

Supporting Information

Systematic screening of transition metal dual-atom doped phthalocyanine electrocatalysts for oxygen reduction reaction

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Table S2. Adsorption energies of O_2 on $\text{Tm}_2\text{-Pc}$

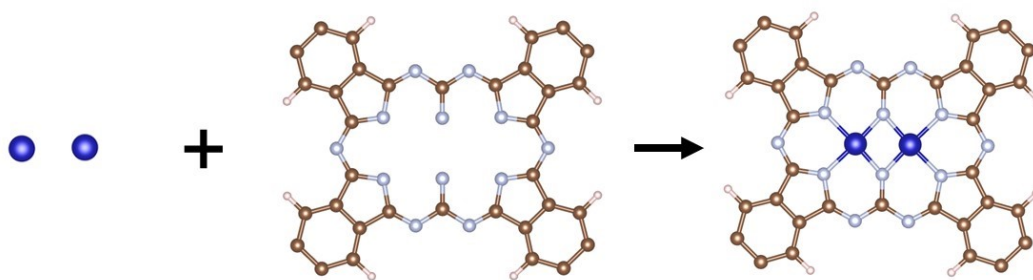


Figure S1. Schematic diagram of Tm₂-Pc formation by doping Pc with dual transition atoms.

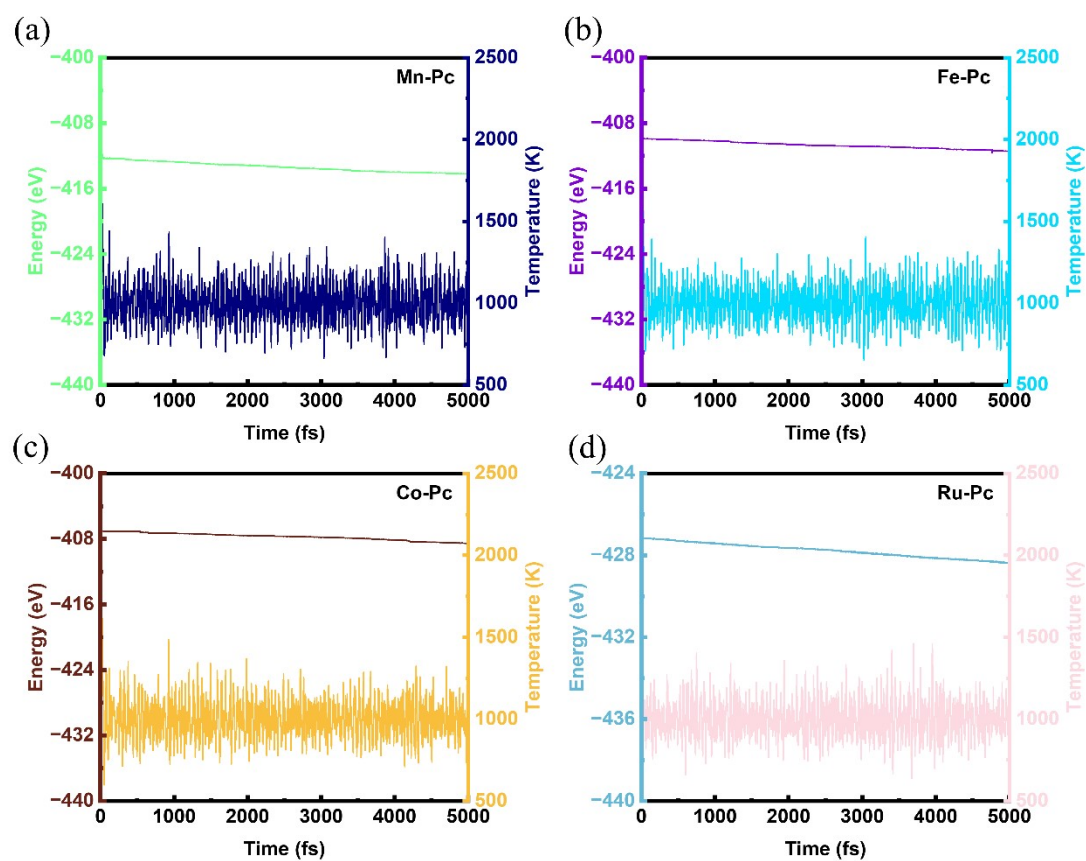


Figure S2. AIMD of Mn₂-Pc, Fe₂-Pc, Co₂-Pc, and Ru₂-Pc at 1000 K, respectively.

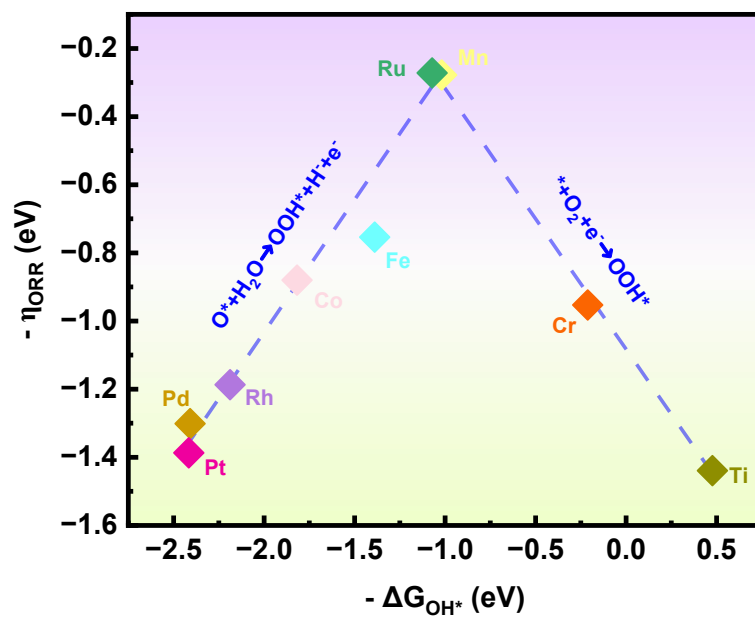


Figure S3. The scaling relation of ΔG_{OOH^*} as ΔG_{OH^*}

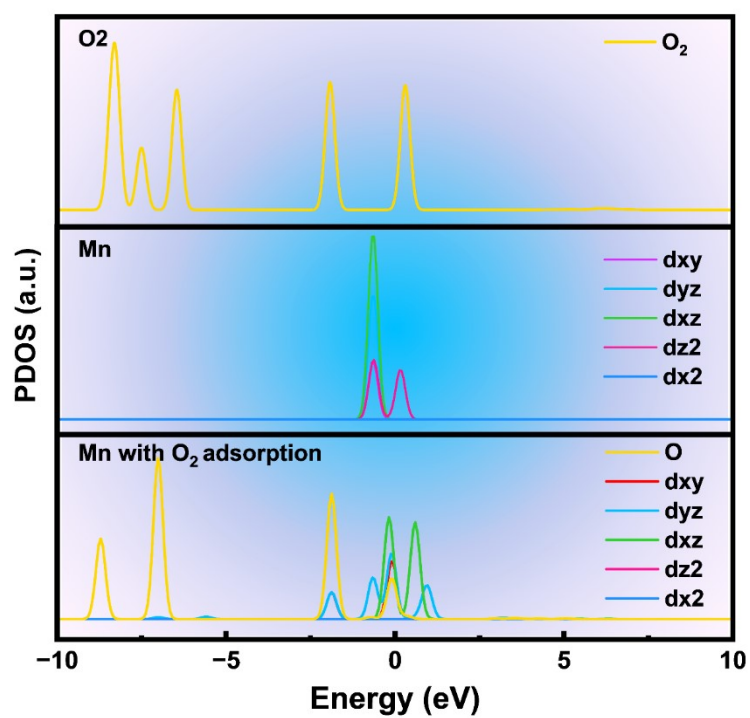


Figure S4. The PDOS of free O_2 , Mn atom, and O_2 adsorbed Mn atom

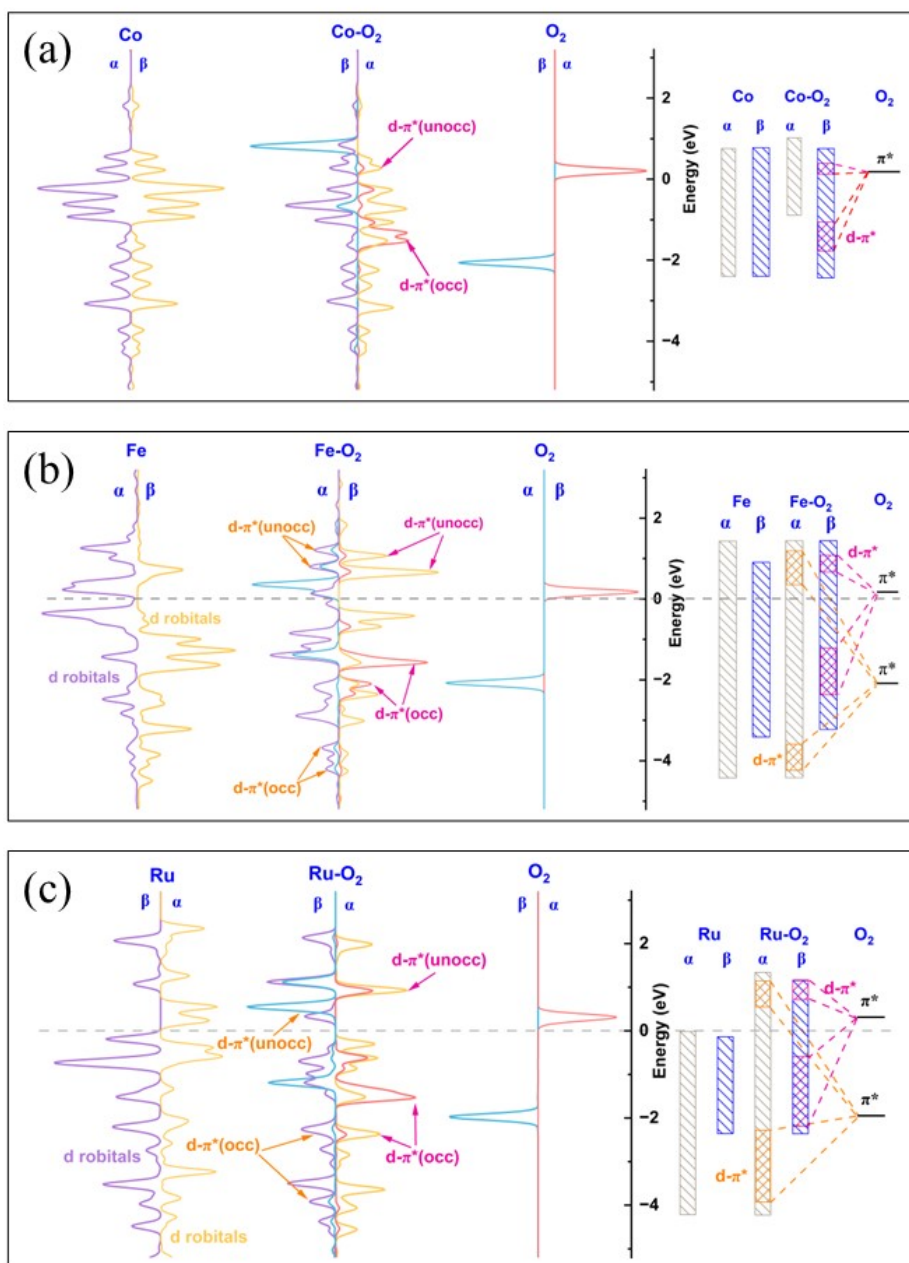


Figure S5. PDOS and schematic illustrations of 3d orbitals of (a) Co₂-Pc, (b) Fe₂-Pc, (c) Ru₂-Pc, 2p-orbitals of O₂ gas molecule, O₂ adsorbed on Co₂-Pc, Fe₂-Pc, Ru₂-Pc, respectively.

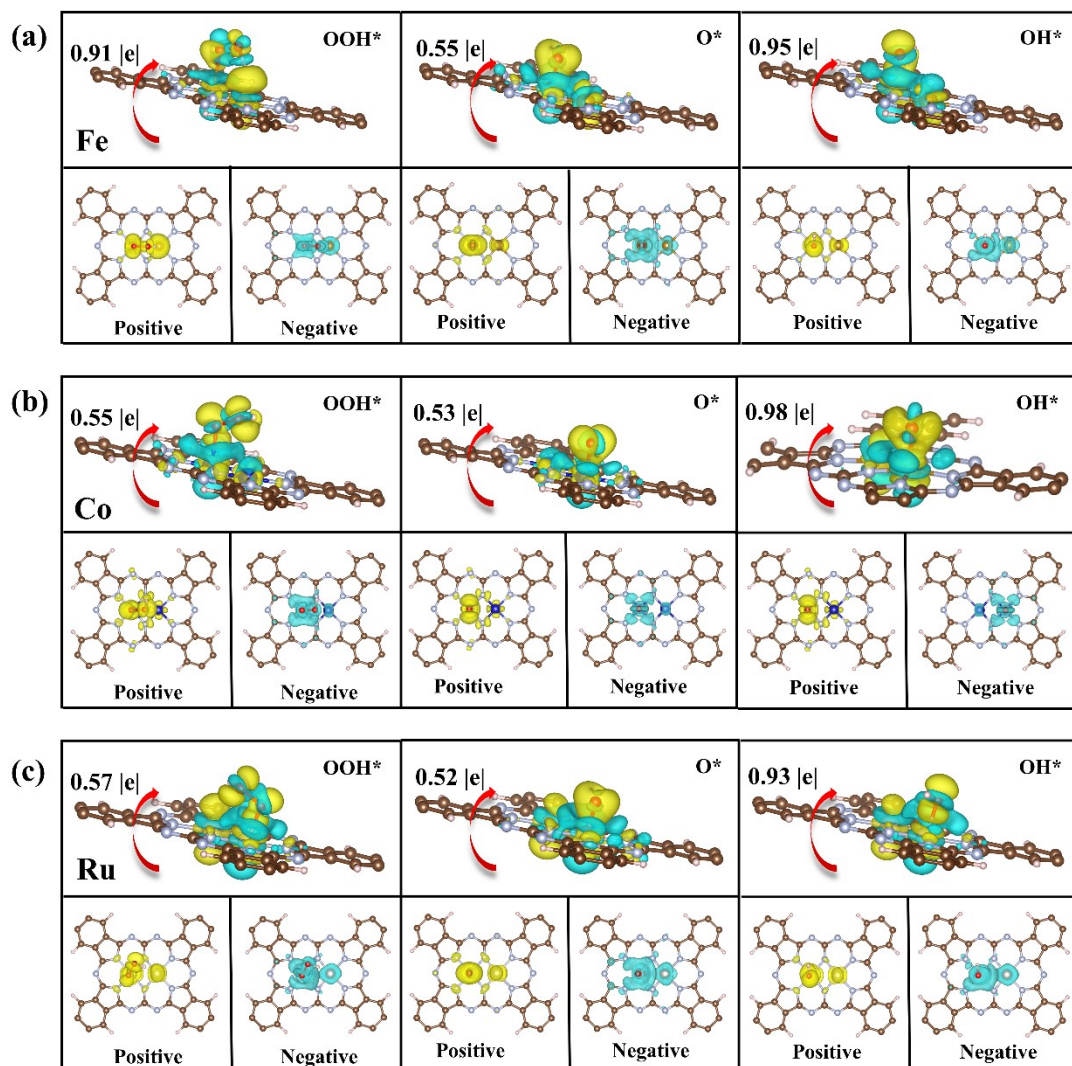


Figure S6. The differential charge density of *OOH, *O and *OH adsorbed on (a) Fe₂-Pc, (b) Co₂-Pc, (c) Ru₂-Pc, respectively.

Table S1. Formation energies of Tm₂-Pc (

$$E_{form} = E_{tot} - E_{Pc} - 2 * E_{Tm\ atom})$$

TM-Pc	E_{tot}	E_{Pc}	$2 * E_{Tm\ atom}$	E_{form}
Sc-Pc	-414.28	-389.54	-13.06	-11.68
Ti-Pc	-418.12	-389.54	-16.60	-11.98
V-Pc	-419.83	-389.54	-19.04	-11.26
Cr-Pc	-420.53	-389.54	-19.88	-11.11
Mn-Pc	-420.17	-389.54	-18.64	-12.00
Fe-Pc	-417.85	-389.54	-17.10	-11.21
Co-Pc	-414.96	-389.54	-14.77	-10.66
Ni-Pc	-412.20	-389.54	-11.74	-10.92
Cu-Pc	-405.99	-389.54	-8.48	-7.97
Zn-Pc	-410.15	-389.54	-2.93	-17.68
Y-Pc	-412.15	-389.54	-13.40	-9.21
Zr-Pc	-416.02	-389.54	-17.90	-8.58
Nb-Pc	-419.12	-389.54	-21.55	-8.03
Mo-Pc	-420.48	-389.54	-22.93	-8.01
Tc-Pc	-420.30	-389.54	-21.79	-8.97
Ru-Pc	-417.75	-389.54	-25.33	-2.88
Rh-Pc	-414.45	-389.54	-9.79	-15.11
Pd-Pc	-409.23	-389.54	-11.60	-8.09
Ag-Pc	-400.09	-389.54	-6.42	-4.13
Cd-Pc	-394.97	-389.54	-2.17	-3.26
Hf-Pc	-419.21	-389.54	-20.65	-9.02
Ta-Pc	-422.02	-389.54	-24.81	-7.68
W-Pc	-423.82	-389.54	-27.13	-7.15
Re-Pc	-423.65	-389.54	-26.02	-8.09
Os-Pc	-421.20	-389.54	-23.68	-7.98
Ir-Pc	-417.03	-389.54	-19.12	-8.37
Pt-Pc	-411.74	-389.54	-13.73	-8.47
Au-Pc	-402.66	-389.54	-7.75	-5.37
Hg-Pc	-391.23	-389.54	-1.24	-0.45

Table S2. Dissolution potential of O2 on Tm2-Pc (

$$U_{diss} = U_{diss^o} - E_{form}/Ne$$
)

TM-Pc	E_{form}	U_{diss}^o	Ne	U_{diss}
Sc-Pc	-11.68	-2.08	3	1.81
Ti-Pc	-11.98	-1.63	2	2.36
V-Pc	-11.26	-1.18	2	2.57
Cr-Pc	-11.11	-0.91	2	2.79
Mn-Pc	-12.00	-1.19	2	2.81
Fe-Pc	-11.21	-0.45	2	3.29
Co-Pc	-10.66	-0.28	2	3.27
Ni-Pc	-10.92	-0.26	2	3.38
Cu-Pc	-7.97	0.34	2	3.00
Zn-Pc	-17.68	-0.76	2	5.13
Y-Pc	-9.21	-2.37	3	0.70
Zr-Pc	-8.58	-1.45	4	1.41
Nb-Pc	-8.03	-1.10	3	1.58
Mo-Pc	-8.01	-0.20	3	2.47
Tc-Pc	-8.97	-	-	-
Ru-Pc	-2.88	0.46	2	1.42
Rh-Pc	-15.11	0.6	2	5.64
Pd-Pc	-8.09	0.95	2	3.65
Ag-Pc	-4.13	0.8	1	2.18
Cd-Pc	-3.26	-	-	-
Hf-Pc	-9.02	-0.14	4	2.87
Ta-Pc	-7.68	-0.6	3	1.96
W-Pc	-7.15	0.1	3	2.48
Re-Pc	-8.09	0.3	3	3.00
Os-Pc	-7.98	0.84	8	3.50
Ir-Pc	-8.37	1.16	3	3.95
Pt-Pc	-8.47	1.18	2	4.00
Au-Pc	-5.37	1.5	3	3.29
Hg-Pc	-0.45	-	-	-

Table S3. Adsorption energies of O₂ on Tm₂-Pc (

$$E_{ads} = E_{tot} - E_{Tm_2-Pc} - E_{O_2})$$

TM-Pc	E_{tot}	E_{Tm_2-Pc}	E_{O_2}	E_{ads}
Sc-Pc	-429.99	-414.28	-9.86	-5.86
Ti-Pc	-433.46	-418.12	-9.86	-5.48
V-Pc	-437.55	-419.83	-9.86	-7.86
Cr-Pc	-433.39	-420.53	-9.86	-3.00
Mn-Pc	-430.20	-420.17	-9.86	-0.16
Fe-Pc	-428.17	-417.85	-9.86	-0.46
Co-Pc	-425.09	-414.96	-9.86	-0.26
Ni-Pc	-422.18	-412.20	-9.86	-0.11
Cu-Pc	-416.30	-405.99	-9.86	-0.46
Zn-Pc	-411.07	-410.15	-9.86	8.95
Y-Pc	-429.97	-412.15	-9.86	-9.96
Zr-Pc	-434.65	-416.02	-9.86	-8.77
Nb-Pc	-439.79	-419.12	-9.86	-10.81
Mo-Pc	-439.87	-420.48	-9.86	-9.53
Tc-Pc	-435.33	-420.30	-9.86	-5.17
Ru-Pc	-427.78	-417.75	-9.86	-0.18
Rh-Pc	-424.43	-414.45	-9.86	-0.12
Pd-Pc	-419.45	-409.23	-9.86	-0.36
Ag-Pc	-411.29	-400.09	-9.86	-1.34
Cd-Pc	-408.16	-394.97	-9.86	-3.34
Hf-Pc	-437.86	-419.21	-9.86	-8.79
Ta-Pc	-443.19	-422.02	-9.86	-11.31
W-Pc	-443.97	-423.82	-9.86	-10.29
Re-Pc	-435.18	-423.65	-9.86	-1.67
Os-Pc	-431.20	-421.20	-9.86	-0.14
Ir-Pc	-427.01	-417.03	-9.86	-0.12
Pt-Pc	-421.98	-411.74	-9.86	-0.38
Au-Pc	-413.30	-402.66	-9.86	-0.78
Hg-Pc	-404.47	-391.23	-9.86	-3.38

The POSCAR of Mn-Pc

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The POSCAR of Fe-Pc

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The POSCAR of Co-Pc

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Direct			
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0.4672129145005481	0.8841661389725564	0.5000000000000000
0.7896274714405868	0.0276439986970161	0.5000000000000000
0.4457572559703265	0.0551457678070122	0.5000000000000000

The POSCAR of Ru-Pc

1.0000000000000000

14.8579998016000001	0.0000000000000000	0.0000000000000000
3.0172031940999999	14.5484240723999996	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

C	N	Ru	H
30	12	2	8

Direct

0.5198640644691397	0.0483289430462931	0.5000000000000000
0.7160618926450093	0.0308125537318732	0.5000000000000000
0.6567270801663698	0.1143148173483993	0.5000000000000000
0.5594524698721683	0.1240214975306172	0.5000000000000000
0.5203363302056409	0.2220654652278211	0.5000000000000000
0.6772300430642670	0.2053347496570806	0.5000000000000000
0.7768560726108892	0.3074228020590378	0.5000000000000000
0.8789466567409725	0.4070485370875935	0.5000000000000000
0.3945989644014941	0.3478021650946087	0.5000000000000000
0.8622134829925993	0.5639409563428154	0.5000000000000000
0.7364863314268093	0.6896746790980117	0.5000000000000000
0.6973847318108944	0.7877191268449919	0.5000000000000000
0.7369945671227202	0.8634024097104935	0.5000000000000000
0.6781516299184368	0.9511979713856565	0.5000000000000000
0.5787205220404881	0.9605435112032202	0.5000000000000000
0.5407968257800082	0.8809396024069275	0.5000000000000000
0.6001092198990035	0.7974269335392099	0.5000000000000000
0.5795982746759544	0.7064063237087337	0.5000000000000000
0.4799678409774652	0.6043129482200593	0.5000000000000000
0.3778683338415876	0.5046933759382127	0.5000000000000000

0.2868468193770211	0.4841896243636772	0.5000000000000000
0.2965539455432040	0.3869137872687231	0.5000000000000000
0.2208655497903768	0.3473154661913538	0.5000000000000000
0.1330755809042820	0.4061636900887403	0.5000000000000000
0.1237301082955117	0.5055956591709588	0.5000000000000000
0.2033383265320420	0.5435147206411534	0.5000000000000000
0.0359385007225245	0.5644439531137388	0.5000000000000000
0.0534717349307304	0.3682398994103492	0.5000000000000000
0.9602559011538819	0.5248360396619647	0.5000000000000000
0.9699639202758946	0.4275613293376361	0.5000000000000000
0.4305866831499472	0.2580532055620558	0.5000000000000000
0.5916693586875087	0.2681392361550295	0.5000000000000000
0.7612936088058311	0.2197273625883230	0.5000000000000000
0.8645516828579508	0.3229855928330438	0.5000000000000000
0.8161394948406353	0.4926079174306272	0.5000000000000000
0.7072258815964404	0.3770510024639921	0.5000000000000000
0.4406717294416060	0.4191356450489149	0.5000000000000000
0.5495934619204496	0.5346841567146590	0.5000000000000000
0.6651541507565474	0.6436009954779397	0.5000000000000000
0.8262324054893326	0.6536879318886243	0.5000000000000000
0.4955389089209803	0.6920032449261224	0.5000000000000000
0.3922731556476355	0.5887525198026903	0.5000000000000000
0.5765873583694044	0.4040509563854621	0.5000000000000000
0.6802303073484933	0.5076901957611605	0.5000000000000000
0.2272419610928194	0.2728937416980959	0.5000000000000000
0.1988697673641437	0.6176842507813931	0.5000000000000000
0.0295560182793370	0.6388676324150114	0.5000000000000000
0.0579419775732821	0.2940699133363560	0.5000000000000000
0.8114179564384435	0.8570252533552586	0.5000000000000000
0.4666259072086761	0.8854286541159748	0.5000000000000000
0.7902283997961804	0.0263697757760678	0.5000000000000000
0.4454441022269781	0.0546972770532321	0.5000000000000000