961	F	F	F
0.4180599929999999	0.7820899850000924	0.0870100030000032	F	F	F
0.9180600400000002	0.2820900179999983	0.0870100030000032	F	F	F
0.9174989010484126	0.7661983487004245	0.2848052441010189	F	F	F
0.4176605009448591	0.2669754788291179	0.2829164524250300	F	F	F
0.6819400070000015	0.4224300250000457	0.1752299990000026	F	F	F
0.1819400070000015	0.9224299590001034	0.1752299990000026	F	F	F
0.1819400070000015	0.1275800049999987	0.1841400010000029	F	F	F
0.6819400070000015	0.6275799969999982	0.1841400010000029	F	F	F
0.6518797124764344	0.3929290529495804	0.3457060297208102	F	F	F
0.1376764744653825	0.8968286833370612	0.3514411818168991	F	F	F
0.9567844917620799	0.0117763966748524	0.2705230094023416	F	F	F
0.4567106115005784	0.5142787125642826	0.2711459601200586	F	F	F
0.1504428420309520	0.6516243866934585	0.3636060670211907	F	F	F
0.6457345689800624	0.1512146716199164	0.3629925991891272	F	F	F
0.4545100160000004	0.5361400390000048	0.0984700050000029	F	F	F
0.9545099699999966	0.0361399980000030	0.0984700050000029	F	F	F
0.4096599940000019	0.0137100000000048	0.0896599969999983	F	F	F
0.9096599470000013	0.5137100339999991	0.0896599969999983	F	F	F
0.7145865945249815	0.9169553531329022	0.3675778384928580	F	F	F
0.3071379086077928	0.3953139530262360	0.3960348036843744	F	F	F
0.2011403799991777	0.1316607536865542	0.3568549231543219	F	F	F
0.6931254230947330	0.6455294883992200	0.3606863490828504	F	F	F
0.8978047982040588	0.5387544300066690	0.2827357515742225	F	F	F
0.4065235115562428	0.0387352667569918	0.2780262647788972	F	F	F
0.6317579235754788	0.6528350093211998	0.5669053335071630	T	T	T
0.4141170109505529	0.6155898058371974	0.5044061365279372	T	T	T
0.7999999999999972	0.7581899820000910	0.1902599909999978	F	F	F
0.3000000230000026	0.7918100090000958	0.1691199950000026	F	F	F
0.3000000230000026	0.2581899979999991	0.1902599909999978	F	F	F
0.7999999999999972	0.2918100090000028	0.1691199950000026	F	F	F
0.8336300499999965	0.0250000010000051	0.1796899989999972	F	F	F
0.7749063077098519	0.2681307210088158	0.3491138272529333	F	F	F
0.3336300030000032	0.5249999790000024	0.1796899989999972	F	F	F
0.2652381919272515	0.7751699040495025	0.3500392723926820	F	F	F
0.5449431634330608	0.9169241786330882	0.2811629878308925	F	F	F
0.5499999999999972	0.1331900059999997	0.0905399970000005	F	F	F
0.0330096964348105	0.4128158603273161	0.2791182903417063	F	F	F
0.0499999999999972	0.6331899899999991	0.0905399970000005	F	F	F
0.7949834617891955	0.0449792321708886	0.3415875432201256	F	F	F
0.2818008091405120	0.9999462341025116	0.3538667030740400	F	F	F
0.3028281661474920	0.5463896684449194	0.3466596137833833	F	F	F
0.7935823934670586	0.5026833804400176	0.3696914477999483	F	F	F

0.7620390788083122	0.7825332052005970	0.3487152986552199	F	F	F
0.8336300499999965	0.5249999790000024	0.1796899989999972	F	F	F
0.2710489552697479	0.2674421911638680	0.3537684815197054	F	F	F
0.3336300030000032	0.0250000010000051	0.1796899989999972	F	F	F
0.0490631280144158	0.8814576285554385	0.2581410382905127	F	F	F
0.0499999999999972	0.1668099999999982	0.1116699999999966	F	F	F
0.5489154737029990	0.3818211002960385	0.2562501294776874	F	F	F
0.5499999999999972	0.6668099509999977	0.1116699999999966	F	F	F
0.5499999999999972	0.4000000200000470	0.1011099950000016	F	F	F
0.0487742801901584	0.1477926625037067	0.2713733061980418	F	F	F
0.5499999999999972	0.8999999540001065	0.1011099950000016	F	F	F
0.0491827527240432	0.6466289932794609	0.2726125203680507	F	F	F
0.0499999999999972	0.4000000200000470	0.1011099950000016	F	F	F
0.0499999999999972	0.8999999540001065	0.1011099950000016	F	F	F
0.5492065720535728	0.6504247008875828	0.2672816153877448	F	F	F
0.5517529448641874	0.1495617162157409	0.2697560466815759	F	F	F
0.3293412915054466	0.5042402586217934	0.4694959668370262	F	F	F
0.5152561534490373	0.4349577524854827	0.4127282265636640	F	F	F
0.6888555477608055	0.5023470237077200	0.4889329709371231	F	F	F
0.5418326480650720	0.6419866509518360	0.4300637530355966	F	F	F
0.5965571594265239	0.6214711014146411	0.5173353189155168	T	T	T

Pd4/In2O3

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

50 32 1 3 1

Selective dynamics

Direct

0.1819400070000015	0.5179200199999985	0.1152000000000015	F	F	F
0.6819400070000015	0.0179200010000003	0.1152000000000015	F	F	F
0.6800806884961519	0.0297287034679657	0.2532715828180243	F	F	F
0.1824425915816819	0.5182922676817440	0.2645412868235001	F	F	F
0.9125411230182372	0.3763655011380964	0.3578021818504473	F	F	F
0.4104838407387491	0.8845179447058278	0.3583709012678181	F	F	F
0.4311832460677445	0.6759857426614266	0.3480286884662410	F	F	F
0.9160217736280721	0.1628997636363408	0.3497147308738220	F	F	F
0.9545099699999966	0.3958000000000613	0.1866899999999987	F	F	F
0.4545100160000004	0.8957999670001365	0.1866899999999987	F	F	F
0.6425545356559822	0.7869163360408624	0.2641387896609924	F	F	F
0.1445741094808557	0.2866422757147586	0.2732298221605439	F	F	F

0.4545100160000004	0.1542000070000000	0.1726800109999971	F	F	F
0.9545099699999966	0.6542000230000017	0.1726800109999971	F	F	F
0.1454900069999994	0.7638599680001186	0.1037499959999977	F	F	F
0.6454899840000010	0.2638599840000011	0.1037499959999977	F	F	F
0.1903399939999985	0.2862900060000015	0.1125700079999987	F	F	F
0.6903399589999992	0.7862899730001225	0.1125700079999987	F	F	F
0.9096599470000013	0.8817800340001344	0.1725899979999994	F	F	F
0.4096599940000019	0.3817800010000628	0.1725899979999994	F	F	F
0.4096599940000019	0.6682199560000017	0.1867800019999990	F	F	F
0.9096599470000013	0.1682200059999988	0.1867800019999990	F	F	F
0.6896560264427848	0.2666243914270641	0.2536231482925949	F	F	F
0.1861287637859272	0.7612884936117850	0.2531612954517954	F	F	F
0.4180599929999999	0.7820899850001191	0.0870100030000032	F	F	F
0.9180600400000002	0.2820900179999983	0.0870100030000032	F	F	F
0.9154985504535083	0.7648521882983763	0.2879979544280560	F	F	F
0.4181559650991990	0.2665537090536633	0.2819727864604147	F	F	F
0.6819400070000015	0.4224300250000596	0.1752299990000026	F	F	F
0.1819400070000015	0.9224299590001332	0.1752299990000026	F	F	F
0.1819400070000015	0.1275800049999987	0.1841400010000029	F	F	F
0.6819400070000015	0.6275799969999982	0.1841400010000029	F	F	F
0.6365343319139942	0.3897966792892794	0.3518682021071061	F	F	F
0.1389495818348866	0.8965510422857034	0.3514002291198571	F	F	F
0.9571651040248672	0.0116375797157954	0.2705478541984851	F	F	F
0.4569012294210820	0.5141571694035977	0.2698648578880074	F	F	F
0.1592719782411348	0.6504928619796735	0.3649034054091356	F	F	F
0.6427663161222924	0.1498667338208725	0.3630376275437211	F	F	F
0.4545100160000004	0.5361400390000048	0.0984700050000029	F	F	F
0.9545099699999966	0.0361399980000030	0.0984700050000029	F	F	F
0.4096599940000019	0.0137100000000053	0.0896599969999983	F	F	F
0.9096599470000013	0.5137100339999991	0.0896599969999983	F	F	F
0.7108906566768677	0.9181653702369720	0.3655394288296940	F	F	F
0.3095221584361021	0.3981545794643059	0.3945537322476378	F	F	F
0.2021015958313748	0.1327333135662969	0.3572630822725861	F	F	F
0.6975939445326955	0.6338850917898796	0.3456549541661548	F	F	F
0.9018207472096155	0.5365346662315266	0.2825574295838982	F	F	F
0.4065942763478618	0.0389163264462881	0.2778737828830407	F	F	F
0.6840658058854671	0.6709559131195645	0.5571039767168403	T	T	T
0.4642336496030481	0.6447648073113442	0.5031493928191128	T	T	T
0.7999999999999972	0.7581899820001177	0.1902599909999978	F	F	F
0.3000000230000026	0.7918100090001225	0.1691199950000026	F	F	F
0.3000000230000026	0.2581899979999991	0.1902599909999978	F	F	F
0.7999999999999972	0.2918100090000028	0.1691199950000026	F	F	F
0.8336300499999965	0.0250000010000060	0.1796899989999972	F	F	F
0.7698539634935860	0.2662922442202967	0.3506611447361169	F	F	F

0.3336300030000032	0.5249999790000024	0.1796899989999972	F	F	F
0.2690284647385333	0.7756420319146465	0.3496994906003550	F	F	F
0.5462539140344361	0.9173863748546097	0.2813644420240292	F	F	F
0.5499999999999972	0.1331900059999997	0.0905399970000005	F	F	F
0.0346229245143293	0.4126494591536694	0.2784985475799825	F	F	F
0.0499999999999972	0.6331899899999991	0.0905399970000005	F	F	F
0.7945630600163588	0.04463629223049728	0.3414500548362583	F	F	F
0.2819445597301199	1.0004070155063214	0.3537574316168670	F	F	F
0.3104938448049171	0.5451810881840551	0.3486185536273785	F	F	F
0.7909633837197939	0.4974383456600052	0.3674169247244934	F	F	F
0.7544611109473277	0.7805607366357986	0.3515364969791659	F	F	F
0.8336300499999965	0.5249999790000024	0.1796899989999972	F	F	F
0.2746120828176056	0.2677771602335810	0.3533847647641463	F	F	F
0.3336300030000032	0.0250000010000060	0.1796899989999972	F	F	F
0.0465899231268347	0.8800449624736710	0.2592436061184357	F	F	F
0.0499999999999972	0.1668099999999982	0.1116699999999966	F	F	F
0.5481012265777592	0.3822169335170977	0.2569286985318820	F	F	F
0.5499999999999972	0.6668099509999977	0.1116699999999966	F	F	F
0.5499999999999972	0.4000000200000603	0.1011099950000016	F	F	F
0.0482735267478367	0.1478515418738492	0.2718248767232317	F	F	F
0.5499999999999972	0.8999999540001363	0.1011099950000016	F	F	F
0.0506425527914712	0.6461536544723760	0.2743435369153040	F	F	F
0.0499999999999972	0.4000000200000603	0.1011099950000016	F	F	F
0.0499999999999972	0.8999999540001363	0.1011099950000016	F	F	F
0.5498555966278696	0.6500960131192290	0.2644709530533224	F	F	F
0.5519853599279755	0.1495145374414768	0.2691349276129530	F	F	F
0.3442033379094241	0.5365118988354254	0.4837687286362465	F	F	F
0.5009568016593009	0.4400468836573624	0.4198343399339292	F	F	F
0.5736276299340437	0.6561972784912226	0.4218741659473937	F	F	F
0.6882133016259484	0.5065707375377896	0.4841500522288948	F	F	F
0.6321815921162111	0.6381323886822842	0.5108409139853215	T	T	T

PdPt3/In2O3

1.000000000000000

10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9857006073000001

O	In	Pt	C
50	32	4	1

Selective dynamics

Direct

0.1819400070000015	0.5179200199999985	0.1152000000000015	F	F	F
0.6819400070000015	0.0179200010000003	0.1152000000000015	F	F	F

0.6803060597048306	0.0276260756891515	0.2538112003384810	F	F	F
0.1789165111507644	0.5178937219353758	0.2636980259637373	F	F	F
0.9072259261321191	0.3762426661076456	0.3577734443361221	F	F	F
0.4094078977191244	0.8829307685859380	0.3583273453584674	F	F	F
0.4271727156267328	0.6738773823576566	0.3492372627902546	F	F	F
0.9140758436531248	0.1629653008461316	0.3496985820790095	F	F	F
0.9545099699999966	0.3958000000000475	0.1866899999999987	F	F	F
0.4545100160000004	0.8957999670001077	0.1866899999999987	F	F	F
0.6429486552520882	0.7887502438851983	0.2633311883955710	F	F	F
0.1420079206805877	0.2857847348553493	0.2729297889033018	F	F	F
0.4545100160000004	0.1542000070000000	0.1726800109999971	F	F	F
0.9545099699999966	0.6542000230000017	0.1726800109999971	F	F	F
0.1454900069999994	0.7638599680000909	0.1037499959999977	F	F	F
0.6454899840000010	0.2638599840000011	0.1037499959999977	F	F	F
0.1903399939999985	0.2862900060000015	0.1125700079999987	F	F	F
0.6903399589999992	0.7862899730000947	0.1125700079999987	F	F	F
0.9096599470000013	0.8817800340001066	0.1725899979999994	F	F	F
0.4096599940000019	0.3817800010000489	0.1725899979999994	F	F	F
0.4096599940000019	0.6682199560000017	0.1867800019999990	F	F	F
0.9096599470000013	0.1682200059999988	0.1867800019999990	F	F	F
0.6893125966240984	0.2672843273204078	0.2539672617208001	F	F	F
0.1877927343068574	0.7605360003595150	0.2538340076657064	F	F	F
0.4180599929999999	0.7820899850000914	0.0870100030000032	F	F	F
0.9180600400000002	0.2820900179999983	0.0870100030000032	F	F	F
0.9189549902024253	0.7651012569335816	0.2858422151049790	F	F	F
0.4188443577383936	0.2634867223338906	0.2801905422782402	F	F	F
0.6819400070000015	0.4224300250000443	0.1752299990000026	F	F	F
0.1819400070000015	0.9224299590001043	0.1752299990000026	F	F	F
0.1819400070000015	0.1275800049999987	0.1841400010000029	F	F	F
0.6819400070000015	0.6275799969999982	0.1841400010000029	F	F	F
0.6271885707000706	0.3864200628033291	0.3580131857273471	F	F	F
0.1372349742623050	0.8956188458048158	0.3520105995688801	F	F	F
0.9569283104479001	0.0110869053609831	0.2708672646703121	F	F	F
0.4578209258477136	0.5155100981579936	0.2711853410740047	F	F	F
0.1572121947775411	0.6485993756926434	0.3655883072386509	F	F	F
0.6412429024966315	0.1477923082866358	0.3626737951042581	F	F	F
0.4545100160000004	0.5361400390000048	0.0984700050000029	F	F	F
0.9545099699999966	0.0361399980000030	0.0984700050000029	F	F	F
0.4096599940000019	0.0137100000000041	0.0896599969999983	F	F	F
0.9096599470000013	0.5137100339999991	0.0896599969999983	F	F	F
0.7128019257968702	0.9172364964900551	0.3687918215902676	F	F	F
0.3195404590470206	0.3981182317744229	0.3777771691235632	F	F	F
0.1994887613468946	0.1307914662530354	0.3582537245913678	F	F	F
0.6945006004940772	0.6447799807696929	0.3504099959917377	F	F	F

0.8969073777883049	0.5371095479374963	0.2839688474550884	F	F	F
0.4056146379577594	0.0383923445627539	0.2782212258260248	F	F	F
0.4105768731819298	0.3957254747927698	0.5756190688121073	T	T	T
0.6107808720348485	0.4195532123904562	0.5094618627130295	T	T	T
0.7999999999999972	0.7581899820000900	0.1902599909999978	F	F	F
0.3000000230000026	0.7918100090000949	0.1691199950000026	F	F	F
0.3000000230000026	0.2581899979999991	0.1902599909999978	F	F	F
0.7999999999999972	0.2918100090000028	0.1691199950000026	F	F	F
0.8336300499999965	0.0250000010000038	0.1796899989999972	F	F	F
0.7661466645888336	0.2658046211710892	0.3513170992159980	F	F	F
0.3336300030000032	0.5249999790000024	0.1796899989999972	F	F	F
0.2661082904543545	0.7744589481450533	0.3509594456290995	F	F	F
0.5437467415460694	0.9173843693355402	0.2810842235246018	F	F	F
0.5499999999999972	0.1331900059999997	0.0905399970000005	F	F	F
0.0304745283390169	0.4118689682737912	0.2794153881897753	F	F	F
0.0499999999999972	0.6331899899999991	0.0905399970000005	F	F	F
0.7944948483326532	0.0439484778339574	0.3420254155841179	F	F	F
0.2809453598012831	0.9990576756219413	0.3539596850984132	F	F	F
0.3060186904021300	0.5432246896566884	0.3477049215820867	F	F	F
0.7855269392591596	0.4967115136505715	0.3698938037724138	F	F	F
0.7610615396884058	0.7838072824196071	0.3483326767019939	F	F	F
0.8336300499999965	0.5249999790000024	0.1796899989999972	F	F	F
0.2753011385771945	0.2632453422229820	0.3507105743865561	F	F	F
0.3336300030000032	0.0250000010000038	0.1796899989999972	F	F	F
0.0493911740073334	0.8806359011834487	0.2581923009217644	F	F	F
0.0499999999999972	0.1668099999999982	0.1116699999999966	F	F	F
0.5470005307535218	0.3823339966301352	0.2588694456329335	F	F	F
0.5499999999999972	0.6668099509999977	0.1116699999999966	F	F	F
0.5499999999999972	0.4000000200000464	0.1011099950000016	F	F	F
0.0456645202041399	0.1478985758720671	0.2714924247305459	F	F	F
0.5499999999999972	0.8999999540001075	0.1011099950000016	F	F	F
0.0496769256872768	0.6449696309893157	0.2737686776932893	F	F	F
0.0499999999999972	0.4000000200000464	0.1011099950000016	F	F	F
0.0499999999999972	0.8999999540001075	0.1011099950000016	F	F	F
0.5499161276257198	0.6517815522993105	0.2652684654448184	F	F	F
0.5534795123613458	0.1484216388166602	0.2681096285988829	F	F	F
0.3805742940350573	0.5511333557409449	0.4931169434791267	F	F	F
0.4827704087021610	0.4048475996242475	0.4337302908376112	F	F	F
0.7119357662883505	0.5330229856471761	0.4885033948387754	F	F	F
0.5521489614352386	0.6157554550992715	0.4180747486898646	F	F	F
0.4514888332307765	0.4303046232470590	0.5273798397209215	T	T	T

Pt4/In2O3

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
 50 32 3 1 1

Selective dynamics

Direct

0.1819400070000015	0.5179200199999985	0.1152000000000015	F	F	F
0.6819400070000015	0.0179200010000003	0.1152000000000015	F	F	F
0.6795664257040763	0.0279973488141038	0.2540094967017761	T	T	T
0.1802512298950760	0.5181914491879532	0.2629936357873948	T	T	T
0.9177204331588205	0.3791932425172004	0.3600504813139958	T	T	T
0.4095714011675828	0.8834466120814753	0.3582180437438539	T	T	T
0.4219198374535268	0.6740659738830214	0.3478137962937300	T	T	T
0.9169003480751835	0.1633683209272971	0.3494097682010006	T	T	T
0.9545099699999966	0.3958000000000982	0.1866899999999987	F	F	F
0.4545100160000004	0.8957999670002250	0.1866899999999987	F	F	F
0.6418757488071873	0.7857818427112294	0.2646118978997443	T	T	T
0.1434244329609922	0.2863144764646416	0.2722087875700391	T	T	T
0.4545100160000004	0.1542000070000000	0.1726800109999971	F	F	F
0.9545099699999966	0.6542000230000017	0.1726800109999971	F	F	F
0.1454900069999994	0.7638599680001995	0.1037499959999977	F	F	F
0.6454899840000010	0.2638599840000011	0.1037499959999977	F	F	F
0.1903399939999985	0.2862900060000015	0.1125700079999987	F	F	F
0.6903399589999992	0.7862899730002034	0.1125700079999987	F	F	F
0.9096599470000013	0.8817800340002226	0.1725899979999994	F	F	F
0.4096599940000019	0.3817800010000997	0.1725899979999994	F	F	F
0.4096599940000019	0.6682199560000017	0.1867800019999990	F	F	F
0.9096599470000013	0.1682200059999988	0.1867800019999990	F	F	F
0.6892912432393193	0.2644799279744970	0.2526329749784031	T	T	T
0.1863049478906429	0.7617296283793947	0.2527414285254825	T	T	T
0.4180599929999999	0.7820899850002001	0.0870100030000032	F	F	F
0.9180600400000002	0.2820900179999983	0.0870100030000032	F	F	F
0.9171386745631508	0.7658392086204555	0.2850232477571236	T	T	T
0.4175510482191085	0.2667460312146444	0.2827809265947032	T	T	T
0.6819400070000015	0.4224300250001038	0.1752299990000026	F	F	F
0.1819400070000015	0.9224299590002216	0.1752299990000026	F	F	F
0.1819400070000015	0.1275800049999987	0.1841400010000029	F	F	F
0.6819400070000015	0.6275799969999982	0.1841400010000029	F	F	F
0.6487813117951416	0.3927760092113070	0.3470374011958466	T	T	T
0.1373757004526129	0.8963772865194746	0.3514444463671854	T	T	T
0.9564131793375947	0.0115170439337202	0.2706106306126170	T	T	T
0.4565806593244047	0.5140438324809918	0.2712445630287043	T	T	T

0.1498640353807450	0.6511510017228458	0.3639249109794223	T	T	T
0.6449766959022971	0.1508969641668355	0.3629349817689991	T	T	T
0.4545100160000004	0.5361400390000048	0.0984700050000029	F	F	F
0.9545099699999966	0.0361399980000030	0.0984700050000029	F	F	F
0.4096599940000019	0.0137100000000053	0.0896599969999983	F	F	F
0.9096599470000013	0.5137100339999991	0.0896599969999983	F	F	F
0.7144492994148848	0.9162037618949129	0.3673399935499024	T	T	T
0.3035123266939095	0.3949752019758835	0.3947507728425682	T	T	T
0.1999036493012072	0.1308872118380543	0.3567286818018777	T	T	T
0.6937992701626976	0.6434379173188760	0.3597590349221990	T	T	T
0.8978931479942280	0.5386237819743964	0.2827812400295708	T	T	T
0.4064064664484364	0.0386483482227480	0.2780528080841583	T	T	T
0.4221920232117244	0.6094261922979297	0.506436777637732	T	T	T
0.6397663357260868	0.6472269805770700	0.5646713672503557	T	T	T
0.799999999999972	0.7581899820001987	0.1902599909999978	F	F	F
0.3000000230000026	0.7918100090002035	0.1691199950000026	F	F	F
0.3000000230000026	0.2581899979999991	0.1902599909999978	F	F	F
0.799999999999972	0.2918100090000028	0.1691199950000026	F	F	F
0.8336300499999965	0.0250000010000061	0.1796899989999972	F	F	F
0.7736600704196352	0.2681596450213434	0.3492913194547624	T	T	T
0.3336300030000032	0.5249999790000024	0.1796899989999972	F	F	F
0.2650184462825064	0.7748000881920721	0.3500286083728129	T	T	T
0.5448945395120455	0.9165631477380862	0.2812818885234984	T	T	T
0.549999999999972	0.1331900059999997	0.0905399970000005	F	F	F
0.0331525850773392	0.4127674162289730	0.2790235756995094	T	T	T
0.049999999999972	0.6331899899999991	0.0905399970000005	F	F	F
0.7944358258912843	0.0447220555986704	0.3416946676901182	T	T	T
0.2815864035560554	-0.0005874480963113	0.3537676686659365	T	T	T
0.3030424425804303	0.5465551922893092	0.3467706108293110	T	T	T
0.7933419516541913	0.5021061098965679	0.3691699193028184	T	T	T
0.7614879072472526	0.7813649026472914	0.3490218862412213	T	T	T
0.8336300499999965	0.5249999790000024	0.1796899989999972	F	F	F
0.2702944616478543	0.2660853016540380	0.3530650225131833	T	T	T
0.3336300030000032	0.0250000010000061	0.1796899989999972	F	F	F
0.0486809327173457	0.8811598256013832	0.2581870306284499	T	T	T
0.049999999999972	0.1668099999999982	0.1116699999999966	F	F	F
0.5489895353082396	0.3818950602782222	0.2564673862885742	T	T	T
0.549999999999972	0.6668099509999977	0.1116699999999966	F	F	F
0.549999999999972	0.4000000200000973	0.1011099950000016	F	F	F
0.0479881056523774	0.1474793782495208	0.2712808071785746	T	T	T
0.549999999999972	0.8999999540002249	0.1011099950000016	F	F	F
0.0492603213800048	0.6465386719977058	0.2726179950209028	T	T	T
0.049999999999972	0.4000000200000973	0.1011099950000016	F	F	F
0.049999999999972	0.8999999540002249	0.1011099950000016	F	F	F

0.5486885313574423	0.6502670741364778	0.2672262860303929	T	T	T
0.5518845900730449	0.1493595252488980	0.2695485240881539	T	T	T
0.3261989464565964	0.5033055029696976	0.4707411973656492	T	T	T
0.5066432031590680	0.4280418594520152	0.4149339307882080	T	T	T
0.5437363033814945	0.6387486530322889	0.4299513187692930	T	T	T
0.6859213393940028	0.4921954498899050	0.4862363128545337	T	T	T
0.6024575645370576	0.6105166444264783	0.5168213914300883	T	T	T

CO and O co-adsorption on Pd_nPt(4-n)/In₂O₃ catalysts

Pd₂Pt₂/In₂O₃

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
 50 32 2 2 1

Selective dynamics

Direct

0.1819400070000015	0.5179200199999983	0.1152000000000015	F	F	F
0.6819400070000015	0.0179200010000002	0.1152000000000015	F	F	F
0.6797118614789166	0.0286555211434135	0.2533888366132040	T	T	T
0.1804970670577834	0.5185066718945308	0.2620042994007155	T	T	T
0.9173690748398395	0.3760763781997258	0.3575963693562678	T	T	T
0.4086999472450688	0.8842609356252452	0.3582018534522659	T	T	T
0.4244639361306626	0.6741500345966273	0.3468467741578656	T	T	T
0.9169955966989161	0.1625248688199032	0.3495693135261938	T	T	T
0.9545099699999966	0.3958000000000013	0.1866899999999987	F	F	F
0.4545100160000004	0.8957999670000021	0.1866899999999987	F	F	F
0.6410167486360818	0.7858028943605337	0.2642250754886561	T	T	T
0.1460282253768798	0.2869468706602050	0.2726158199186081	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
0.6894765302772755	0.2651948325853008	0.2528009055914961	T	T	T
0.1860321665543957	0.7621644768141327	0.2531510360836263	T	T	T
0.4180599930000000	0.7820899849999989	0.0870100030000032	F	F	F
0.9180600400000003	0.2820900179999981	0.0870100030000032	F	F	F
0.9145556679693939	0.7658407140928356	0.2864083609057350	T	T	T
0.4185128509982188	0.2667712111296457	0.2822964499956088	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

0.6431701475568989	0.3903642765483543	0.3500970976381186	T	T	T
0.1373434632654619	0.8972376789242441	0.3518187476539573	T	T	T
0.9574119493705097	0.0118840866239754	0.2702591847458522	T	T	T
0.4568314008250920	0.5136045184659913	0.2706056288136598	T	T	T
0.1517391514736707	0.6506796532998457	0.3632845831948443	T	T	T
0.6445672426848186	0.1499983663141050	0.3627420748188573	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
0.7119163109544671	0.9170425203830461	0.3656825201074599	T	T	T
0.3120570431794707	0.4008085343225201	0.3948554155766363	T	T	T
0.2032426546522750	0.1338122350632463	0.3568234583107762	T	T	T
0.6956636783149064	0.6369463027740372	0.3520962785025117	T	T	T
0.8996873612113643	0.5371963048545657	0.2822742910625746	T	T	T
0.4063567740907518	0.0386996400656841	0.2778634125985063	T	T	T
0.7467091877425109	0.6723994707293218	0.5313432530700036	T	T	T
0.4053021676476128	0.6555306997058583	0.4833830607444036	T	T	T
0.799999999999972	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
0.799999999999972	0.2918100090000024	0.1691199950000026	F	F	F
0.8336300499999965	0.0250000010000022	0.1796899989999972	F	F	F
0.7724261027862341	0.2668080383541751	0.3493632100669078	T	T	T
0.3336300030000032	0.5249999790000004	0.1796899989999972	F	F	F
0.2655319796679140	0.7750805293559696	0.3514173847389442	T	T	T
0.5451611970143849	0.9168065790489802	0.2816270374139245	T	T	T
0.549999999999972	0.1331900059999995	0.0905399970000005	F	F	F
0.0346055411280766	0.4124655843656096	0.2781712477120308	T	T	T
0.049999999999972	0.6331899899999982	0.0905399970000005	F	F	F
0.7950467427858854	0.0442613441060587	0.3411566424087564	T	T	T
0.2813611273309901	0.9991322973107448	0.3539032948078248	T	T	T
0.3034298646825172	0.5448459317656776	0.3455432122121458	T	T	T
0.7931998355931500	0.4974002779006440	0.3675340760398492	T	T	T
0.7553195309590983	0.7801691012221483	0.3505236628643465	T	T	T
0.8336300499999965	0.5249999790000004	0.1796899989999972	F	F	F
0.2745164906269194	0.2701186430723987	0.3539446153019182	T	T	T
0.3336300030000032	0.0250000010000022	0.1796899989999972	F	F	F
0.0474136252852071	0.8806394947904279	0.2590811718314229	T	T	T
0.049999999999972	0.1668099999999981	0.1116699999999966	F	F	F
0.5489412533993867	0.3817596691788093	0.2572989251012425	T	T	T
0.549999999999972	0.6668099509999976	0.1116699999999966	F	F	F
0.549999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0493571005114864	0.1481545960620215	0.2719290654647620	T	T	T

0.549999999999972	0.899999954000019	0.1011099950000016	F	F	F
0.0483534553956840	0.6472193006721983	0.2732252443736168	T	T	T
0.049999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.049999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.5498999384695923	0.6493479971344231	0.2656935610039474	T	T	T
0.5517757562135662	0.1492411585689807	0.2694356601930998	T	T	T
0.3322981976309853	0.5333777805967546	0.4717862175625072	T	T	T
0.5102672868813312	0.4376902852145825	0.4212629252207001	T	T	T
0.5548645138254573	0.6562379425180163	0.4248638660662821	T	T	T
0.7057312341298725	0.4972343583954467	0.4855375642315188	T	T	T
0.6825843499908598	0.6335572630316161	0.4913366004611821	T	T	T

Pd3Pt/In2O3

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
50	32	3	1	1

Selective dynamics

Direct

0.1819400070000015	0.5179200199999983	0.1152000000000015	F	F	F
0.6819400070000015	0.0179200010000002	0.1152000000000015	F	F	F
0.6795153641101581	0.0278260952629352	0.2538563757942963	T	T	T
0.1799308342189091	0.5177778521677154	0.2619700630025217	T	T	T
0.9182661468959923	0.3781275303970656	0.3587165363592802	T	T	T
0.4088090360790916	0.8832386941139400	0.3582531082246134	T	T	T
0.4205813799735557	0.6734398360141494	0.3478896962039997	T	T	T
0.9167903491657895	0.1629863413425169	0.3495026803610752	T	T	T
0.9545099699999966	0.3958000000000013	0.1866899999999987	F	F	F
0.4545100160000004	0.8957999670000021	0.1866899999999987	F	F	F
0.6412706035847080	0.7854741447497827	0.2646694745513139	T	T	T
0.1454727207839079	0.2864024102130961	0.2728642946719164	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

0.6894645105901210	0.2647959145471313	0.2527359402856765	T	T	T
0.1864909682472710	0.7621440018931497	0.2527714862611411	T	T	T
0.4180599930000000	0.7820899849999989	0.0870100030000032	F	F	F
0.9180600400000003	0.2820900179999981	0.0870100030000032	F	F	F
0.9162151534737791	0.7661766916735355	0.2847908458740460	T	T	T
0.4182796496063403	0.2666004817594532	0.2825626425589815	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
0.6474651891809777	0.3920920695946405	0.3484661441352309	T	T	T
0.1366752999590227	0.8965194440544455	0.3517421777250846	T	T	T
0.9567755588401662	0.0116964486366527	0.2704489698249552	T	T	T
0.4566427832207755	0.5138484617093326	0.2711750799476155	T	T	T
0.1475277575587431	0.6511227068889694	0.3627452400601390	T	T	T
0.6449761261289880	0.1505649454862108	0.3628509768669864	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
0.7138971959695457	0.9160177999300801	0.3668123162461948	T	T	T
0.3121172419817942	0.3946501836483581	0.3969351809876578	T	T	T
0.2011208970240883	0.1313757119428695	0.3567010663674319	T	T	T
0.6935311512702860	0.6427242362861629	0.3594963431760372	T	T	T
0.8980032998207447	0.5383856217461104	0.2822879331660743	T	T	T
0.4064081524906306	0.0384738159270203	0.2780569752594756	T	T	T
0.3894697604775529	0.6328955141074527	0.4896730643770852	T	T	T
0.7276725895712425	0.6702285989886182	0.5356676938052073	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
0.7735917536852935	0.2678472800652862	0.3492972150970902	T	T	T
0.3336300030000032	0.5249999790000004	0.1796899989999972	F	F	F
0.2638697051939380	0.7744641281173629	0.3509723873036319	T	T	T
0.5446225417690737	0.9163149144112450	0.2815419192029914	T	T	T
0.5499999999999972	0.1331900059999995	0.0905399970000005	F	F	F
0.0338559669647838	0.4120936730927854	0.2785010149582947	T	T	T
0.0499999999999972	0.6331899899999982	0.0905399970000005	F	F	F
0.7945089801409715	0.0444496193586803	0.3415167824360547	T	T	T
0.2813540266045586	-0.0005843844243046	0.3538467277674050	T	T	T
0.3011372776338108	0.5463560322394448	0.3453650910312595	T	T	T
0.7942408518623625	0.5010121274764714	0.3679595516031957	T	T	T

0.7607700624058704	0.7808726115001529	0.3492539019195043	T	T	T
0.8336300499999965	0.5249999790000004	0.1796899989999972	F	F	F
0.2734393648716382	0.2667546316183997	0.3540554466115257	T	T	T
0.3336300030000032	0.0250000010000022	0.1796899989999972	F	F	F
0.0487033189521693	0.8812199264215106	0.2583249256663269	T	T	T
0.0499999999999972	0.1668099999999981	0.1116699999999966	F	F	F
0.5490349378347776	0.3817961313565161	0.2570190059580109	T	T	T
0.5499999999999972	0.6668099509999976	0.1116699999999966	F	F	F
0.5499999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0487606161413479	0.1477533845551059	0.2717117330171802	T	T	T
0.5499999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.0485584497546660	0.6470602334470139	0.2721692023082691	T	T	T
0.0499999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0499999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.5486256900316843	0.6501222344662538	0.2675502337113079	T	T	T
0.5520582234970239	0.1491418570870770	0.2694969644557548	T	T	T
0.3223182096710349	0.5142598185712545	0.4679528921174439	T	T	T
0.5106931414660411	0.4320457352691432	0.4190349107815175	T	T	T
0.5407951458348605	0.6457954854139298	0.4303652405625458	T	T	T
0.7028584629668027	0.4923043469955994	0.4856356708601181	T	T	T
0.6694669104214772	0.6252768997983624	0.4970729778436879	T	T	T

Pd4/In2O3

1.0000000000000000

10.2175998688000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4497995377000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9857006073000001

O In Pd C
50 32 4 1

Selective dynamics

Direct

0.1819400070000015	0.5179200199999983	0.1152000000000015	F	F	F
0.6819400070000015	0.0179200010000002	0.1152000000000015	F	F	F
0.6798282046542177	0.0281668762752469	0.2539770342014862	T	T	T
0.1795790590656354	0.5177756193249816	0.2618126746454076	T	T	T
0.9195121072696407	0.3783195818163183	0.3597190503718554	T	T	T
0.4094262577206114	0.8832067767169468	0.3580216186611623	T	T	T
0.4212367657948487	0.6730506320922668	0.3489727000093880	T	T	T
0.9180092020069617	0.1630789151848938	0.3496235503751471	T	T	T
0.9545099699999966	0.3958000000000013	0.1866899999999987	F	F	F
0.4545100160000004	0.8957999670000021	0.1866899999999987	F	F	F
0.6410029515388166	0.7859670212764873	0.2643291361992278	T	T	T
0.1455740841779246	0.2866244088156399	0.2727740441705189	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
0.6896327184685076	0.2644658162682471	0.2525700705003154	T	T	T
0.1868894580410388	0.7621541265003630	0.2527882693485630	T	T	T
0.4180599930000000	0.7820899849999989	0.0870100030000032	F	F	F
0.9180600400000003	0.2820900179999981	0.0870100030000032	F	F	F
0.9165037896416208	0.7665305116465685	0.2844048602677851	T	T	T
0.4182306435579322	0.2667999374230763	0.2827738589674543	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
0.6505629078168899	0.3923157464368632	0.3466515931914164	T	T	T
0.1372446793712750	0.8968229519670867	0.3517412049910265	T	T	T
0.9570408910829485	0.0117675454405949	0.2704714957921512	T	T	T
0.4563931476411465	0.5142714717660167	0.2710077589961815	T	T	T
0.1476545013355113	0.6517082704011538	0.3624751993396494	T	T	T
0.6460207402609102	0.1510606242029600	0.3629230581974212	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
0.7146116184119204	0.9167690383582194	0.3672984133408282	T	T	T
0.3112696487160299	0.3941650346142729	0.3975155842380088	T	T	T
0.2014155471946807	0.1313828558198738	0.3564872401817698	T	T	T
0.6926237880269667	0.6453299912788351	0.3607196093256921	T	T	T
0.8976573801580199	0.5385276185147679	0.2824271502804891	T	T	T
0.4067243305534184	0.0387199083862851	0.2780087345403818	T	T	T
0.7218324341066399	0.6738747871882115	0.5397652031000127	T	T	T
0.3856567574627496	0.6316798555681670	0.4898413946168602	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
0.7748643066066767	0.2679774312981862	0.3490108744403214	T	T	T

0.3336300030000032	0.5249999790000004	0.1796899989999972	F	F	F
0.2642309680093794	0.7747301978337267	0.3508874290702454	T	T	T
0.5447323132488768	0.9168356863765772	0.2811221062877760	T	T	T
0.5499999999999972	0.1331900059999995	0.0905399970000005	F	F	F
0.0334086497735925	0.4122032414832366	0.2787132978809623	T	T	T
0.0499999999999972	0.6331899899999982	0.0905399970000005	F	F	F
0.7952083635171081	0.0448076385795576	0.3415511812691603	T	T	T
0.2819482449401530	-0.0003858831702654	0.3538993402849825	T	T	T
0.3001801222164222	0.5462549586951212	0.3451860883471813	T	T	T
0.7944415318320110	0.5017479732633618	0.3688238089555035	T	T	T
0.7613605415392726	0.7821822759748340	0.3487173055681268	T	T	T
0.8336300499999965	0.5249999790000004	0.1796899989999972	F	F	F
0.2729226694300825	0.2670083226267000	0.3543781363007067	T	T	T
0.3336300030000032	0.0250000010000022	0.1796899989999972	F	F	F
0.0492812075612389	0.8814575024059064	0.2582550688825706	T	T	T
0.0499999999999972	0.1668099999999981	0.1116699999999966	F	F	F
0.5489802394547615	0.3818190738347589	0.2565937665531712	T	T	T
0.5499999999999972	0.6668099509999976	0.1116699999999966	F	F	F
0.5499999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0492236478790459	0.1478396525475109	0.2715736596351688	T	T	T
0.5499999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.0483307084335733	0.6471021490038059	0.2720907405662253	T	T	T
0.0499999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0499999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.5489885011302670	0.6503360488810799	0.2677743656631202	T	T	T
0.5522124097209050	0.1495113578083306	0.2696752926316902	T	T	T
0.3239070099309564	0.5120691397153636	0.4665694820997430	T	T	T
0.5155135081915329	0.4365355948209371	0.4149752628227276	T	T	T
0.6999173948836421	0.5002768721232875	0.4876760549684944	T	T	T
0.5388281502186225	0.6467596774291460	0.4311594050907955	T	T	T
0.6630375117201532	0.6340722634411201	0.4993700273561507	T	T	T

PdPt3/In2O3

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
50	32	1	3	1

Selective dynamics

Direct

0.1819400070000015	0.5179200199999983	0.1152000000000015	F	F	F
0.6819400070000015	0.0179200010000002	0.1152000000000015	F	F	F

0.6795766836423482	0.0282986906695936	0.2533329345456494	T	T	T
0.1808828305404527	0.5179156198186556	0.2627953389389139	T	T	T
0.9136070780901149	0.3755152822985671	0.3570371800008681	T	T	T
0.4084848561160984	0.8838096793679455	0.3581585894352526	T	T	T
0.4253215936049020	0.6746978662652138	0.3469562314937025	T	T	T
0.9161459736018591	0.1619453024403499	0.3497988943125845	T	T	T
0.9545099699999966	0.3958000000000013	0.1866899999999987	F	F	F
0.4545100160000004	0.8957999670000021	0.1866899999999987	F	F	F
0.6415043750322024	0.7858071945684352	0.2643093416053917	T	T	T
0.1449736399631841	0.2865038300669678	0.2730033382017296	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
0.6894442754666014	0.2658099108004698	0.2532772431216714	T	T	T
0.1860787522534353	0.7617641129960089	0.2531823736358636	T	T	T
0.4180599930000000	0.7820899849999989	0.0870100030000032	F	F	F
0.9180600400000003	0.2820900179999981	0.0870100030000032	F	F	F
0.9146800469883805	0.7653194387144210	0.2865667820181803	T	T	T
0.4181840230514174	0.2660923289757586	0.2819456703922503	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
0.6378862192715923	0.3887351551790541	0.3518345721503942	T	T	T
0.1367984056939812	0.8964583485285778	0.3519590721863654	T	T	T
0.9571634012303268	0.0115146027964364	0.2702432779048120	T	T	T
0.4572138977660333	0.5138454115020892	0.2701059190660885	T	T	T
0.1525654254434924	0.6500940079961108	0.3636390920879491	T	T	T
0.6433848583791203	0.1489720522808521	0.3627109798569484	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
0.7117692649434945	0.9166913279925256	0.3658942318045586	T	T	T
0.3112699378504838	0.3983372057733005	0.3941225732245962	T	T	T
0.2018195701180200	0.1324284680343727	0.3568985929713830	T	T	T
0.6954444280285318	0.6369143342642511	0.3527118834187386	T	T	T

0.8992479418768448	0.5368578998157092	0.2826217528959470	T	T	T
0.4061179208212748	0.0384718747981497	0.2779083978267165	T	T	T
0.7388403287836306	0.6668820316257564	0.5359560532417608	T	T	T
0.4052872402173295	0.6574150367033493	0.4835185494813490	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
0.7706953840399313	0.2656583850524708	0.3501298684201036	T	T	T
0.3336300030000032	0.5249999790000004	0.1796899989999972	F	F	F
0.2654557005759176	0.7747022276114227	0.3514755165706078	T	T	T
0.5449573217542381	0.9164553839645053	0.2816568142962380	T	T	T
0.5499999999999972	0.1331900059999995	0.0905399970000005	F	F	F
0.0339288352116546	0.4122370983876011	0.2784111812965337	T	T	T
0.0499999999999972	0.6331899899999982	0.0905399970000005	F	F	F
0.7947364335241551	0.0436245404491883	0.3412177381353321	T	T	T
0.2808202734118850	0.9997954327690687	0.3537271318177085	T	T	T
0.3055611600930972	0.5450196622206925	0.3462949208007905	T	T	T
0.7918976386224575	0.4972426215002260	0.3681334275257020	T	T	T
0.7556014841845287	0.7798925492940696	0.3507718337448819	T	T	T
0.8336300499999965	0.5249999790000004	0.1796899989999972	F	F	F
0.2745586597067521	0.2676219756377304	0.3535147597959619	T	T	T
0.3336300030000032	0.0250000010000022	0.1796899989999972	F	F	F
0.0472503858723039	0.8801272724259777	0.2590373612106525	T	T	T
0.0499999999999972	0.1668099999999981	0.1116699999999966	F	F	F
0.5481981641788137	0.3816417200715365	0.2572293403731067	T	T	T
0.5499999999999972	0.6668099509999976	0.1116699999999966	F	F	F
0.5499999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0485167156385825	0.1477709869366845	0.2719419764623153	T	T	T
0.5499999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.0487167662792407	0.6466583692252152	0.2734679264410160	T	T	T
0.0499999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0499999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.5498839123968565	0.6496203403887569	0.2656962860053845	T	T	T
0.5517668587963130	0.1488314134669840	0.2692341309227697	T	T	T
0.3301039804123411	0.5356480681943500	0.4744403283379883	T	T	T
0.5038647470550743	0.4381240408371078	0.4212141560873319	T	T	T
0.5554144128844153	0.6578662653816116	0.4251386168283245	T	T	T
0.6993507834577977	0.4950071879114189	0.4849509477627080	T	T	T
0.6785810313954986	0.6316358594400874	0.4930592513618491	T	T	T

1.000000000000000

10.2175998688000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4497995377000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9857006073000001

O	In	Pt	C
50	32	4	1

Selective dynamics

Direct

0.1819400070000015	0.5179200199999983	0.1152000000000015	F	F	F
0.6819400070000015	0.0179200010000002	0.1152000000000015	F	F	F
0.6803122443635218	0.0276154722415163	0.2536519376065069	T	T	T
0.1807476803716748	0.5178039291305805	0.2648439749360441	T	T	T
0.9111986793033063	0.3776579487036690	0.3573973906233909	T	T	T
0.4094525307553357	0.8836044373960932	0.3583554357278121	T	T	T
0.4278591068214132	0.6762161768101683	0.3488558681151242	T	T	T
0.9139165522705219	0.1638475663345448	0.3495936121015584	T	T	T
0.9545099699999966	0.3958000000000013	0.1866899999999987	F	F	F
0.4545100160000004	0.8957999670000021	0.1866899999999987	F	F	F
0.6421710193611757	0.7876588109990195	0.2634227656601233	T	T	T
0.1434698672401568	0.2855954922225461	0.2724183524665281	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
0.6898604234031306	0.2674192287112850	0.2540316526094733	T	T	T
0.1878768241025571	0.7615923953907471	0.2532736767292494	T	T	T
0.4180599930000000	0.7820899849999989	0.0870100030000032	F	F	F
0.9180600400000003	0.2820900179999981	0.0870100030000032	F	F	F
0.9185200561772994	0.7654655257000075	0.2851355142456600	T	T	T
0.4191622984120002	0.2633788408695266	0.2799042045613174	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
0.6326949944640592	0.3894532205122345	0.3560244284940347	T	T	T
0.1374534244432397	0.8965782387962656	0.3516171258940390	T	T	T
0.9567865210291615	0.0116358652375833	0.2707046466689936	T	T	T
0.4565870403795312	0.5155386780031332	0.2715677389578812	T	T	T

0.1541293086048725	0.6513352992431023	0.3643571711510023	T	T	T
0.6419669821689887	0.1484137477267409	0.3626496603744233	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
0.7137219610624261	0.9165564557704727	0.3678300949688861	T	T	T
0.3247813255742081	0.3947681617247081	0.3797966989844389	T	T	T
0.1994565390629255	0.1309413792462907	0.3573711472161012	T	T	T
0.6969705056513439	0.6429053274654604	0.3515348405997024	T	T	T
0.8984296139009090	0.5376921498506760	0.2825708486135934	T	T	T
0.4064457964062915	0.0385458568500152	0.2779212533398257	T	T	T
0.3131206833227818	0.3982218310117077	0.5479349160353012	T	T	T
0.6509271825975189	0.4017570222320234	0.4907214567357703	T	T	T
0.799999999999972	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
0.799999999999972	0.2918100090000024	0.1691199950000026	F	F	F
0.8336300499999965	0.0250000010000022	0.1796899989999972	F	F	F
0.7669442935735321	0.2675363943490242	0.3521183483872499	T	T	T
0.3336300030000032	0.5249999790000004	0.1796899989999972	F	F	F
0.2657196606431648	0.7751681319454167	0.3508287616358859	T	T	T
0.5441860014099863	0.9171291661051316	0.2811608369186604	T	T	T
0.549999999999972	0.1331900059999995	0.0905399970000005	F	F	F
0.0331971655840007	0.4120070600535558	0.2789306430061796	T	T	T
0.049999999999972	0.6331899899999982	0.0905399970000005	F	F	F
0.7942022555107333	0.0446224208419716	0.3419048095972004	T	T	T
0.2815756072377594	-0.0003014275906365	0.3536534534157749	T	T	T
0.3038563360194764	0.5420871657014933	0.3514415497202487	T	T	T
0.7881985695886469	0.4976784339090694	0.3673781970478519	T	T	T
0.7609470883729507	0.7825874751735046	0.3479837781430370	T	T	T
0.8336300499999965	0.5249999790000004	0.1796899989999972	F	F	F
0.2760176436357398	0.2632243016335283	0.3511826879098146	T	T	T
0.3336300030000032	0.0250000010000022	0.1796899989999972	F	F	F
0.0491809996144016	0.8811010570402127	0.2582858943070825	T	T	T
0.049999999999972	0.1668099999999981	0.1116699999999966	F	F	F
0.5465697317398330	0.3826495921934733	0.2596958850788268	T	T	T
0.549999999999972	0.6668099509999976	0.1116699999999966	F	F	F
0.549999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.0458352541096937	0.1484951755678611	0.2716646142019538	T	T	T
0.549999999999972	0.8999999540000019	0.1011099950000016	F	F	F
0.0511818030223961	0.6455612165342005	0.2732255702169881	T	T	T
0.049999999999972	0.4000000200000002	0.1011099950000016	F	F	F
0.049999999999972	0.8999999540000019	0.1011099950000016	F	F	F

0.5492941679232997	0.6506629917394036	0.2656504955479537	T	T	T
0.5541604268267747	0.1489493584162317	0.2681667788632910	T	T	T
0.3523375808137570	0.5618995636386720	0.4832781764601866	T	T	T
0.4938759123953599	0.3965722403650698	0.4360058408982842	T	T	T
0.7059020331073668	0.5265350823084834	0.4849030414154673	T	T	T
0.5467341795582419	0.6155533251051224	0.4178845769641208	T	T	T
0.3746542343031350	0.4289039570438839	0.5040300679106602	T	T	T