

Identifying Key Descriptors for the Single-atom Catalyzed CO Oxidation

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Table S1. EXAFS fitting parameters of different metal oxides and M₁/CsPMA. The fits corresponding to the Figures 2B and S1-10 were performed within the following k and r ranges: Cr k 2.0-9.5, R 1.0-2.3; Mn k 2.0-8.0, R 1.0-2.9; Fe k 2.0-9.7, R 1.0-2.3; Co k 2.2-9.5, R 1.0-2.1; Ni k 2.0-8.0, R 1.0-3.0; Cu k 2.0-9.0, R 1.0-2.4; Ru k 3.0-10.0, R 1.0-2.2; Rh k 3.0-13.5, R 1.2-2.0; Pd k 2.7-12.0, R 1.1-2.2; Pt k 2.0-10.0, R 1.2-2.4.

Catalyst	Coordination shell	CN	R (Å)	σ ²
Cr ₂ O ₃	Cr-O	6	2.00 ± 0.02	0.002 ± 0.003
Cr ₁ /CsPMA		7.0 ± 1.1	1.96 ± 0.02	0.003 ± 0.003
MnO	Mn-O	6	2.23 ± 0.03	0.010 ± 0.005
Mn ₁ /CsPMA		5.0 ± 1.3	2.13 ± 0.02	0.003 ± 0.005
Fe ₂ O ₃	Fe-O	6	1.98 ± 0.03	0.016 ± 0.005
Fe ₁ /CsPMA		6.4 ± 1.2	1.98 ± 0.02	0.009 ± 0.003
CoO	Co-O	6	2.10 ± 0.04	0.017 ± 0.008
Co ₁ /CsPMA		6.0 ± 1.9	2.03 ± 0.04	0.009 ± 0.007
NiO	Ni-O	6	2.10 ± 0.02	0.006 ± 0.002
Ni ₁ /CsPMA		5.9 ± 1.1	2.03 ± 0.02	0.007 ± 0.004
CuO	Cu-O	4	1.94 ± 0.01	0.003 ± 0.001
Cu ₁ /CsPMA		3.4 ± 0.8	1.93 ± 0.02	0.001 ± 0.004
RuO ₂	Ru-O	6	1.96 ± 0.02	0.002 ± 0.003
Ru ₁ /CsPMA		4.6 ± 1.7	1.98 ± 0.03	0.001 ± 0.004
Rh ₂ O ₃	Rh-O	6	2.04 ± 0.01	0.003 ± 0.001
Rh ₁ /CsPMA		6.8 ± 0.9	2.02 ± 0.01	0.003 ± 0.002
PdO	Pd-O	4	2.02 ± 0.01	0.004 ± 0.001
Pd ₁ /CsPMA		4.3 ± 0.3	2.02 ± 0.01	0.001 ± 0.001
PtO ₂	Pt-O	6	2.14 ± 0.02	0.001 ± 0.002
Pt ₁ /CsPMA		3.9 ± 0.7	2.13 ± 0.01	0.001 ± 0.002

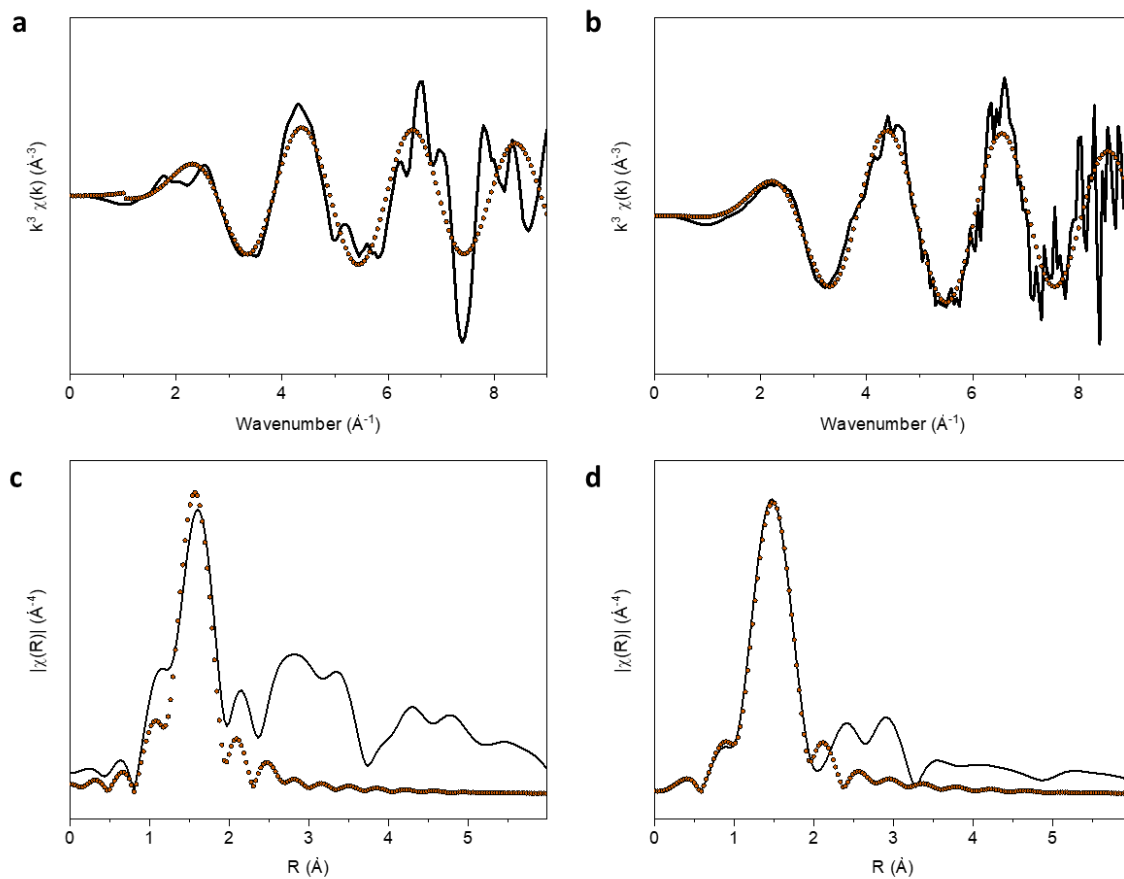


Figure S1. EXAFS fitting of Cr_2O_3 and Cr_1/CsPMA . Experimental EXAFS spectra (solid black lines) and the fit of the first coordination shell (coloured dots) in the k (a, b) and R (c, d) for Cr_2O_3 (a, c) and Cr_1/CsPMA (b, d). Higher scattering contributions for Cr_1/CsPMA can be attributed to Cr-Mo scattering similar to what we reported previously.¹

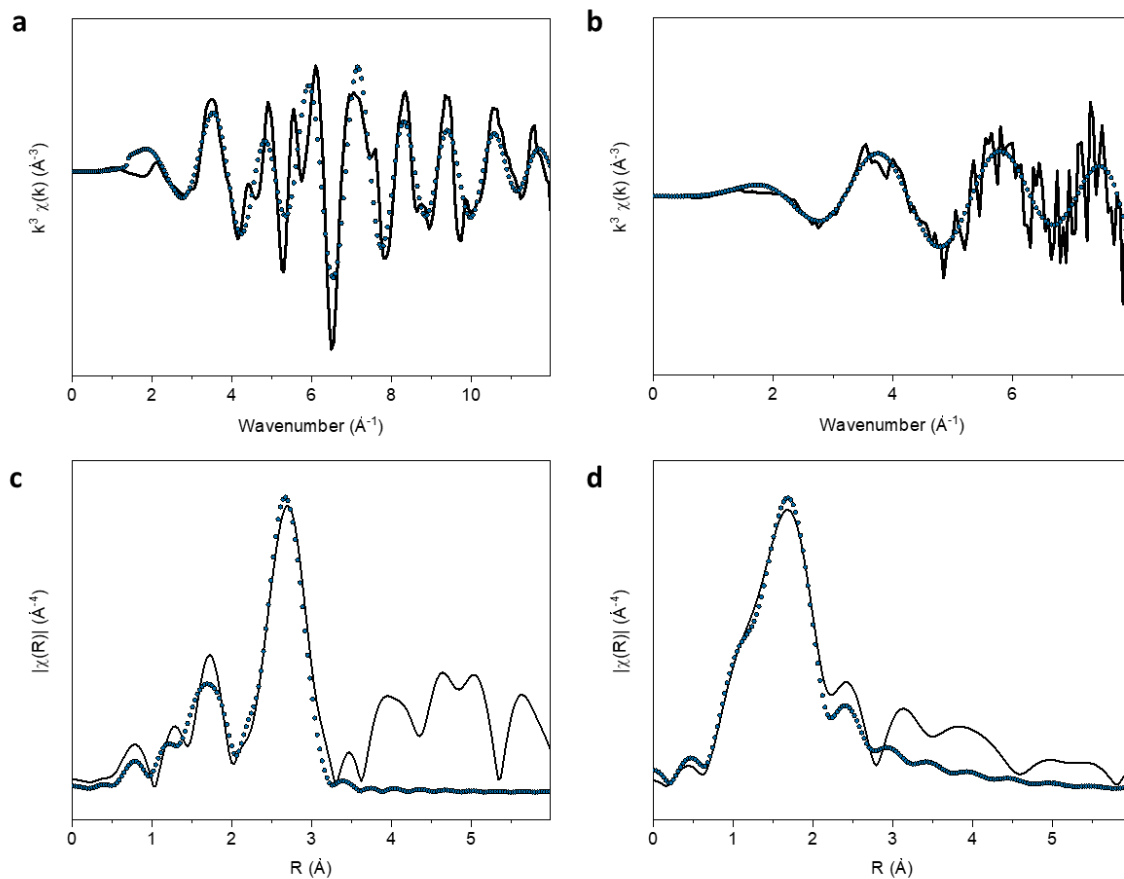


Figure S2. EXAFS fitting of MnO and Mn₁/CsPMA. Experimental EXAFS spectra (solid black lines) and the fit of the first coordination shell (coloured dots) in the k (a, b) and R (c, d) for MnO (a, c) and Mn₁/CsPMA (b, d). Higher scattering contributions for Mn₁/CsPMA can be attributed to Mn–Mo scattering similar to what we reported previously.¹

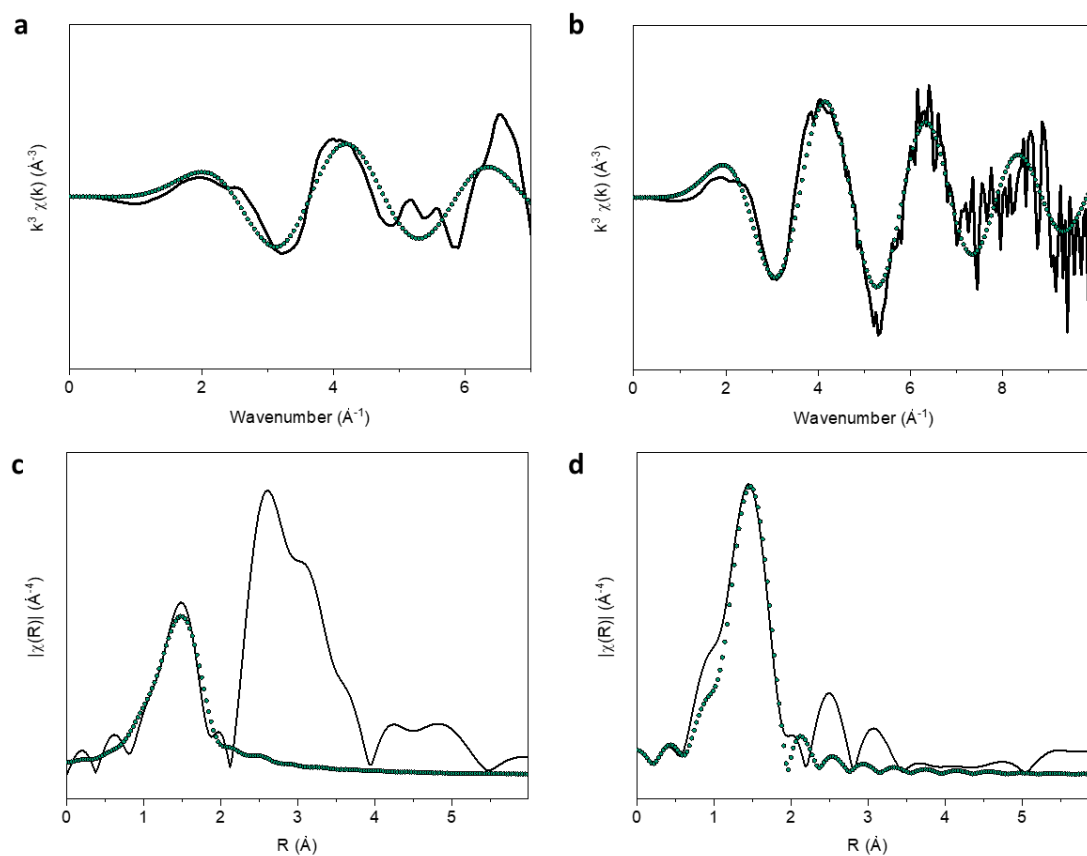


Figure S3. EXAFS fitting of Fe_2O_3 and Fe_1/CsPMA . Experimental EXAFS spectra (solid black lines) and the fit of the first coordination shell (coloured dots) in the k (a, b) and R (c, d) for Fe_2O_3 (a, c) and Fe_1/CsPMA (b, d). Higher scattering contributions for Fe_1/CsPMA can be attributed to Fe–Mo scattering similar to what we reported previously.¹

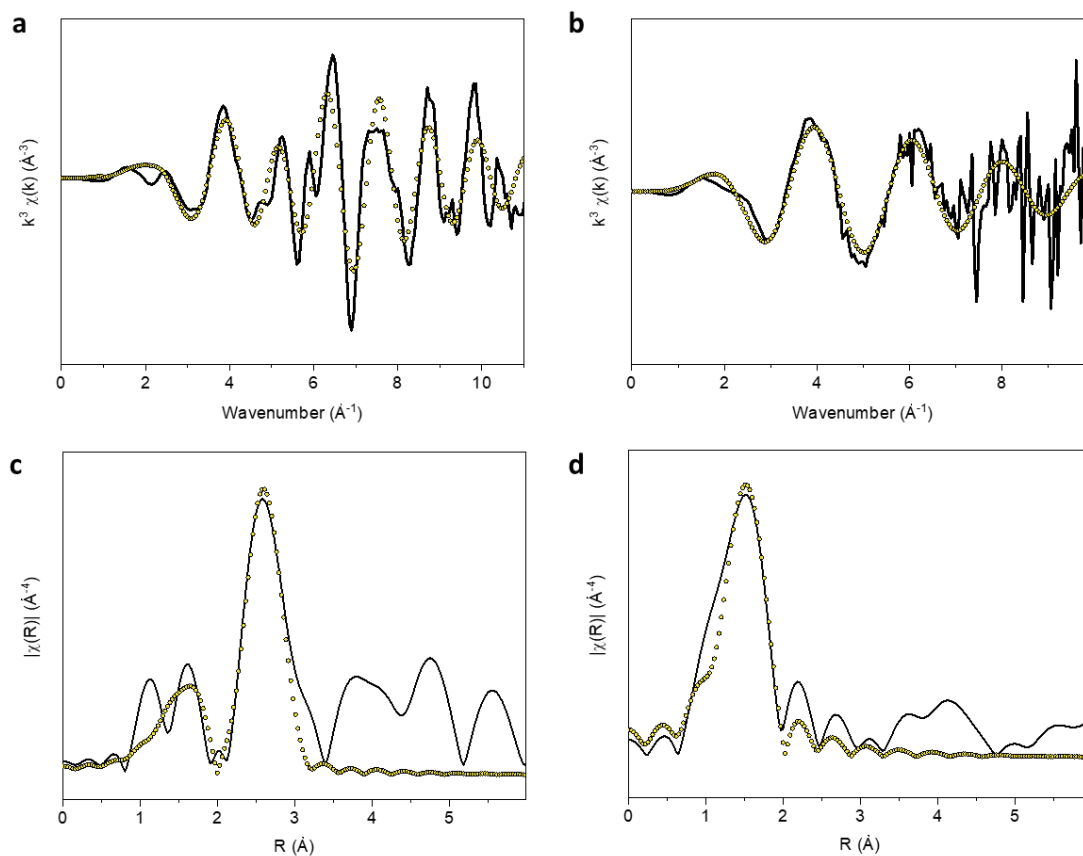


Figure S4. EXAFS fitting of CoO and Co₁/CsPMA. Experimental EXAFS spectra (solid black lines) and the fit of the first coordination shell (coloured dots) in the k (a, b) and R (c, d) for CoO (a, c) and Co₁/CsPMA (b, d). Higher scattering contributions for Co₁/CsPMA can be attributed to Co–Mo scattering similar to what we reported previously.¹

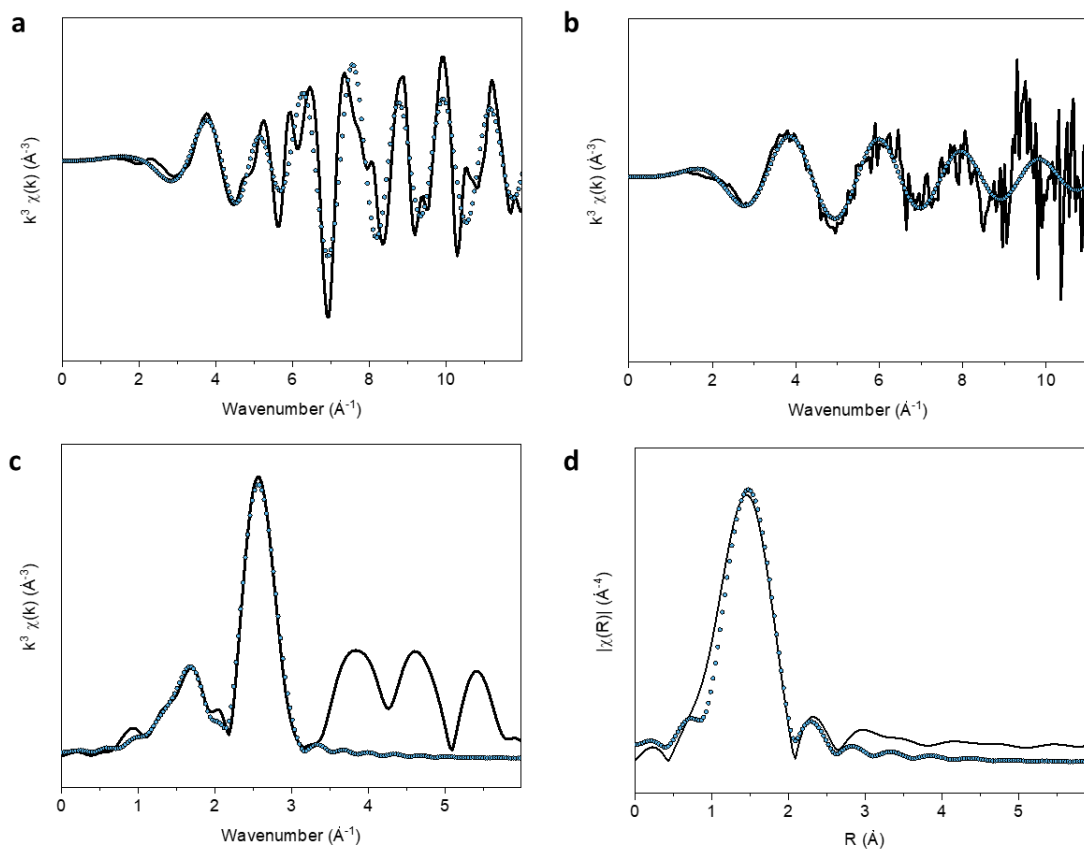


Figure S5. EXAFS fitting of NiO and Ni₁/CsPMA. Experimental EXAFS spectra (solid black lines) and the fit of the first coordination shell (coloured dots) in the k (a, b) and R (c, d) for NiO (a, c) and Ni₁/CsPMA (b, d). Higher scattering contributions for Ni₁/CsPMA can be attributed to Ni–Mo scattering similar to what we reported previously.¹

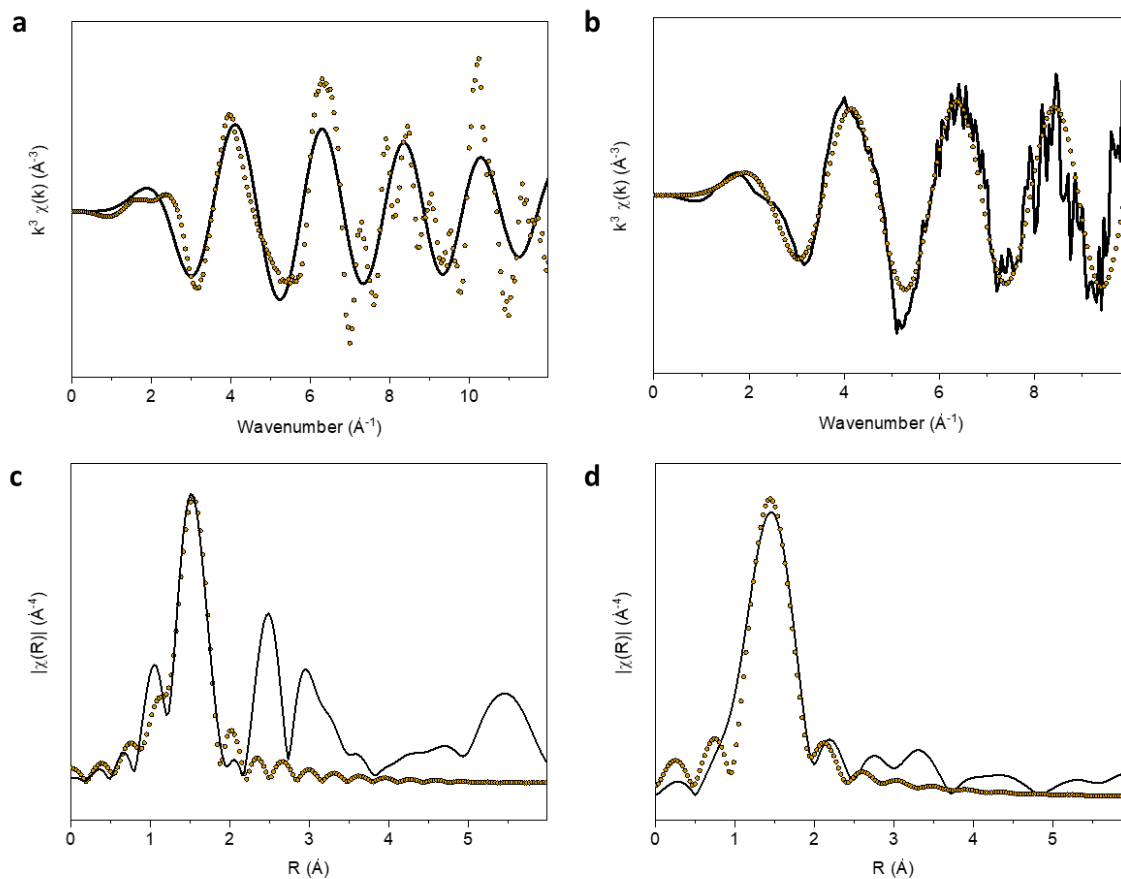


Figure S6. EXAFS fitting of CuO and Cu₁/CsPMA. Experimental EXAFS spectra (solid black lines) and the fit of the first coordination shell (coloured dots) in the k (a, b) and R (c, d) for CuO (a, c) and Cu₁/CsPMA (b, d). Higher scattering contributions for Cu₁/CsPMA can be attributed to Cu–Mo scattering similar to what we reported previously.¹

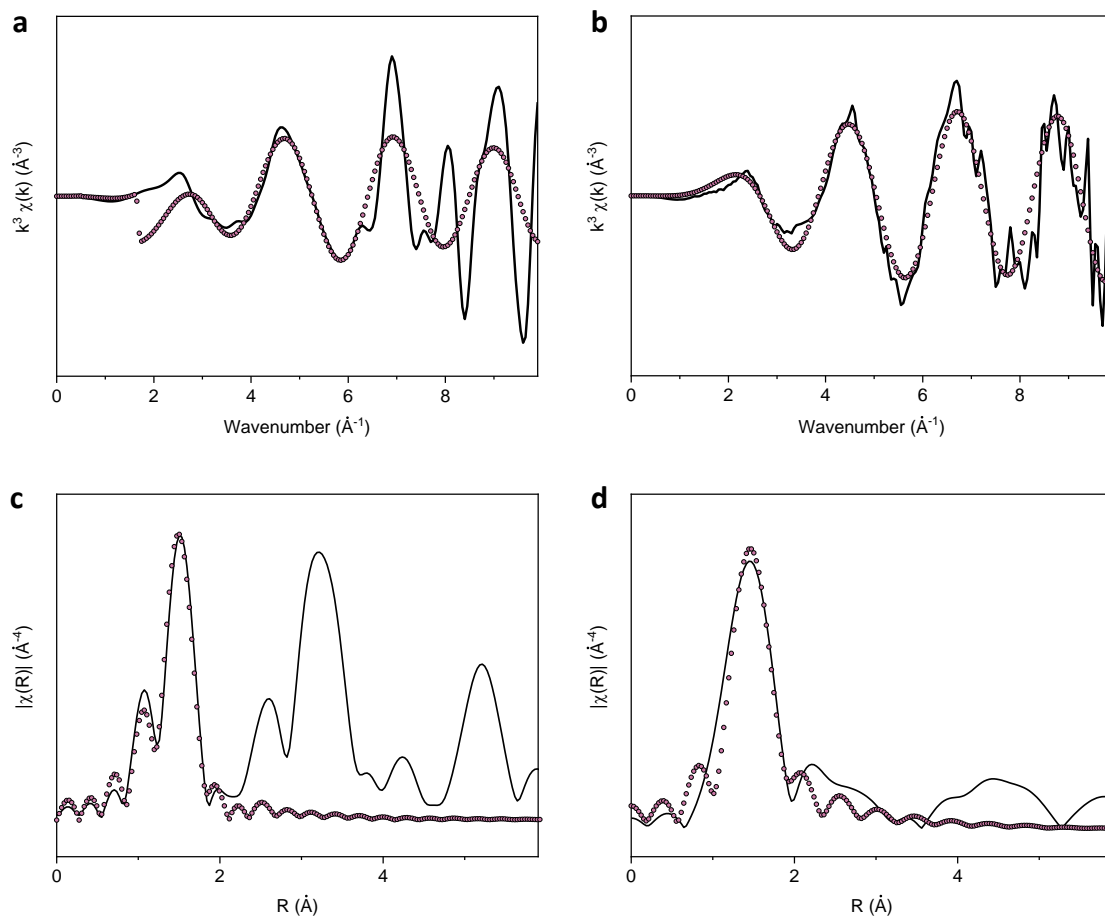


Figure S7. EXAFS fitting of RuO₂ and Ru₁/CsPMA. Experimental EXAFS spectra (solid black lines) and the fit of the first coordination shell (coloured dots) in the k (a, b) and R (c, d) for RuO₂ (a, c) and Ru₁/CsPMA (b, d). Higher scattering contributions for Ru₁/CsPMA can be attributed to Ru–Mo scattering similar to what we reported previously.¹

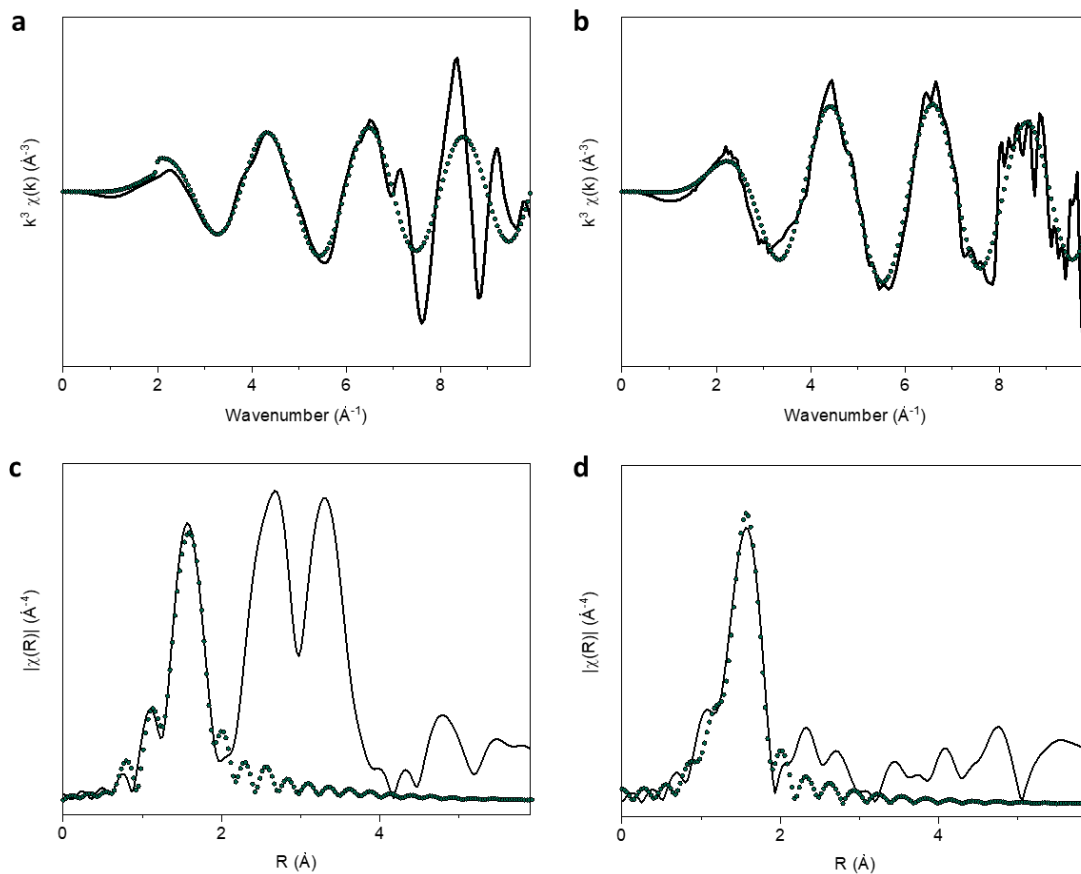


Figure S8. EXAFS fitting of Rh_2O_3 and Rh_1/CsPMA . Experimental EXAFS spectra (solid black lines) and the fit of the first coordination shell (coloured dots) in the k (a, b) and R (c, d) for Rh_2O_3 (a, c) and Rh_1/CsPMA (b, d). Higher scattering contributions for Rh_1/CsPMA can be attributed to Rh–Mo scattering similar to what we reported previously.¹

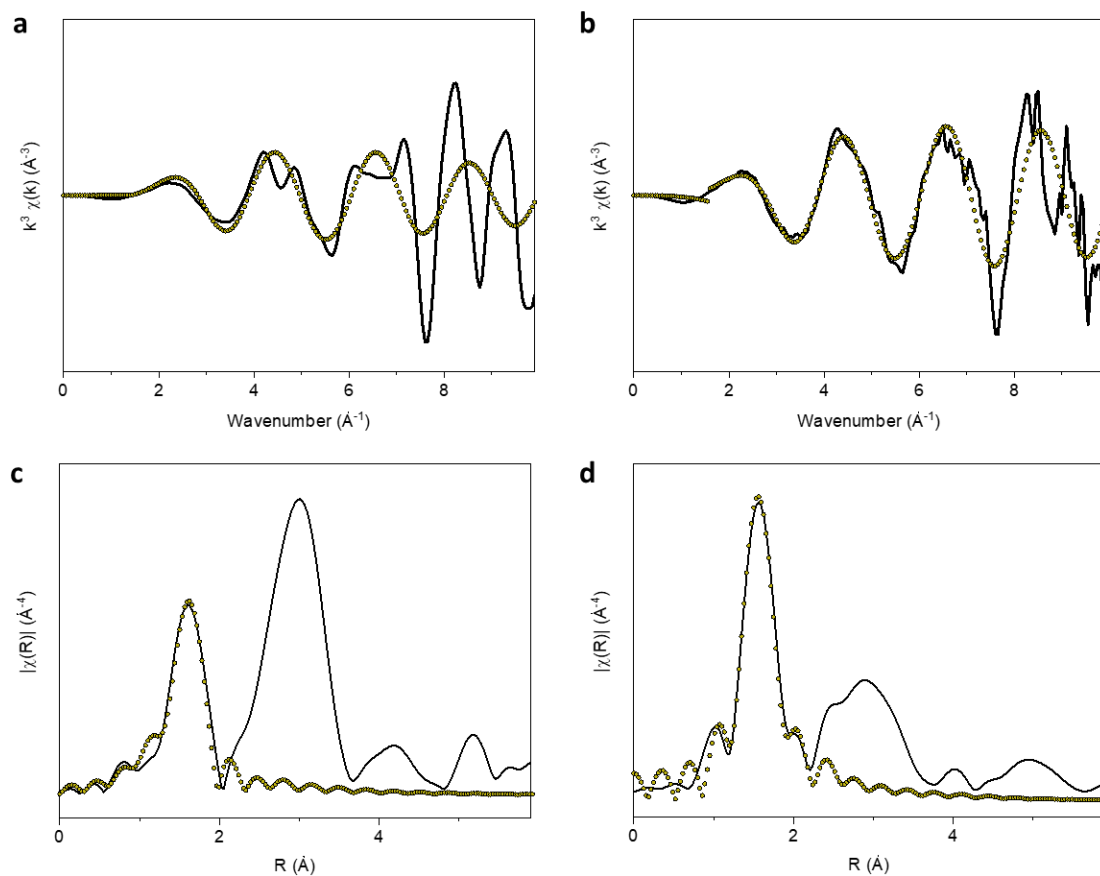


Figure S9. EXAFS fitting of PdO and Pd₁/CsPMA. Experimental EXAFS spectra (solid black lines) and the fit of the first coordination shell (coloured dots) in the k (a, b) and R (c, d) for PdO (a, c) and Pd₁/CsPMA (b, d). Higher scattering contributions for Pd₁/CsPMA can be attributed to Pd–Mo scattering similar to what we reported previously.¹

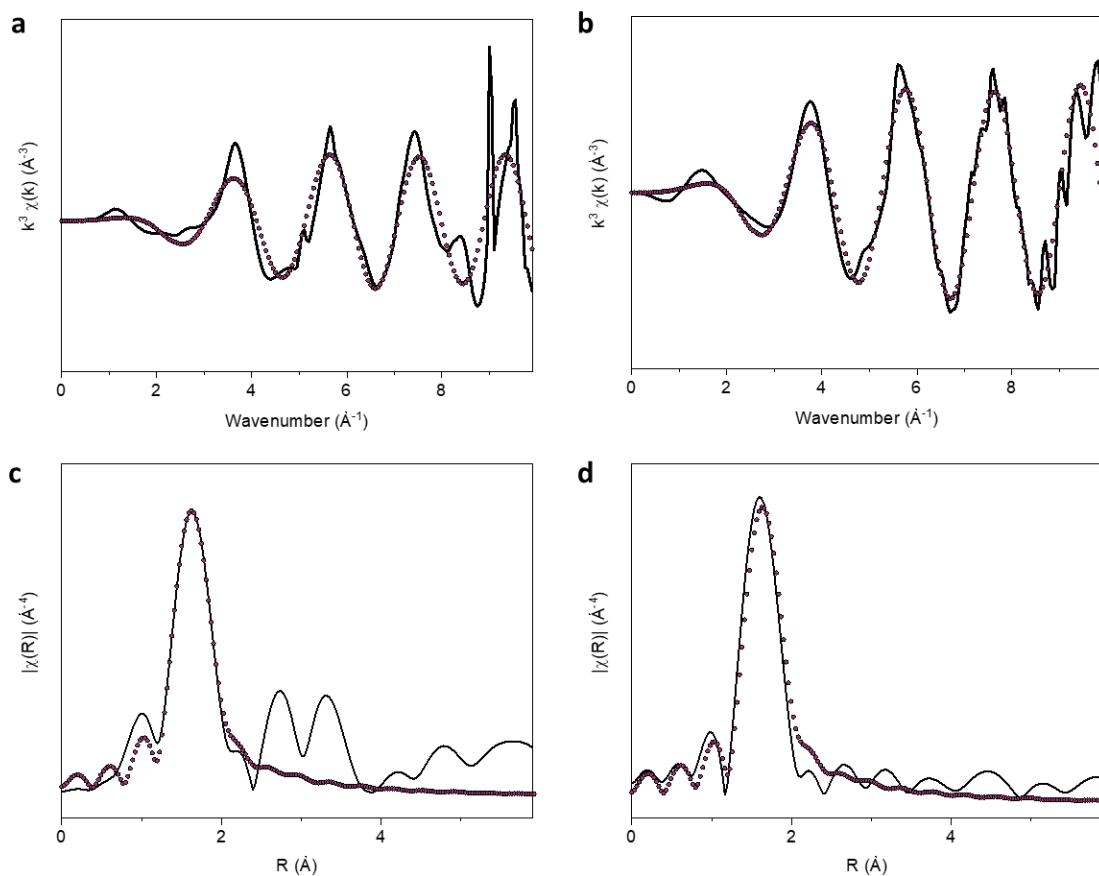


Figure S10. EXAFS fitting of PtO_2 and Pt_1/CsPMA . Experimental EXAFS spectra (solid black lines) and the fit of the first coordination shell (coloured dots) in the k (a, b) and R (c, d) for PtO_2 (a, c) and Pt_1/CsPMA (b, d). Higher scattering contributions for Pt_1/CsPMA can be attributed to Pt–Mo scattering similar to what we reported previously.¹

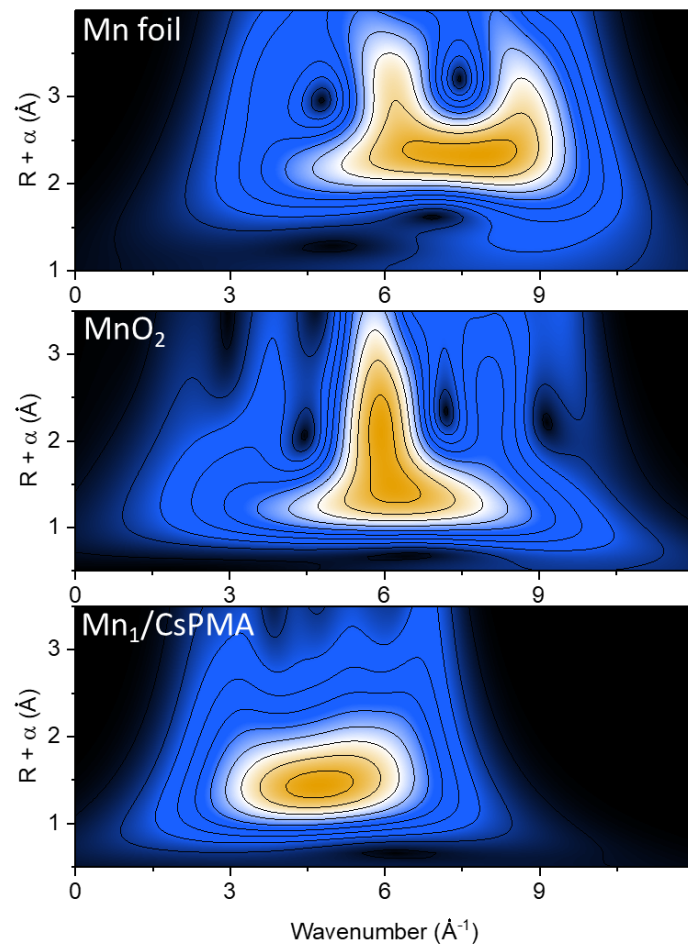


Figure S11. Morlet Wavelet analysis of Mn-containing materials.

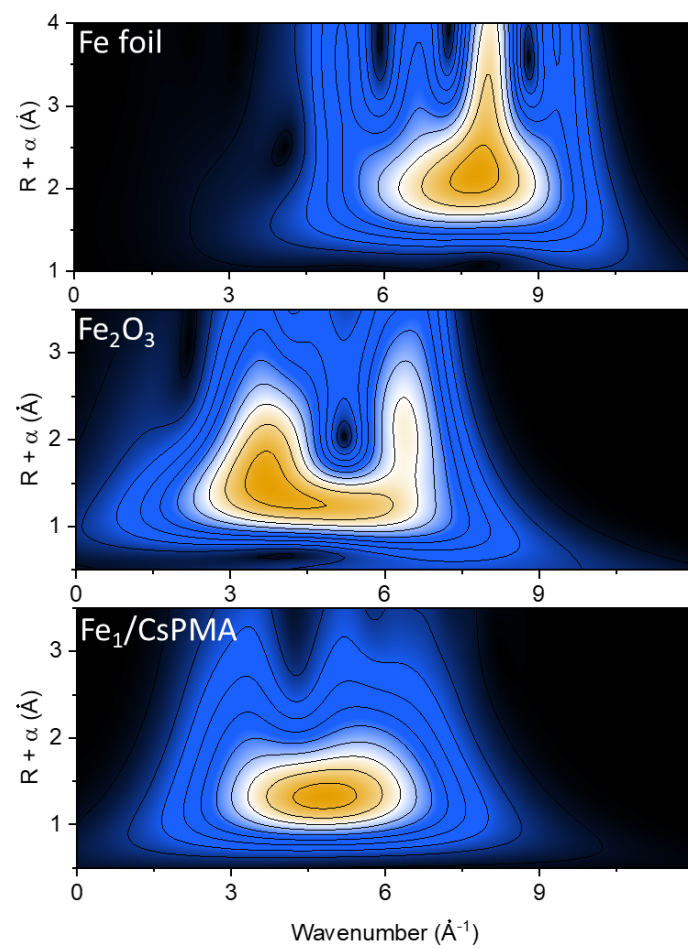


Figure S12. Morlet Wavelet analysis of Fe-containing materials.

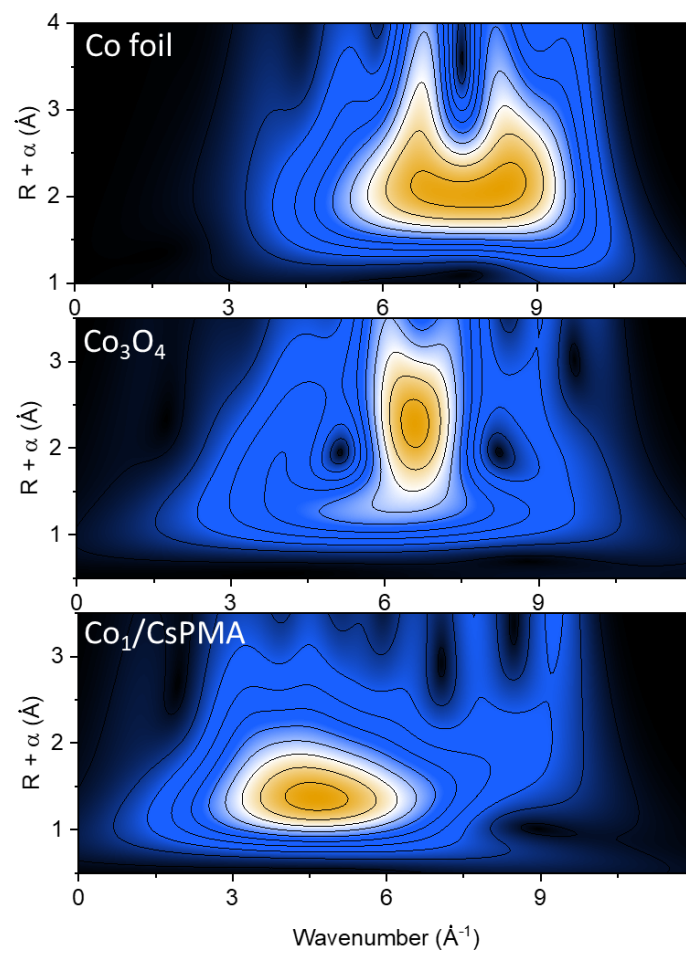


Figure S13. Morlet Wavelet analysis of Co-containing materials.

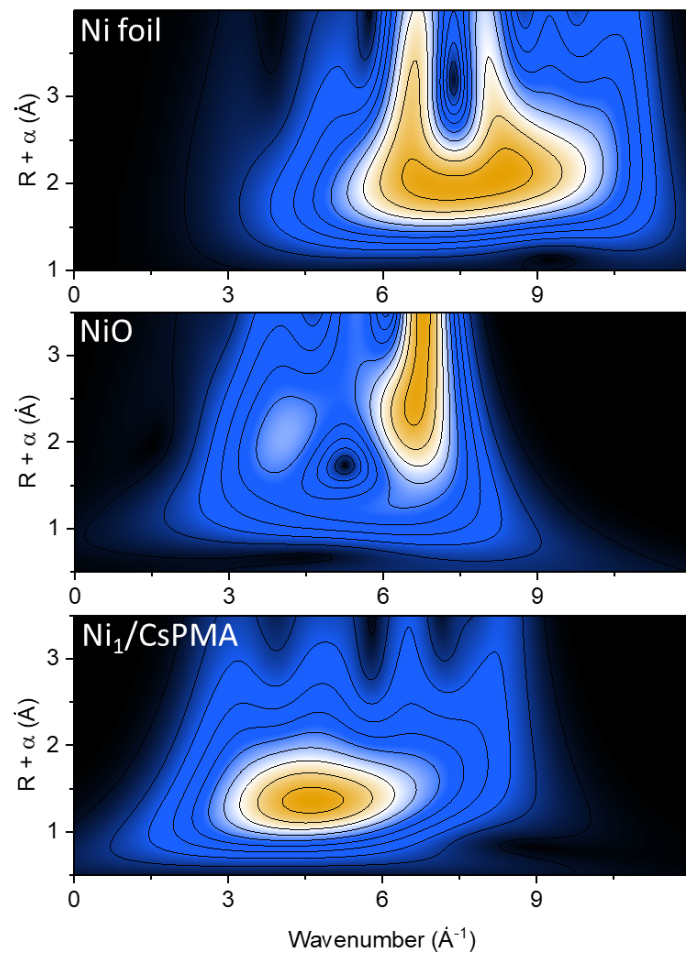


Figure S14. Morlet Wavelet analysis of Ni-containing materials.

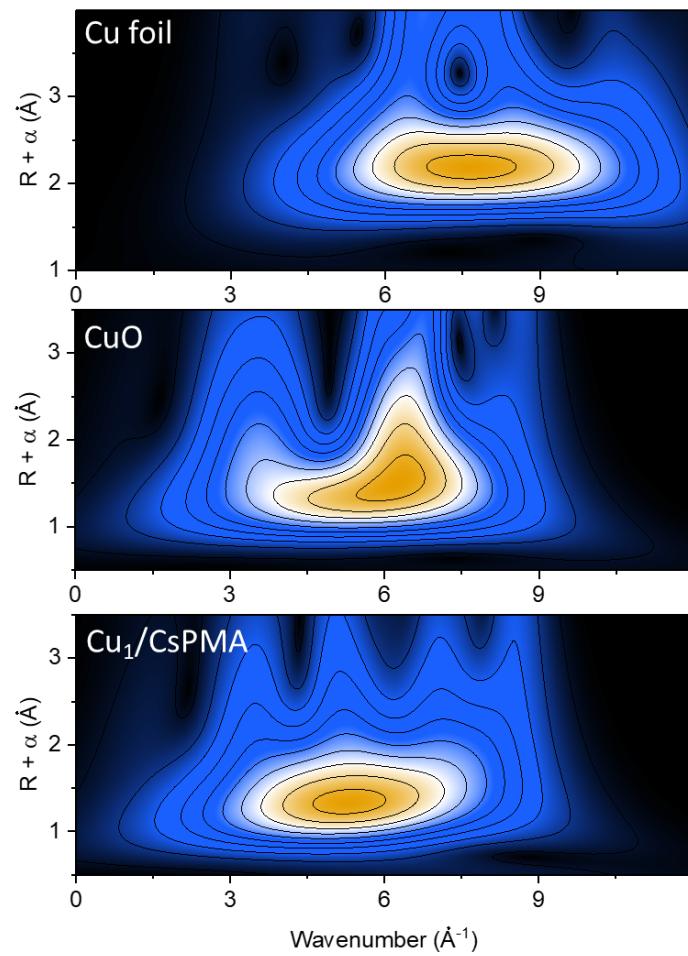


Figure S15. Morlet Wavelet analysis of Cu-containing materials.

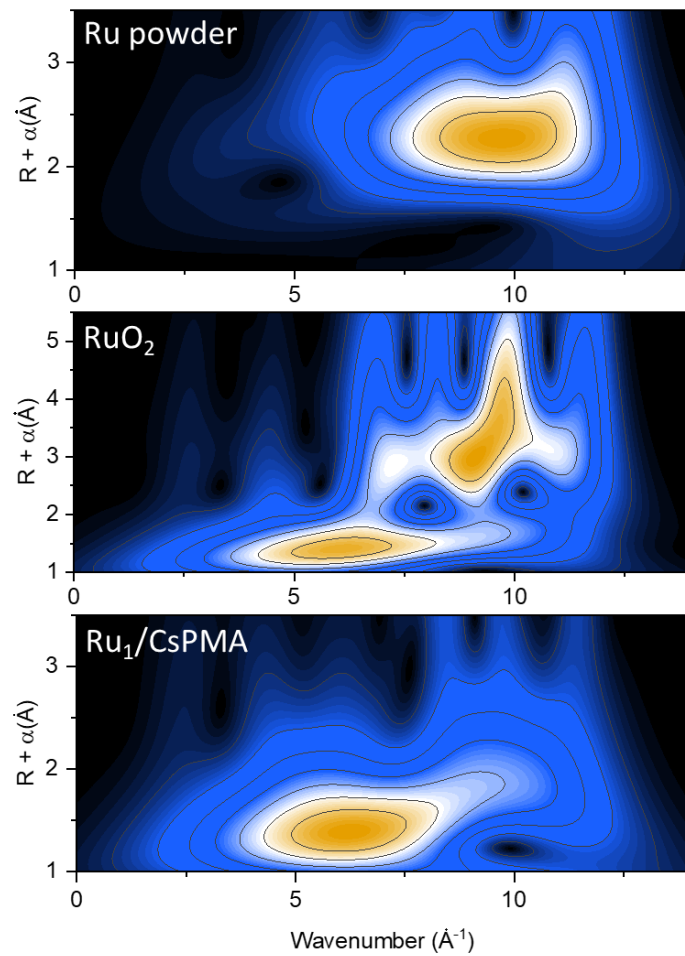


Figure S16. Morlet Wavelet analysis of Ru-containing materials.

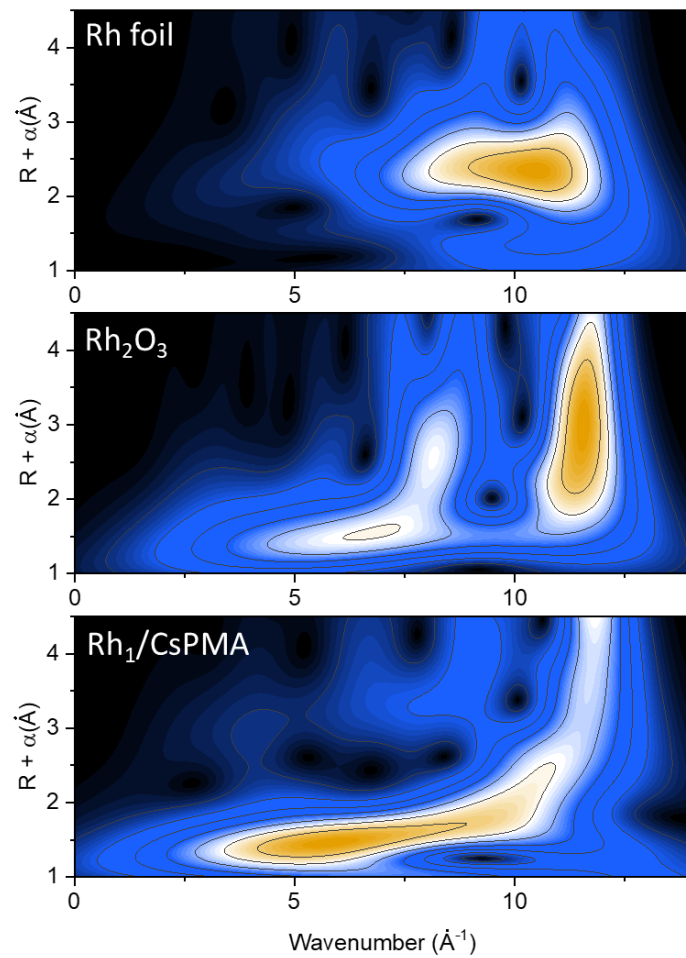


Figure S17. Morlet Wavelet analysis of Rh-containing materials.

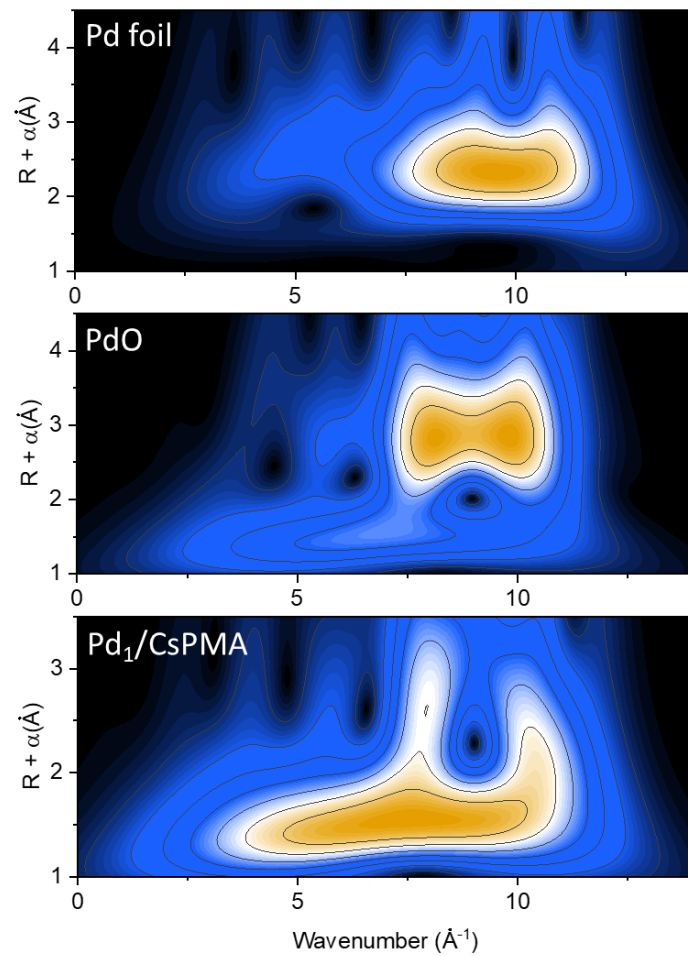


Figure S18. Morlet Wavelet analysis of Pd-containing materials.

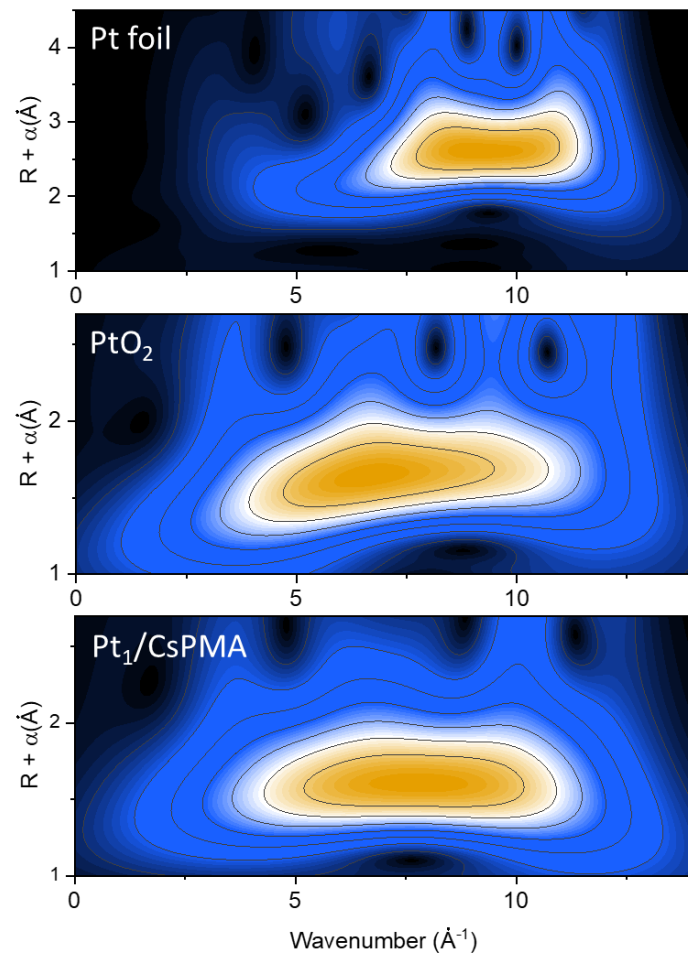


Figure S19. Morlet Wavelet analysis of Pt-containing materials.

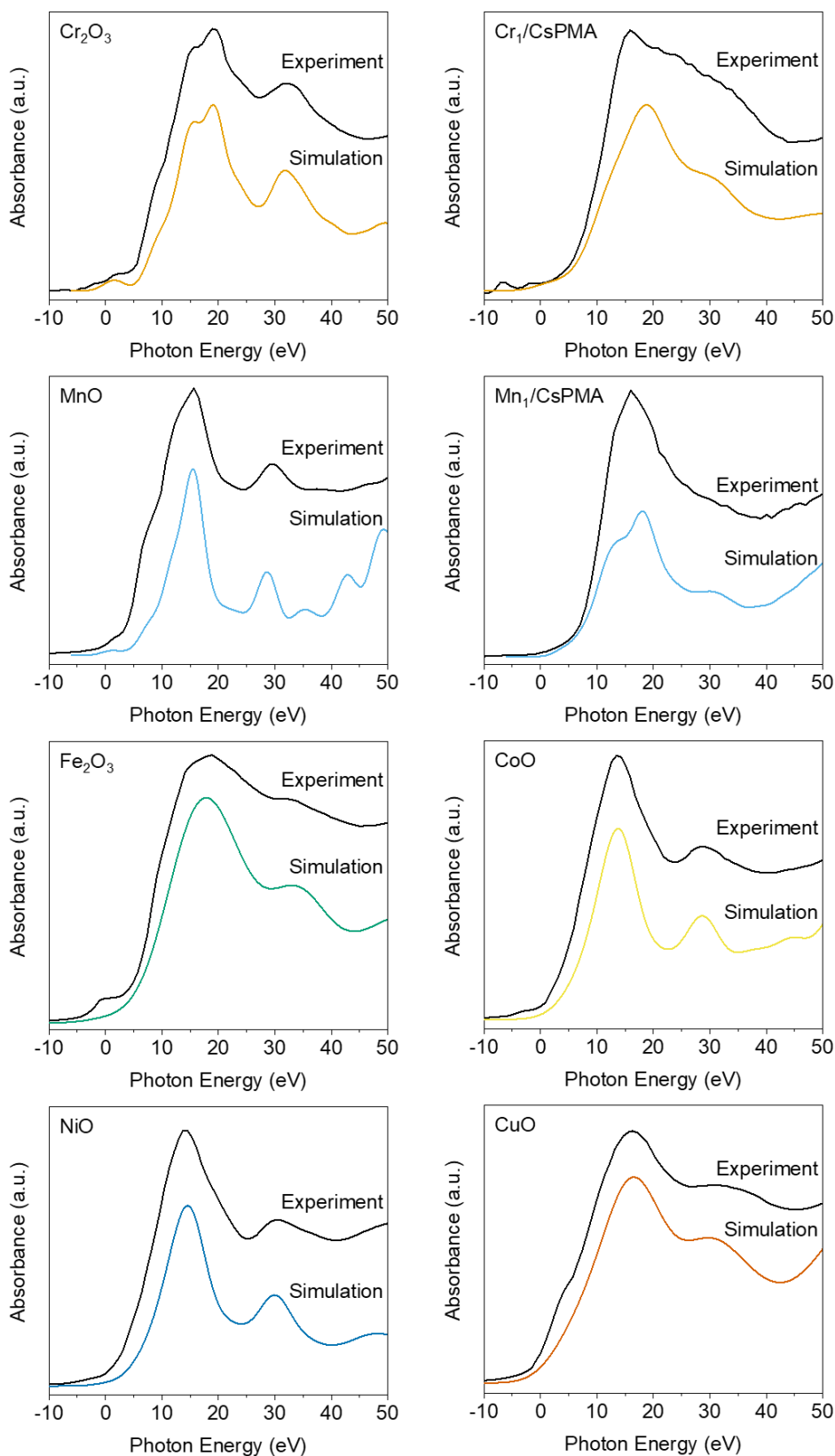


Figure S20. XANES simulations for different materials. XANES simulations were performed on metal oxide reference materials and the same approach was used for the simulation of $M_1/CsPMA$. Experimental data (black solid lines) and simulated data (coloured solid lines) show excellent overlap for all investigated materials.

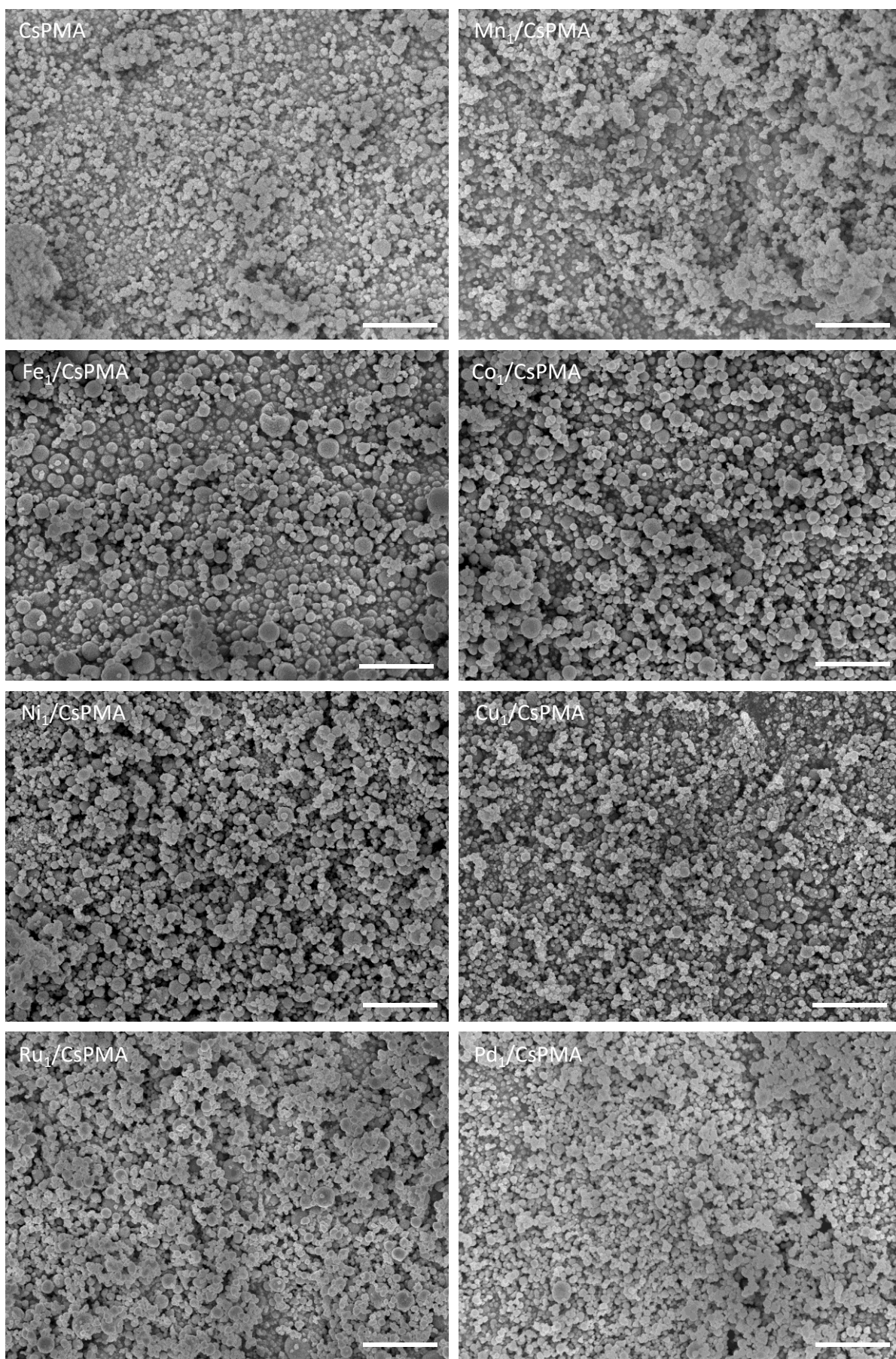


Figure S21. FESEM images of CspPMA and different $M_1/CspPMA$ materials. The scale bar indicates a length of 2 μm .

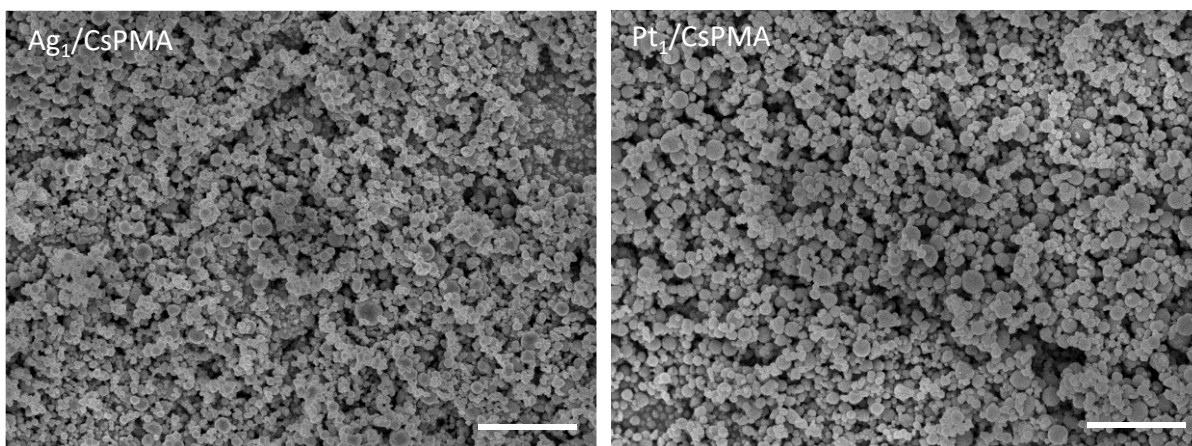


Figure S21 cont'd. FESEM images of CsPMA and different M₁/CsPMA materials. The scale bar indicates a length of 2 μ m.

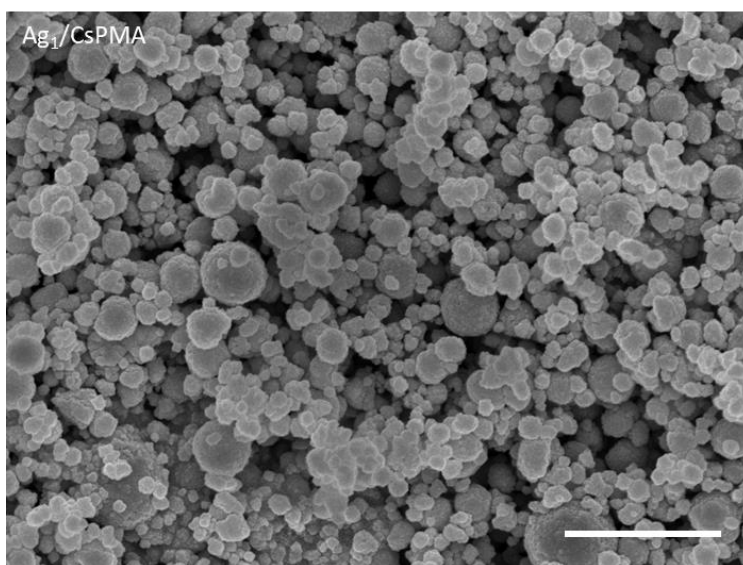
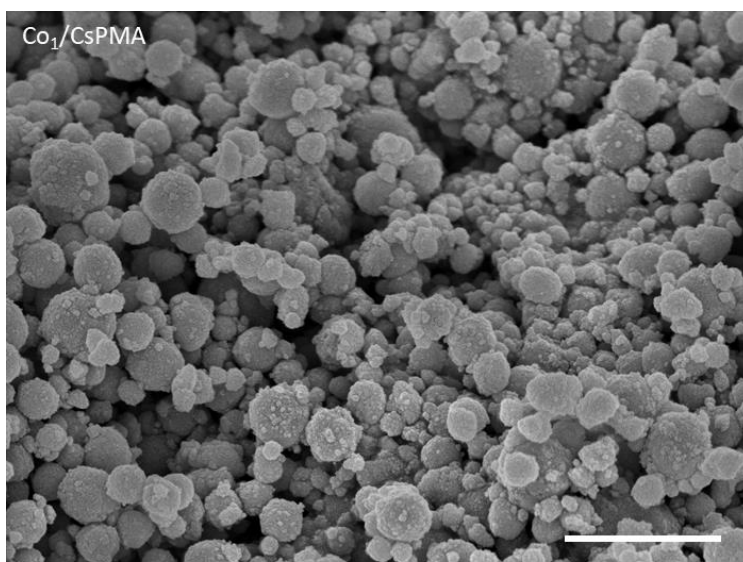


Figure S22. High resolution FESEM images of Co₁/CsPMA and Ag₁/CsPMA. The scale bar indicates a length of 1 μ m.

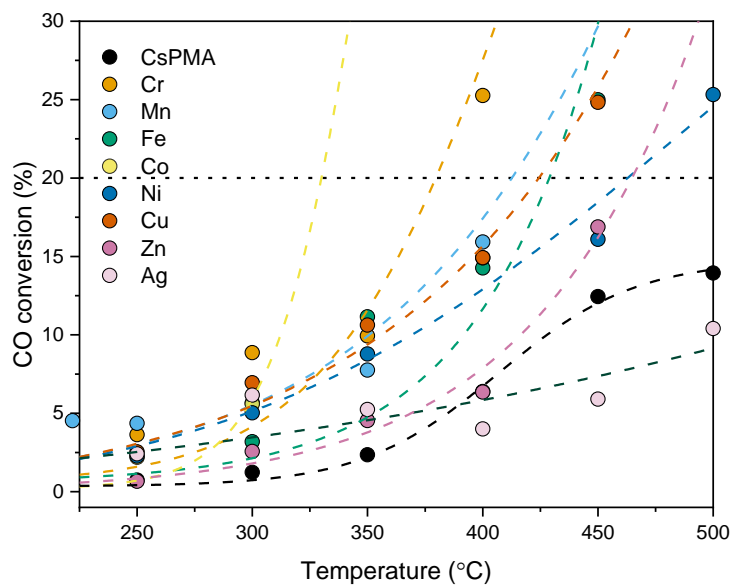


Figure S23. Additional CO oxidation activity of different M_1 /CsPMA catalysts. Light-off curves of select M_1 /CsPMA catalysts. The horizontal line at 20% CO conversion serves to guide the eye.

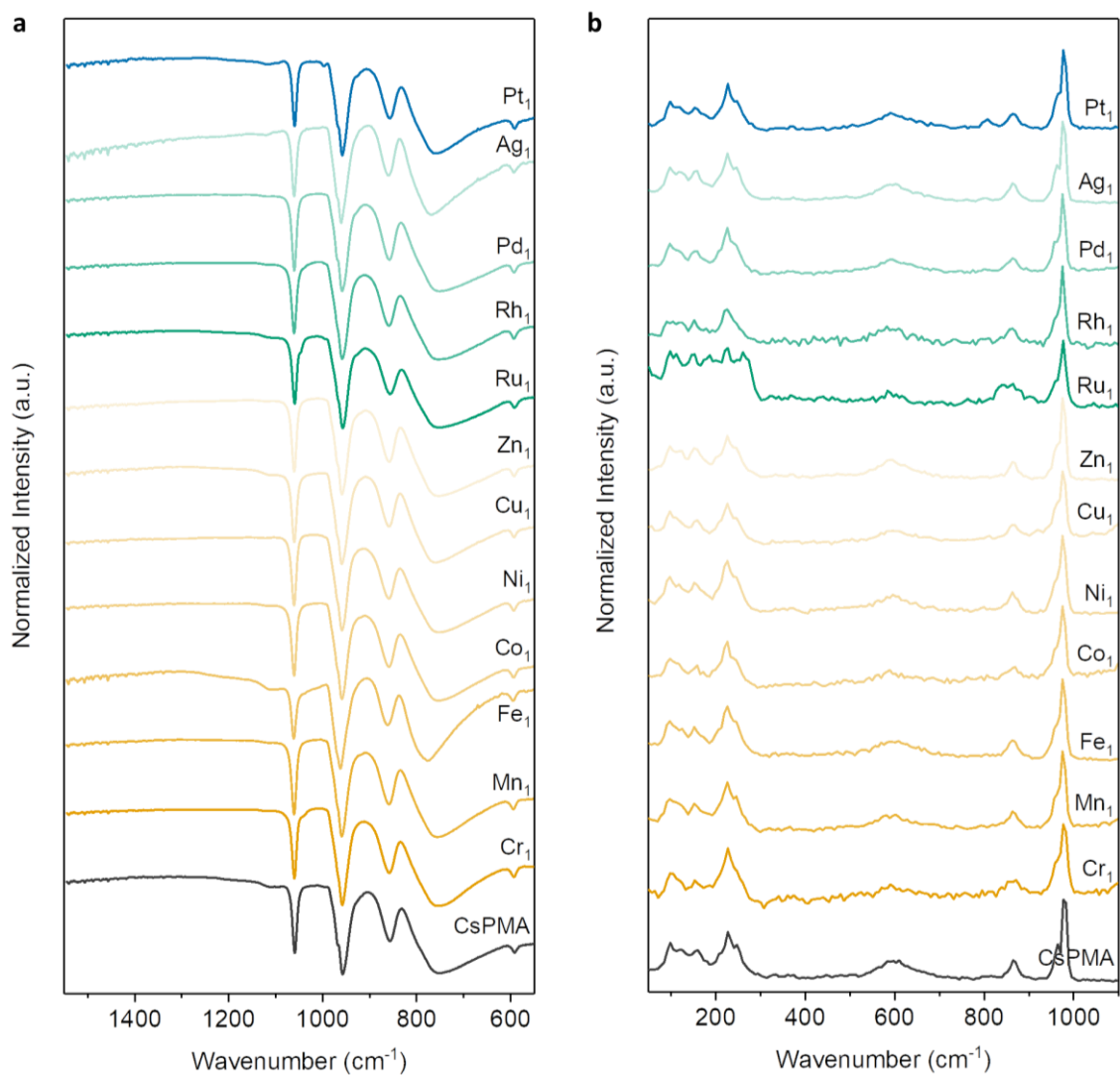


Figure S24. (a) ATR and (b) Raman spectroscopy of the used catalysts. The testing for all catalysts was performed up to 500 °C for a total reaction time of ~12 hours.

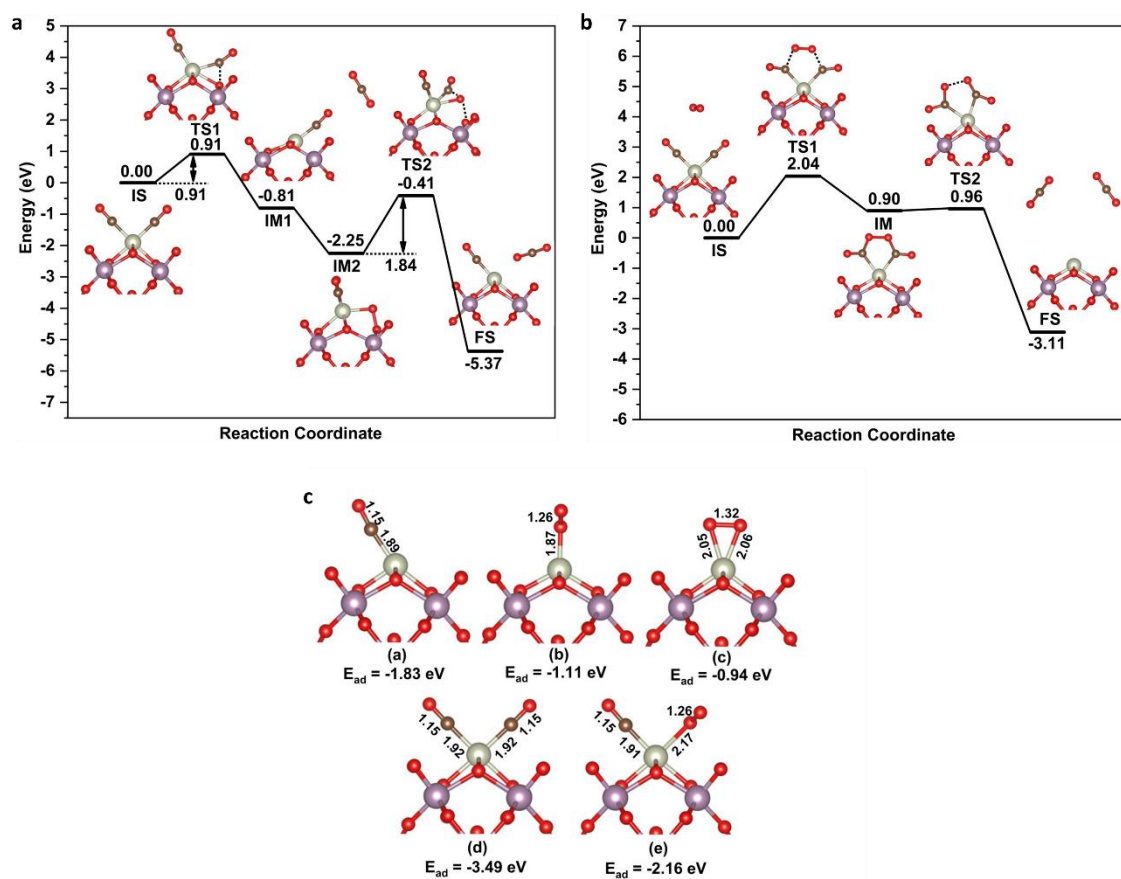


Figure S25. DFT calculations on Rh₁/CsPMA. Calculated reaction energies and barriers for the (a), Mars-van Krevelen and the (b), Eley-Rideal mechanisms. (c), Adsorption geometries and energies of one CO molecule on Rh, one O₂ molecule adsorbed end-on(η^1) or side-on(η^2), two CO molecules or the co-adsorption of one CO and one O₂(η^1) molecule. Those structures are representative for the adsorption modes on all the M₁/CsPMA materials.

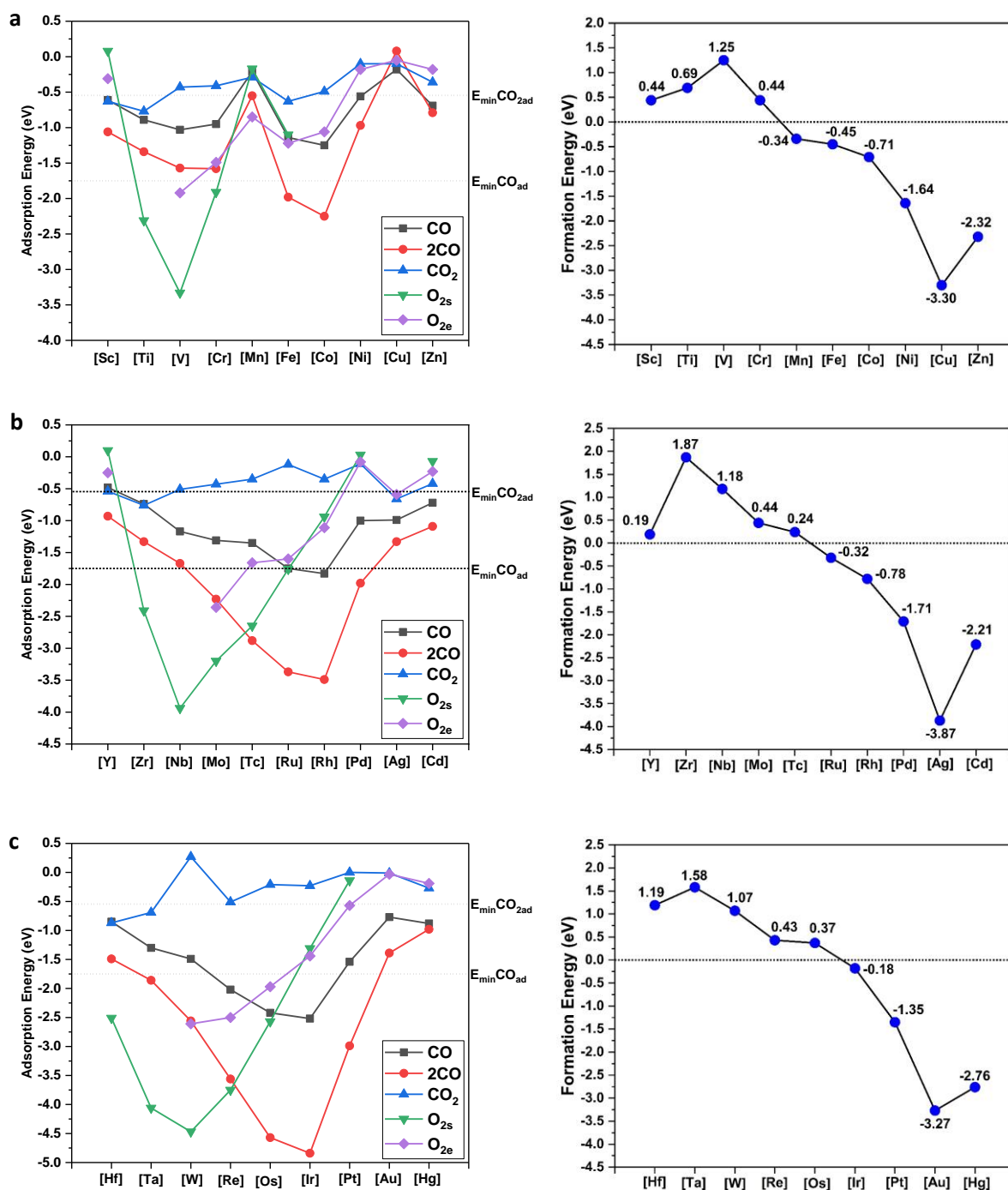


Figure S26. Trends for the adsorption and oxygen vacancy formation energies across the transition metals. Adsorption energies for one CO molecule (CO), two CO molecules (2CO), one CO₂ molecule (CO₂), one O₂ molecule adsorbed side-on (O_{2s}) or end-on (O_{2e}) and the oxygen vacancy formation energies adjacent to the single-atom site for (a), 3d, (b), 4d, and (c), 5d transition metals.

General trends arise that enable us to categorize different TM SACs based on their adsorption properties. Groups 3-6 include metals that are very oxophilic with low CO adsorption energies and endothermic oxygen vacancy formation rendering them rather bad CO oxidation catalysts.

Group 7 and in particular Mn exhibit almost endothermic CO adsorption behaviour and thus are poor CO oxidation catalysts as well. Metals in group 8 adsorb the substrates strongly enough but do not have sufficiently large OV formation energies. Group 9 is located at an ideal point among the transition metals with ample adsorption energies for both CO and O₂ and moderate OV formation energies rendering them the most efficient CO oxidation SACs in our study. Groups 10-12, however, contain metals that mostly do not adsorb CO strongly enough and have very high OV formation energies potentially leading to the formation of thermodynamic sinks.

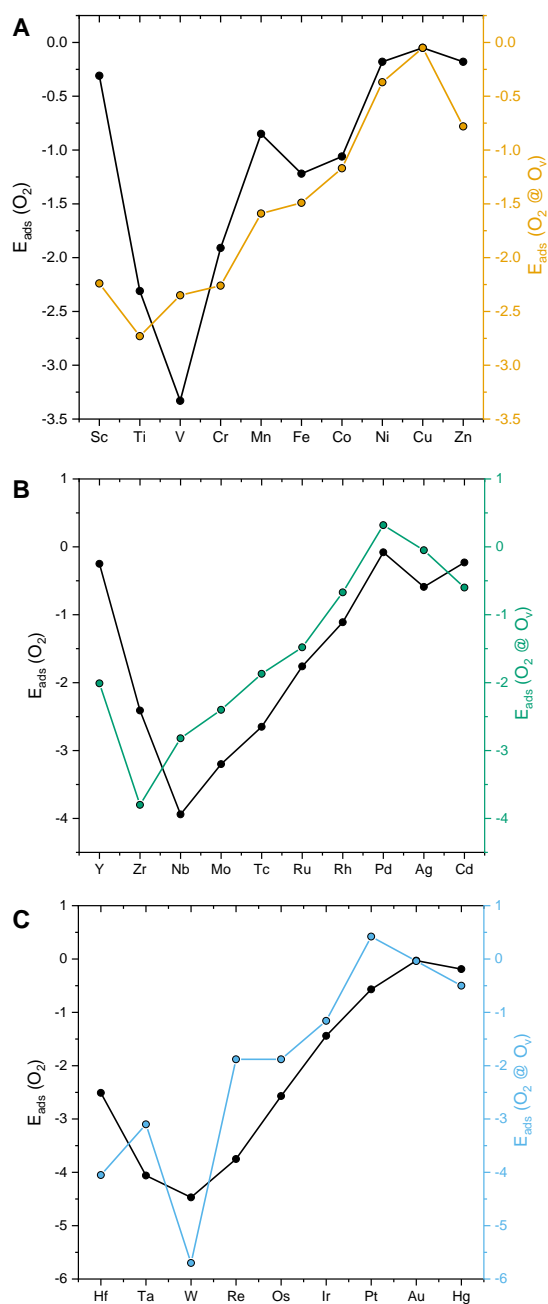


Figure S27. Trends for the adsorption energies of O_2 on the metal site or into the oxygen vacant interface between the metal and the support. Adsorption energies are almost independent of the exact adsorption site for (a), 3d, (b), 4d, and (c), 5d metals.

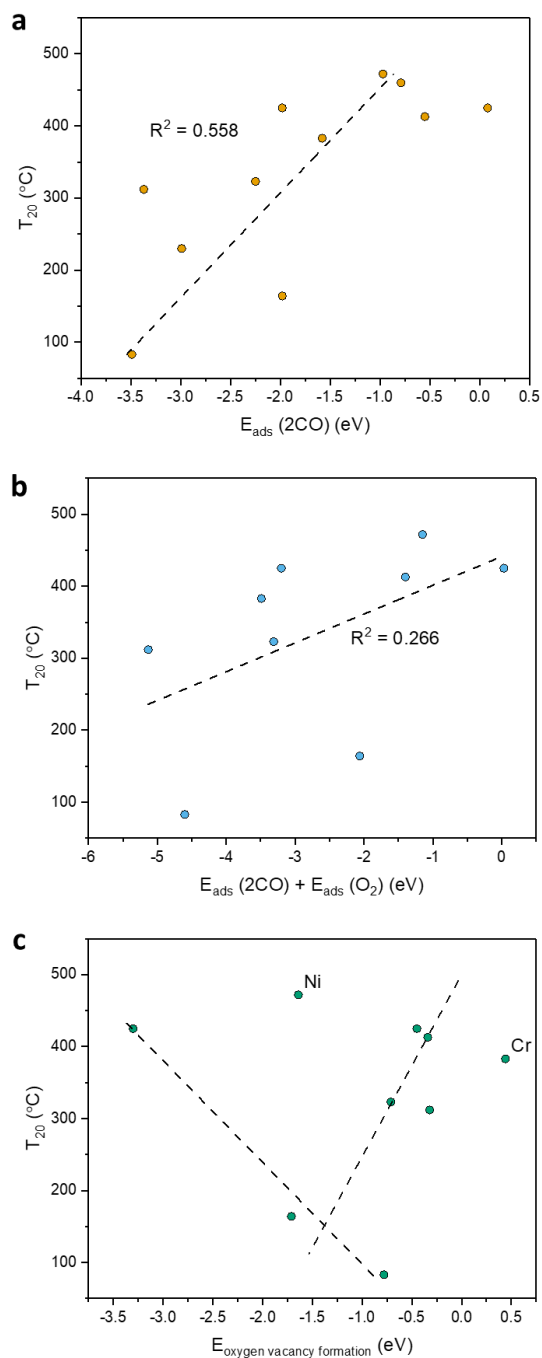


Figure S28. Scaling relation between reaction energies the T_{20} values of different M_1/CsPMA . (a) Scaling relations between the adsorption energy of two CO molecules and the T_{20} values and (b) scaling relations between the sum of the adsorption energies of two CO molecules and one O_2 molecules as well as the T_{20} values. R^2 values of a linear fit are indicated at the graphs. (c) Scaling relations between the oxygen vacancy formation energy and the T_{20} values.

Calculated Adsorption energies (eV)

Table S2-1. Calculated Adsorption energies of CO O₂, CO₂ and O, formation energy on 3d TM supported on PMA.

Calculated Adsorption energies (eV)						
PMA@TM	O _v	CO	2CO	O ₂ _side	O ₂ _end	CO ₂
PMA@Sc	0.44	-0.61	-1.06	0.08	-0.31	-0.63
PMA@Ti	0.69	-0.89	-1.34	-2.31	--	-0.77
PMA@V	1.25	-1.03	-1.57	-3.33	-1.92	-0.43
PMA@Cr	0.44	-0.95	-1.58	-1.91	-1.49	-0.41
PMA@Mn	-0.34	-0.21	-0.55	-0.17	-0.85	-0.29
PMA@Fe	-0.45	-1.14	-1.98	-1.1	-1.22	-0.63
PMA@Co	-0.71	-1.25	-2.25	--	-1.06	-0.49
PMA@Ni	-1.64	-0.56	-0.97	--	-0.18	-0.1
PMA@Cu	-3.30	-0.18	0.08	--	-0.05	-0.1
PMA@Zn	-2.32	-0.69	-0.79	--	-0.18	-0.36

Table S2-2. Calculated Adsorption energies of CO O₂, CO₂ and O, formation energy on 4d TM supported on PMA.

Calculated Adsorption energies (eV)						
PMA@TM	O _v	CO	2CO	O ₂ _side	O ₂ _end	CO ₂
PMA@Y	0.19	-0.48	-0.93	0.10	-0.25	-0.54
PMA@Zr	1.87	-0.74	-1.33	-2.41	--	-0.76
PMA@Nb	1.18	-1.17	-1.67	-3.94	--	-0.51
PMA@Mo	0.44	-1.31	-2.23	-3.2	-2.36	-0.43
PMA@Tc	0.24	-1.35	-2.88	-2.65	-1.66	-0.35
PMA@Ru	-0.32	-1.75	-3.37	-1.76	-1.6	-0.12
PMA@Rh	-0.78	-1.83	-3.49	-0.94	-1.11	-0.35
PMA@Pd	-1.71	-1.00	-1.98	0.03	-0.08	-0.11
PMA@Ag	-3.87	-0.99	-1.33	--	-0.59	-0.66
PMA@Cd	-2.21	-0.72	-1.09	-0.07	-0.23	-0.42

Table S2-3. Calculated Adsorption energies of CO O₂, CO₂ and O, formation energy on 5d TM supported on PMA.

Calculated Adsorption energies (eV)						
PMA@TM	O _v	CO	2CO	O ₂ _side	O ₂ _end	CO ₂
PMA@Hf	1.19	-0.85	-1.49	-2.51	--	-0.87
PMA@Ta	1.58	-1.3	-1.86	-4.06	--	-0.69
PMA@W	1.07	-1.49	-2.56	-4.47	-2.61	0.27
PMA@Re	0.43	-2.02	-3.56	-3.75	-2.5	-0.51
PMA@Os	0.37	-2.42	-4.57	-2.57	-1.97	-0.21
PMA@Ir	-0.18	-2.52	-4.84	-1.31	-1.44	-0.23
PMA@Pt	-1.35	-1.54	-2.99	-0.14	-0.57	0.00
PMA@Au	-3.27	-0.77	-1.39	--	-0.03	-0.01
PMA@Hg	-2.76	-0.88	-0.98	--	-0.19	-0.27

Calculated total energies (eV)

Table S2-4. Calculated total energies of 3d,4d,5d-TM supported on PMA, free PMA and small molecules (CO, O₂ and CO₂).

Calculated total energies (eV)					
3d-TM supported on PMA		4d-TM supported on PMA		5d-TM supported on PMA	
Systems	Energies (eV)	Systems	Energies (eV)	Systems	Energies (eV)
PMA4H-Sc	-444.99145	PMA4H-Y	-445.16382	PMA4H-Hf	-448.07773
PMA4H-Ti	-444.97976	PMA4H-Zr	-446.26842	PMA4H-Ta	-447.49969
PMA4H-V	-444.29476	PMA4H-Nb	-445.29220	PMA4H-W	-445.98667
PMA4H-Cr	-444.00252	PMA4H-Mo	-443.83317	PMA4H-Re	-443.53630
PMA4H-Mn	-443.49345	PMA4H-Tc	-442.03737	PMA4H-Os	-441.12661
PMA4H-Fe	-441.00700	PMA4H-Ru	-439.99351	PMA4H-Ir	-438.77689
PMA4H-Co	-439.26582	PMA4H-Rh	-438.10497	PMA4H-Pt	-436.23257
PMA4H-Ni	-437.76065	PMA4H-Pd	-435.72620	PMA4H-Au	-433.01104
PMA4H-Cu	-435.55341	PMA4H-Ag	-432.09478	PMA4H-Hg	-429.87492
PMA4H-Zn	-433.39170	PMA4H-Cd	-432.12032		
Free PMA					
PMA	-427.82210				
Small Molecules					
CO	-14.833623				
O ₂	-9.7727403				
CO ₂	-23.029384				

Table S2-5. Calculated total energies of Ov systems of 3d,4d,5d-TM supported on PMA.

3d-TM@PMA-Ov		4d-TM@PMA-Ov		5d-TM@PMA-Ov	
System	Energies (eV)	System	Energies (eV)	System	Energies (eV)
PMA4H-Sc_CO_Ov	-452.25617	PMA4H-Y_CO_Ov	-452.54603	PMA4H-Hf_CO_Ov	-455.01744
PMA4H-Ti_CO_Ov	-452.27239	PMA4H-Zr_CO_Ov	-452.36460	PMA4H-Ta_CO_Ov	-454.41874
PMA4H-V_CO_Ov	-451.25114	PMA4H-Nb_CO_Ov	-452.42003	PMA4H-W_CO_Ov	-454.10825
PMA4H-Cr_CO_Ov	-451.78165	PMA4H-Mo_CO_Ov	-452.26579	PMA4H-Re_CO_Ov	-453.30062
PMA4H-Mn_CO_Ov	-451.03889	PMA4H-Tc_CO_Ov	-451.32340	PMA4H-Os_CO_Ov	-451.96363
PMA4H-Fe_CO_Ov	-450.07513	PMA4H-Ru_CO_Ov	-450.32228	PMA4H-Ir_CO_Ov	-450.43816
PMA4H-Co_CO_Ov	-448.86564	PMA4H-Rh_CO_Ov	-449.01385	PMA4H-Pt_CO_Ov	-447.20988
PMA4H-Ni_CO_Ov	-447.00896	PMA4H-Pd_CO_Ov	-446.04894	PMA4H-Au_CO_Ov	-444.30652
PMA4H-Cu_CO_Ov	-445.41118	PMA4H-Ag_CO_Ov	-443.93670	PMA4H-Hg_CO_Ov	-440.26068
PMA4H-Zn_CO_Ov	-443.13458	PMA4H-Cd_CO_Ov	-442.06132		

Table S2-6. Total energies of CO, 2CO, O₂_sideon, O₂_endon and CO₂ adsorbed on 3d-TM@PMA.

Systems	CO	2CO	O ₂ _sideon	O ₂ _endon	CO ₂
PMA4HSc	-460.43227	-475.72239	-454.67979	-455.07484	-468.65363
PMA4HTi	-460.69955	-475.99189	-457.06304	---	-468.78389
PMA4HV	-460.15370	-475.53289	-457.40084	-455.98863	-467.75828
PMA4HCr	-459.79031	-475.24650	-455.68855	-455.26515	-467.44061
PMA4HMn	-458.53704	-473.71082	-453.43702	-454.11732	-466.80850
PMA4HFe	-456.98082	-472.65866	-451.88338	-452.00015	-464.66607
PMA4HCo	-455.35051	-471.18745	---	-450.09677	-462.79020
PMA4HNi	-453.15401	-468.39665	---	-447.70995	-460.89347
PMA4HCu	-450.56357	-465.14485	---	-445.37679	-458.68700
PMA4HZn	-448.91440	-463.84767	---	-443.34841	-456.77940

Table S2-7. Total energies of CO, 2CO, O₂_sideon, O₂_endon and CO₂ adsorbed on 4d-TM@PMA.

Systems	CO	2CO	O ₂ _sideon	O ₂ _endon	CO ₂
PMA4H-Y	-460.47617	-475.76173	-454.83701	-455.18624	-468.72986
PMA4HZr	-461.84306	-477.26143	-458.44796	---	-470.06138
PMA4HNb	-461.29403	-476.63111	-459.00894	---	-468.83735
PMA4HMo	-459.97504	-475.73216	-457.20699	-455.96207	-467.29788
PMA4HTc	-458.21723	-474.58949	-454.46486	-453.46845	-465.42161
PMA4HRu	-456.58126	-473.03261	-451.52387	-451.36945	-463.13974
PMA4HRh	-454.77171	-471.25995	-448.81847	-448.98765	-461.48208
PMA4HPd	-451.56325	-467.37201	-445.46976	-445.58187	-458.86816
PMA4HAg	-447.92017	-463.09330	---	-442.45725	-455.77942
PMA4HCd	-447.67100	-462.88256	-441.96631	-442.12552	-455.57274
Systems	CO	2CO	O ₂ _sideon	O ₂ _endon	CO ₂
PMA4HHf	-463.76279	-479.23673	-460.35559	---	-471.97379
PMA4HTa	-463.63638	-479.02351	-461.33455	---	-471.21479
PMA4HW	-462.30653	-478.21028	-460.22939	-458.36492	-468.74862
PMA4HRe	-460.38623	-476.76368	-457.05465	-455.80673	-467.07672
PMA4HOs	-458.37747	-475.36221	-453.47256	-452.87027	-464.36207
PMA4HIr	-456.13234	-473.28863	-449.86023	-449.99276	-462.03666
PMA4HPt	-452.60330	-468.88684	-446.14175	-446.57772	-459.25785
PMA4HAu	-448.61390	-464.06376	---	-442.81024	-456.05442
PMA4HHg	-445.58695	-460.52572	---	-439.83367	-453.17102

Table S2-8. Total energies of CO, 2CO, O₂_sideon, O₂_endon and CO₂ adsorbed on 4d-TM@PMA.

Atomic fractional coordinates of optimized geometries

Phosphomolybdic acid (PMA)

PMA

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0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo

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Direct

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0.5716036285543464 0.6511278955569348 0.4453924070279804
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0.6571038026449956 0.4361360805424329 0.3341017019937420
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PMA-4H-3d_TM

PMA-4H@Sc

PMA4HSc

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O P Mo Sc

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PMA-4H@Ti

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O P Mo Ti

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PMA-4H@V

PMA4HV

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O P Mo V

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0.4020565454981098 0.4116778081004218 0.5058858175574499
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0.5997027934265122 0.5915879585069823 0.2611859072935691
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0.5062109869530489 0.3172076160689669 0.3814447067414945
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PMA-4H@Cr

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0.5131441806525675 0.3909151565808582 0.2207008835839181
0.5092646576727933 0.5633981302093810 0.3425183278610801
0.4415305672288206 0.5021724981947856 0.4302505957373295
0.5084104308275813 0.4365878900218317 0.3449966699085600
0.5689336248482743 0.5014197654948059 0.4354250900532429
0.4383150591723344 0.3539905260524066 0.4464909386032809
0.5782939794081797 0.6722430819658622 0.3120718883904087
0.3607377709990942 0.5666726445997606 0.3225101037650340
0.3598599196236673 0.4343623389568225 0.3251753378240910
0.4288832642412420 0.4982960604289555 0.2359309482631811
0.6590210155246049 0.5649417828570724 0.3347290933750773
0.5014290983015838 0.5844565480785979 0.5386062744822132

0.5691136681306430 0.3532094072775149 0.4517971134072944
0.5710931827998514 0.6502885147806921 0.4459431196130477
0.5003580030745375 0.4236340097829054 0.5418750433048358
0.6580292861362123 0.4326241560289362 0.3373323282068207
0.3770269308681676 0.6229238178347255 0.1920355693845343
0.3277413385255206 0.5683427532906958 0.4556862190357940
0.3269552838471492 0.4386039821062733 0.4583194069444720
0.2416140196084868 0.5021041865843755 0.3610577703444623
0.3751781992652323 0.3728674491153347 0.1969403942436764
0.4401857008691062 0.6510208941727565 0.4406678716420752
0.5084100882875410 0.7664551690436571 0.3897549765821354
0.4040062504697619 0.5049945573046587 0.5567283368872481
0.3700240146762891 0.3645970750273752 0.5685652142304862
0.5972419737433676 0.4973599113887507 0.2428494587714976
0.5760151416823511 0.3256496043009751 0.3188297695983022
0.6523535545039043 0.3713442192858374 0.2082184271570724
0.6541218506391993 0.6213370263903120 0.2035559385994482
0.3716378239266422 0.6461416646386423 0.5628955135039130
0.5049878944776530 0.2356657455916810 0.4003779369626603
0.6810231671627790 0.5662681343312973 0.4700731442103563
0.6801066536021619 0.4365460601335390 0.4727867864908863
0.7737987913477730 0.4988290471732856 0.3827636353196187
0.6294659468368745 0.6447077728071128 0.5733069298570621
0.5961490416277081 0.5038887742409744 0.5645500292828797
0.6272905556303724 0.3630327598223566 0.5790421915221147
0.5070449263660870 0.5008704257496416 0.3881049112660838
0.4266159097347389 0.5927034931329681 0.2539263961159295
0.3244558363840886 0.5019058880422770 0.3796518338043454
0.4252165762175715 0.4047592348099667 0.2576013074573896
0.5084809722783508 0.6827202663672669 0.3758116531400465
0.4014005360294997 0.4139958598895595 0.5068086607598863
0.5979265153809592 0.4038117225500825 0.2646669810612777
0.5993063208967675 0.5917541765157308 0.2611875150206631
0.4024628947669612 0.5938700222312023 0.5032579747938768
0.5061460335468708 0.3186872682519077 0.3829010462542451
0.6897292108398252 0.4996527039759345 0.3945986079071879
0.6029735778675758 0.5927480621603738 0.5113609336875146
0.6016288753066952 0.4128027082455185 0.5149896794040807
0.4992237134230523 0.5049165916256998 0.5818635807869910

PMA-4H@Mn

PMA4HMn

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Mn

40 1 12 1

Direct

0.5146540115063822 0.6038854532126801 0.2166358880826840
0.4418054532795851 0.3258410078643535 0.3129831659595410
0.4440976498278390 0.6735283083010888 0.3061780957265358
0.5131459886624984 0.3908980692532315 0.2207115456953374
0.5092670898307670 0.5634235163155192 0.3421114835168638
0.4420905013569491 0.5020906993214265 0.4302900512624198
0.5084225292134901 0.4364489693723053 0.3445360299622646

0.5683968462443664 0.5013560320146305 0.4354159502254320
 0.4381939745367864 0.3520791699638955 0.4462441279755850
 0.5783157838353714 0.6727871530191322 0.3117046788488432
 0.3615598955276254 0.5666387211902845 0.3230264227798286
 0.3606393426023424 0.4343453097424138 0.3256602890501464
 0.4288643349599223 0.4982885221891049 0.2357697960992492
 0.6581656040213246 0.5649265607373046 0.3351983952233925
 0.5013577780257870 0.5913070337841773 0.5414186575240827
 0.5692050655807299 0.3513403359530261 0.4515700852915215
 0.5711955998957245 0.6521965808739737 0.4456593659159845
 0.5001978271827594 0.4169483558641199 0.5448643074522785
 0.6572089662502207 0.4326332074802203 0.3377923159290889
 0.3768063904814495 0.6226157956272486 0.1921283655626277
 0.3295821886264619 0.5684875029152352 0.4564211999895582
 0.3287216958158190 0.4384922202645528 0.4590923156616135
 0.2428405655569181 0.5021087178543064 0.3628740442618638
 0.3749676910348992 0.3731747622991484 0.1970020277600754
 0.4401281295098201 0.6529422546837308 0.4403977839139570
 0.5084309850169855 0.7678404416789042 0.3881999378322097
 0.4068069686882814 0.5049870135893512 0.5560093904890511
 0.3686196198956745 0.3631470083180209 0.5683628739949800
 0.5972512858109414 0.4973688043506034 0.2427186681345593
 0.5760575461441405 0.3250783439123501 0.3184521947383011
 0.6525862449061198 0.3716724207786054 0.2083182464178331
 0.6543402613910819 0.6210473699431495 0.2036888415119993
 0.3702104738932577 0.6476131835967420 0.5626759051711808
 0.5050276449772232 0.2342905188624236 0.3988842422284352
 0.6791449924880989 0.5664444703773968 0.4706675888272817
 0.6783028678915414 0.4364182152916445 0.4734249857370780
 0.7724369347452643 0.4988514338653411 0.3845290604056016
 0.6309209699123712 0.6461655357384730 0.5731985310977887
 0.5933710400511734 0.5038945727831813 0.5636093829261709
 0.6287034604322753 0.3615240950623421 0.5789823152797845
 0.5070791043009084 0.5008112263172252 0.3875949633841967
 0.4265903848858696 0.5925994766753673 0.2539562573883560
 0.3258214624794410 0.5018840464299441 0.3809005949999941
 0.4252142894066341 0.4048413117640955 0.2576220997253886
 0.5085055034289933 0.6840419677686647 0.3748066052949822
 0.4027278394590721 0.4116396801419159 0.5074298068253589
 0.5979377663688825 0.4039334268270887 0.2646668651075443
 0.5993041267228082 0.5916533157762854 0.2612106967374598
 0.4038063177613744 0.5962671339238346 0.5038344288677311
 0.5062008096443037 0.3174270575765624 0.3819390827346534
 0.6882788277415649 0.4996639795365560 0.3957953551626202
 0.6016093379330567 0.5951982567363130 0.5117960661465517
 0.6002574987231049 0.4104361890140891 0.5155349388918151
 0.4995343375337017 0.5047852812664252 0.5741036752703366

PMA-4H@Fe

PMA4HFe

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Fe

40 1 12 1

Direct

0.5146644343655649 0.6037792260916370 0.2166569519691482
0.4417467215034858 0.3260014123596247 0.3129700340234943
0.4440343040071287 0.6733893481514460 0.3061339230559284
0.5131491499125986 0.3910265587385764 0.2207729238385371
0.5092752440544828 0.5634616047474050 0.3425158669985717
0.4416258458981437 0.5021338882240823 0.4303061966242010
0.5084243109350869 0.4364639962523658 0.3449966793138572
0.5689416519665335 0.5013839800123394 0.4354101277528746
0.4383944475591851 0.3529498111674262 0.4461433985609164
0.5783087045907281 0.6726238771963654 0.3116778969131573
0.3610982303861863 0.5666932107496049 0.3226480329980304
0.3601822226309320 0.4342798669660992 0.3253243719530862
0.4288341732661290 0.4983027284266516 0.2357813670542910
0.6586235106309477 0.5649782626587690 0.3348884643097744
0.5014578185784003 0.5865729683360663 0.5381436367126132
0.5690694116816262 0.3522013873885778 0.4514324413922543
0.5710397081061186 0.6512854954524373 0.4455171572890452
0.5003623031521500 0.4215687628186143 0.5414395311139962
0.6576532729297608 0.4325440817892243 0.3375068109734031
0.3770062366672308 0.6227357266944250 0.1918529097224440
0.3287288630044041 0.5682384667622902 0.4560396231520682
0.3279018214285105 0.4386913326497993 0.4587039882071940
0.2421233944645312 0.5020994695432122 0.3618497504040881
0.3751577288261628 0.3730994620784862 0.1967579334364610
0.4402841232212759 0.6520360200068550 0.4402694432340040
0.5083280637215191 0.7673524969919228 0.3886703616926387
0.4053742884806811 0.5050008420849107 0.5569682266818408
0.3704339359358384 0.3645316242638120 0.5687934343912736
0.5972648930402885 0.4973751269819459 0.2427770888674223
0.5760573827338186 0.3252690976292216 0.3184589023505943
0.6524224415801840 0.3715752825461877 0.2081469791255109
0.6542021209714841 0.6211669767414484 0.2035143870311830
0.3719715215353910 0.6461735339726475 0.5630830438914630
0.5049185544975012 0.2347712565949691 0.3993404731609752
0.6800378163602709 0.5661656323644396 0.4703310061116694
0.6791762237123700 0.4366597558958744 0.4731038820135243
0.7731888104603925 0.4988121189655542 0.3836218289446703
0.6291551270534538 0.6447962027985946 0.5733842161880778
0.5947871036017446 0.5039027529080945 0.5646596311497045
0.6269113320124248 0.3628979520446632 0.5791711988066069
0.5070695813396776 0.5008490927123410 0.3880736014379645
0.4265523929927052 0.5926474437417746 0.2538509593326724
0.3250186462714220 0.5018932784995164 0.3802177060071701
0.4251556687811910 0.4048314704506301 0.2575610502171936
0.5084645828591676 0.6835924281816452 0.3749586221316794
0.4025793565475701 0.4130749616647919 0.5067421431162773
0.5980046409253028 0.4039173063586087 0.2646833344773051
0.5993864928670602 0.5916852040794546 0.2612112777819554
0.4036587778969177 0.5947564651646547 0.5031480588385407
0.5061627757964428 0.3178609821094149 0.3820967742537792
0.6890925299967761 0.4996405706187207 0.3952055947462584
0.6018066214995079 0.5936899077142327 0.5110957593074862
0.6004744411343951 0.4118601741453957 0.5147998343249410
0.4991660476271799 0.5050191545121601 0.5851911536162019

PMA-4H@Co

PMA4HCo

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Co

40 1 12 1

Direct

0.5146607213997262 0.6039103330857991 0.2166656790723042

0.4418275830214928 0.3259628653383493 0.3132327348011464

0.4441208378035786 0.6734281853164300 0.3064207912260505

0.5131472046664385 0.3908497873249510 0.2207508845395974

0.5092784892523735 0.5635332086113043 0.3419967396623825

0.4417051194360436 0.5021322919669715 0.4296840208658945

0.5084255460207879 0.4363958642750605 0.3444641729182281

0.5687797361250794 0.5013859690535781 0.4348676665385233

0.4383043943203017 0.3526839175911571 0.4465077537660192

0.5782876397746196 0.6726671368766296 0.3119219360399177

0.3611670999550618 0.5667461714926096 0.3229640629944090

0.3602801095661252 0.4343081209725074 0.3256087133771698

0.4287867416892994 0.4983013670575456 0.2360678502287776

0.6585793483401056 0.5650076257503767 0.3351734112856918

0.5013795412606172 0.5879229207227052 0.5403349079677572

0.5691052804816108 0.3519144680078999 0.4518294313442552

0.5710884537687810 0.6516161167144403 0.4459417706763709

0.5002699336376177 0.4202175279887041 0.5437040966182779

0.6575805911970085 0.4326059818540013 0.3377585400054618

0.3768591535928220 0.6227417960509271 0.1922396517461524

0.3289184308095325 0.5683350718425499 0.4565677839910562

0.3280862015798161 0.4386452644571360 0.4591819469841486

0.2424417426792228 0.5021288042562652 0.3625937553179668

0.3750207401448462 0.3730091336027452 0.1971463458543727

0.4402031223293936 0.6523480622823743 0.4406697062748179

0.5084236858884029 0.7674270765326778 0.3889713110259418

0.4078115262605858 0.5049622443515646 0.5559456677533106

0.3693939560999456 0.3635292087539561 0.5686321981876074

0.5973106494730522 0.4973709116528238 0.2429919910752531

0.5760363656031837 0.3252218604234213 0.3186849682049328

0.6525097767160949 0.3714966952771324 0.2084410532438422

0.6542783973131648 0.6211519603802051 0.2037755340926400

0.3710340557754872 0.6472249253841783 0.5630014560897041

0.5050222541941930 0.2346936685557063 0.3996103212120677

0.6797822032949371 0.5662895604973107 0.4708704015261878

0.6789143211918013 0.4365749112934424 0.4735802731409413

0.7728700856776451 0.4988670844790165 0.3842433281248871

0.6300428887862966 0.6457771479034626 0.5734765635174650

0.5922841794043621 0.5038873014959903 0.5634824119082810

0.6279006722072412 0.3619185410730908 0.5792049835135591

0.5070640933585007 0.5008394022617505 0.3875159746595754

0.4266229074072623 0.5926884436729019 0.2540577986807415

0.3254262708688558 0.5019131907922294 0.3805552073639035

0.4252349144051649 0.4047621521639854 0.2577409155437300

0.5084975323995503 0.6836775194770003 0.3752972404355004

0.4022214885949905 0.4124162688215261 0.5073046882742448

0.5979060576702184 0.4038378973579865 0.2647774532483091

0.5992877811847444 0.5917371368304101 0.2613206021824667
0.4033066315974446 0.5954961459845639 0.5037507785673214
0.5061891438857944 0.3177859579783424 0.3824259856618218
0.6887146045831333 0.4996744346264338 0.3954752567996550
0.6020984467755672 0.5944348592164133 0.5117417227078552
0.6007692697683926 0.4111621156727117 0.5154288934149895
0.4996518827616688 0.5046934225967534 0.5720006567465357

PMA-4H@Ni

PMA4HNi

1.0000000000000000

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0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Ni

40 1 12 1

Direct

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0.4418111300119414 0.3260290572182704 0.3133239676425799
0.4441123907895167 0.6733332304996831 0.3065205047419196
0.5131417586128930 0.3908003504860627 0.2206853602650413
0.5092962844674901 0.5634837112713952 0.3417471312871535
0.4417871851930894 0.5020856366902392 0.4295475531721728
0.5084354927495073 0.4363815460202150 0.3441885334387609
0.5687251582222629 0.5013310148622038 0.4347087043235365
0.4383177273656633 0.3529277477664854 0.4465907830844243
0.5782946505471459 0.6725823290465396 0.3120242713553641
0.3612442409707859 0.5667841805796245 0.3230684928524147
0.3603236226636831 0.4342290565155600 0.3257277205419943
0.4287153234600000 0.4982969412802634 0.2360892199588538
0.6584882192558651 0.5650574743381291 0.3352722847041018
0.5013326522662521 0.5893395624070962 0.5415584670096704
0.5690890877422129 0.3521545756902398 0.4519148928923393
0.5710591929521076 0.6513856517130455 0.4460634385184230
0.5002084846372888 0.4189114557301255 0.5449264780621972
0.6575207433346988 0.4325288217674693 0.3378683308181432
0.3768568395177342 0.6227330298373859 0.1923116193789128
0.3287984929505021 0.5682868977752249 0.4566947049201704
0.3279302882866259 0.4387129647545628 0.4593457896661944
0.2426071131641626 0.5021293457245872 0.3625154092795182
0.3749907894399243 0.3730543095502262 0.1972118626456567
0.4402120949778462 0.6521340354319446 0.4407788507205166
0.5084064326064343 0.7671965218784771 0.3891056333586947
0.4070039450745662 0.5049774124586122 0.5558283211176848
0.3688740584138168 0.3631182344586412 0.5685165262318074
0.5973827062345856 0.4973746985202407 0.2430245953496137
0.5760350233044707 0.3252987846263296 0.3187745501392789
0.6525109018620159 0.3715496663155117 0.2084921141407615
0.6542797924219154 0.6211642748319717 0.2038569954925185
0.3704533358360625 0.6476243665373099 0.5628564938346576
0.5050111132677205 0.2349233438582305 0.3997635549671368
0.6798981726237060 0.5662414717117182 0.4709944202608662
0.6790659796100694 0.4366367662879428 0.4737378031775989
0.7727014542512605 0.4988589602132008 0.3841604983163383
0.6306651101009905 0.6461661875181145 0.5733623783224377
0.5931388639057211 0.5038940539929465 0.5634123212951841

0.6284336340147729 0.3615215711814068 0.5791190421880138
0.5070758860042067 0.5008211047375383 0.3872679247604345
0.4267055193864484 0.5927220061756793 0.2540471165859575
0.3255671112379464 0.5018979603447222 0.3804683709765956
0.4253135622255801 0.4047398613588479 0.2577483952571307
0.5084887755750952 0.6834627350586221 0.3754487818266397
0.4018922877152115 0.4123654401097986 0.5075651703211996
0.5978118550194145 0.4038343527324618 0.2647569148771023
0.5991968762362577 0.5917734211289413 0.2612948000999504
0.4029788103134415 0.5955679431575893 0.5040134728007273
0.5061818140437565 0.3180007049091295 0.3825322656228997
0.6885654323597892 0.4996592068268916 0.3953669010924701
0.6024264443339618 0.5944789342518073 0.5120365162559917
0.6010855681815350 0.4111221447657105 0.5157013453098904
0.4997978420533783 0.5046396936465500 0.5680719830390428

PMA-4H@Cu

PMA4HCu

1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Cu

40 1 12 1

Direct

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0.4440038187877148 0.6736924114100593 0.3064672764292545
0.5131508038505915 0.3905611882569624 0.2208755539938646
0.5093069355974439 0.5635748540220189 0.3413365942728739
0.4421351583914360 0.5020703912881238 0.4291856156587642
0.5084522686880011 0.4362424980565306 0.3438136328846217
0.5684288991155285 0.5013342051373634 0.4343173146726415
0.4383946351676133 0.3511431959271509 0.4470582230578892
0.5783825287600710 0.6729612567437830 0.3119959008677108
0.3616302489415534 0.5667211756104197 0.3231638674661742
0.3606965117949948 0.4342872076839155 0.3258314957544526
0.4287883333430803 0.4983026643464920 0.2357739491358100
0.6580768499738181 0.5650162717346626 0.3353461479520908
0.5012620467529654 0.5930132175804075 0.5433258227291905
0.5689382287189030 0.3504138294376843 0.4523333756645150
0.5709081697835674 0.6531504036708055 0.4463427921106802
0.5000867392581739 0.4152630156663649 0.5468970014328602
0.6571307209433137 0.4326007651633640 0.3379378296231899
0.3768291840779365 0.6226651434143413 0.1923031311705196
0.3301331687175815 0.5685206207620381 0.4570084314884214
0.3292257760940774 0.4384399005019083 0.4596406162496362
0.2434086409345819 0.5021377946477087 0.3639272830829771
0.3749947865707562 0.3730654830368085 0.1972705436009175
0.4403208951153011 0.6539096575927597 0.4411218644616373
0.5084462012094171 0.7684013599625809 0.3878033048982778
0.4082755045445359 0.5049372020860069 0.5550731466697807
0.3674855389566027 0.3623147423943293 0.5682743763390443
0.5973267263112343 0.4973835232555461 0.2427284033770563
0.5761700805988618 0.3249552765418566 0.3188218600234668
0.6525493470608588 0.3715627585118532 0.2085769163757054

0.6543325253025337 0.6210941608556879 0.2038810579881167
0.3692000607821674 0.6484375967619588 0.5626154258097189
0.5050543939053340 0.2337076147695448 0.3985088863194599
0.6785652324210086 0.5665156690137637 0.4711598048822475
0.6777639850280395 0.4363916682512562 0.4739095324175476
0.7717942379034913 0.4988864955319827 0.3855366924752372
0.6319190446469776 0.6470018796851976 0.5731792069654222
0.5919741721103104 0.5038820863308853 0.5625201832548761
0.6298273080755898 0.3606951804880077 0.5789584216679750
0.5070955827874920 0.5007892288072638 0.3867455963586033
0.4266510054718443 0.5925988334350447 0.2540702560160619
0.3264935749124687 0.5019238129629764 0.3813824691312166
0.4252455832716323 0.4048681321939928 0.2578249155034514
0.5085374405095274 0.6845763235784399 0.3747717361170974
0.4027726292395029 0.4106454377293161 0.5079563090726449
0.5978843915748548 0.4039368807742875 0.2648530533722561
0.5992717783594667 0.5916688311774062 0.2613661018647119
0.4039342369624300 0.5973029139731199 0.5043216526939047
0.5062244773047839 0.3168937762192980 0.3819785844816732
0.6875698857928511 0.4996920822911117 0.3961953656699965
0.6014564091822709 0.5961902420599755 0.5122721767403732
0.6001368361985562 0.4094772252943636 0.5160433241338299
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PMA-4H@Zn

PMA4HZn

1.0000000000000000
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0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Zn

40 1 12 1

Direct

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0.5131461868181024 0.3909801950911154 0.2206530499353786
0.5092894145292861 0.5634849798922549 0.3422664171923946
0.4419197399669869 0.5020904405861208 0.4303152400995729
0.5084246711752500 0.4364084512283788 0.3447402013830899
0.5685735322468232 0.5013346771380479 0.4354386447341050
0.4383239823446463 0.3519480995533570 0.4460738575177983
0.5783564321501243 0.6728032462802473 0.3114803072169214
0.3615502540953585 0.5666794167082505 0.3229711517314403
0.3606160115003882 0.4342505204051210 0.3256522681267483
0.4287548595711481 0.4982835476928750 0.2358613143172217
0.6581615302844953 0.5649761225203861 0.3351697362574223
0.5013897887496401 0.5919870502044176 0.5395150013293233
0.5691460942782131 0.3511918228377704 0.4513597202710842
0.5710828106408371 0.6524018435848584 0.4454709133108232
0.5002389832880267 0.4162266544608812 0.5430013857653527
0.6571999023021857 0.4325544101145682 0.3377699468635399
0.3768997782712150 0.6226044005693449 0.1919954755558887
0.3295570974988047 0.5683756367103836 0.4565831040563930
0.3286899815646936 0.4385729965672872 0.4592683782700438
0.2429536056311106 0.5021017382678676 0.3628656553065661

0.3750046019272889 0.3732160359783300 0.1968999521019047
0.4402322759834677 0.6531101332450672 0.4402108992298703
0.5084257949092618 0.7678819827322567 0.3880167421753531
0.4046825758913649 0.5050194737538066 0.5567024964244141
0.3690301930083534 0.3631684578136885 0.5683344133302085
0.5973481488680650 0.4973608813454546 0.2428151227288769
0.5761100643910521 0.3250640198934666 0.3182304315277356
0.6525111863402719 0.3716944269858444 0.2081826950108328
0.6543149172879186 0.6210275446189600 0.2035894693005365
0.3705658819856375 0.6475405171331606 0.5626352770663824
0.5050272588211790 0.2342723840618852 0.3987645299804516
0.6791336743358599 0.5663301522864040 0.4708061803171995
0.6783285425540045 0.4365631520142538 0.4736167753746320
0.7723165831448300 0.4988176882719251 0.3845535245043587
0.6305923531127295 0.6461000678131460 0.5731188716839617
0.5954089940278620 0.5039213025185989 0.5644755197915665
0.6283173284036904 0.3615565681809281 0.5788857830100941
0.5070644873203733 0.5008047880814672 0.3878113888500056
0.4265960811481131 0.5926320284490293 0.2539024895434324
0.3258921431205104 0.5018770477117628 0.3809238079146362
0.4251815406125622 0.4048278775366846 0.2576074885453534
0.5085219264010483 0.6840808988678457 0.3747098455612534
0.4029538030565948 0.4116765971280482 0.5072849050828404
0.5979435449857652 0.4038806260258834 0.2646497288654052
0.5993722803812116 0.5916948100633462 0.2612218698462470
0.4040298810923587 0.5962299816590015 0.5036662287186215
0.5062128451140763 0.3174093864617422 0.3818324445485552
0.6881834972855108 0.4996187900727476 0.3957731758040522
0.6013988427598373 0.5951411196006411 0.5116229491509325
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PMA-4H-4d_TM

PMA-4H@Y

PMA4HY

1.0000000000000000

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0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Y

40 1 12 1

Direct

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0.4417151817931720 0.3262066698554736 0.3128011799162432
0.4440363961905173 0.6732006089693151 0.3058691572975682
0.5131671442648091 0.3910936812832469 0.2207708662711795
0.5092649178303259 0.5633243365829264 0.3425026664358376
0.4417714191639469 0.5021751089519753 0.4306417021268759
0.5084155836457588 0.4366054301672428 0.3450397734803465
0.5686514137324113 0.5014235625739815 0.4358127238174644
0.4385892413594051 0.3536178899956625 0.4456515205244577
0.5784844417141257 0.6724424367591970 0.3114036061638509
0.3607509303646003 0.5666334164304693 0.3216234538029276
0.3598365955149587 0.4345495635386434 0.3242765868719248
0.4292690134719379 0.4983566545034959 0.2354077933723223

0.6590400212203273 0.5648437450569833 0.3338244798451098
0.5013781032886512 0.5869290231257466 0.5395746034649127
0.5688645649845873 0.3528591408035495 0.4509867520202406
0.5707990020393531 0.6505500793215436 0.4451618729219860
0.5002661394012318 0.4210078730048443 0.5426532449783381
0.6580778060417866 0.4327753694365343 0.3364553661190381
0.3768828868015415 0.6224728039118339 0.1911814010700031
0.3293761272507453 0.5686001858369661 0.4543654819588236
0.3284247082158274 0.4381795289951945 0.4568493985317238
0.2415399107071030 0.5022512960192754 0.3612152648750309
0.3752172248084666 0.3731313612566497 0.1962041444913928
0.4405956311727536 0.6513082653140020 0.4398982559164103
0.5084878319297342 0.7669605917012466 0.3885761228962167
0.4005350170421000 0.5049390118307201 0.5563260224339435
0.3707052981704469 0.3660128221888875 0.5686064771452273
0.5969043470361243 0.4974286206586963 0.2422708639671022
0.5762134908857027 0.3254243731121790 0.3182295421586225
0.6524409927165959 0.3716333131248510 0.2074258439127428
0.6542737332873552 0.6209519312237485 0.2026501563612806
0.3724495425853812 0.6447390549895949 0.5631495086008280
0.5050709157228560 0.2351481121769695 0.3993529698617077
0.6795119618973636 0.5664919129001255 0.4686144695067310
0.6787266594439200 0.4360461194288328 0.4711887889911267
0.7738310662111523 0.4989707965117272 0.3829808354630647
0.6286207193035853 0.6432522068539159 0.5735124822632192
0.5995481321679205 0.5037491313611738 0.5644337463329553
0.6266117577698693 0.3644662654861750 0.5791018847018395
0.5070444209953231 0.5008703414522484 0.3880724147553645
0.4263674201841409 0.5926279256732838 0.2534413004533181
0.3244624454814639 0.5020218367552911 0.3796628619492218
0.4250001394736287 0.4048116667654862 0.2573063406578825
0.5085542141900413 0.6831422380257273 0.3748027310616502
0.4032937494337173 0.4143230532981112 0.5062777333940577
0.5982293144777370 0.4038989233399652 0.2642969147528159
0.5995564926258421 0.5916953903448441 0.2606545112289575
0.4044885475425555 0.5935062700824679 0.5029078322079207
0.5062797830998996 0.3182887527870751 0.3820442583753568
0.6896852829849467 0.4997604452121094 0.3946153885244575
0.6009645347034849 0.5923821363765523 0.5108379090406843
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0.4981783084149163 0.5051800838003693 0.6062108825837287

PMA-4H@Zr

PMA4HZr

1.0000000000000000

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0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Zr

40 1 12 1

Direct

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0.4439950545228999 0.6732656280812537 0.3058345131955386
0.5131345782433764 0.3924033042444849 0.2210199357275076
0.5091586815910469 0.5633855955169285 0.3453150299294904

0.4416881896642350 0.5021837162309211 0.4337220411557674
 0.5082902156804573 0.4364077666954242 0.3479967665532229
 0.5685620864187385 0.5014153170086850 0.4388489561983549
 0.4375428014729666 0.3525460977125366 0.4456403975659096
 0.5785381169921132 0.6725007612713372 0.3113840206821616
 0.3608028288780738 0.5665655580855734 0.3219399278631724
 0.3598567487008008 0.4349887151463814 0.3239100721885113
 0.4301494288461402 0.4984107913565612 0.2353352751235406
 0.6589742668672276 0.5648143257903611 0.3341463556816295
 0.5013374512168399 0.5865829897858826 0.5409560883565444
 0.5699112549790816 0.3517765718826142 0.4510409248064005
 0.5715295179699479 0.6514276321472201 0.4454647154283780
 0.5002375510881745 0.4216668841830206 0.5438230261191889
 0.6580804175045253 0.4331965059253775 0.3361182501422429
 0.3765982482473606 0.6219791576574698 0.1912507297844794
 0.3273379187644058 0.5689564970190982 0.4546966601252651
 0.3264614367357593 0.4381337655957707 0.4569883886075042
 0.2403326726830312 0.5021378244226178 0.3600872291143854
 0.3749106812096082 0.3732001447207525 0.1960396105499444
 0.4398544878115853 0.6522368660825113 0.4401383207678942
 0.5085247717838242 0.7675964248611331 0.3878491062086811
 0.4034029517183584 0.5050630007685818 0.5590574644318508
 0.3692905915075236 0.3649168173878894 0.5679182582088789
 0.5960752602203138 0.4975084649633221 0.2421492297704758
 0.5759258229269353 0.3253909490662387 0.3173302058527976
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 0.6545735292933053 0.6204619583713661 0.2027474513436996
 0.3709373274143427 0.6460036994523117 0.5622966490418101
 0.5050683592210209 0.2346103973784982 0.3990995523797005
 0.6815417160868140 0.5668168603170805 0.4691647774726415
 0.6806890995649065 0.4360281639885560 0.4715245373332518
 0.7750934189534745 0.4988452317931255 0.3819127044652829
 0.6302330104959187 0.6444960963527483 0.5728316221441963
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 0.6280709257992981 0.3633380080894824 0.5785080630863013
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 0.4258604374313094 0.5920398760508190 0.2536254261762691
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 0.4010021073140789 0.4125615128142065 0.5047169209759825
 0.5985581306637475 0.4035374089976278 0.2644523118994191
 0.5999920161862603 0.5911527207147403 0.2608292586257449
 0.4021003302024789 0.5953511003761129 0.5011602052362566
 0.5062343211530815 0.3176606349641270 0.3818781165334394
 0.6911593203714749 0.4996038652261019 0.3943670943927367
 0.6035620672692628 0.5941813970802006 0.5093327897358148
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PMA-4H@Nb

PMA4HCu

1.0000000000000000
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 0.0000000000000000 20.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Nb
40 1 12 1

Direct

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0.5132469992602158 0.3922857206003203 0.2212622302078695
0.5090790678676502 0.5634676957227411 0.3458058026507871
0.4419572975159657 0.5022315313462415 0.4347002402355634
0.5081742403914560 0.4363565383558601 0.3484212142777610
0.5682845770468341 0.5014403018331614 0.4397188714059995
0.4376129803935841 0.3516858918202331 0.4457338405726929
0.5786512095132681 0.6725615780042582 0.3114808255879731
0.3610300803210114 0.5663491480777285 0.3218701571025442
0.3600284807404519 0.4351468049090906 0.3237909501717303
0.4307881239380975 0.4983657849844320 0.2350128072521536
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0.5011884631420216 0.5902212065854520 0.5445276104054282
0.5700618766985608 0.3509580427309312 0.4512318558876913
0.5717672668203754 0.6523384044186141 0.4456196227226260
0.5000509537341331 0.4181729906805061 0.5476582326607360
0.6579392933859706 0.4331485100719054 0.3365077420700325
0.3763559173830986 0.6217799568061040 0.1913746413774986
0.3276390404472510 0.5692784703120896 0.4545188610220918
0.3268075183420638 0.4377769834334186 0.4568261460284644
0.2403843746906455 0.5021065153630989 0.3608623810974467
0.3746866017156391 0.3733507521149472 0.1960899336994816
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0.5084960382894036 0.7680626037571587 0.3872400090047599
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0.5961591123211866 0.4974896892940252 0.2424501684196578
0.5760783896911538 0.3253717437354730 0.3175817735857607
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0.6812925299271058 0.5669698296081357 0.4693451024580945
0.6804365280952225 0.4358883835187836 0.4717730817573833
0.7747641582447574 0.4988521709981986 0.3822106305264116
0.6325080130519044 0.6462861732329983 0.5716665654708749
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0.6304008484352759 0.3614330849991276 0.5773232324142782
0.5069484469774042 0.5008664558135807 0.3907331826242727
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0.5061114864166983 0.3172465325086000 0.3814977543284735
0.6907610747753549 0.4996216283141817 0.3942981390935959
0.6039982264810514 0.5956889324164802 0.5094420308487457
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PMA-4H@Mo

PMA4HMo

1.0000000000000000

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0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Mo

40 1 12 1

Direct

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0.4447006441096511 0.6737153111249187 0.3048715341709763

0.5136103878119235 0.3914933472029818 0.2212071912413930

0.5088872508735882 0.5635898996101891 0.3450272751359845

0.4416401542644996 0.5021926464861558 0.4333663710428971

0.5079416240312777 0.4363946859580148 0.3475149513728938

0.5684362400251809 0.5013758861315213 0.4382994288009791

0.4385419486257048 0.3515229752391996 0.4457845577967655

0.5792945815853646 0.6727070185077256 0.3121560782447099

0.3613254272709377 0.5658016507908801 0.3211063611202976

0.3603609390808722 0.4354370489183428 0.3233076146355048

0.4320698533417666 0.4983076689619545 0.2335869454021727

0.6587742091376293 0.5652194651585120 0.3353273791648345

0.5013476335314391 0.5869103549840297 0.5424640582208130

0.5698899895706656 0.3509928294217158 0.4515430394947638

0.5717146540784596 0.6524352096411624 0.4457982427204926

0.5002768351440287 0.4213206317980643 0.5455782033035766

0.6577497638001790 0.4325047754638884 0.3378087781231160

0.3758215541874914 0.6215964128485207 0.1916885859572176

0.3278616718691936 0.5696360540502180 0.4542911722934758

0.3270428400937955 0.4372310806547755 0.4567691461408044

0.2402889856769386 0.5020940038367152 0.3620971952807074

0.3739969040049183 0.3739373764771412 0.1964074133565003

0.4406295151299063 0.6534359503454763 0.4401264597185868

0.5082621777626053 0.7683381837965146 0.3871400652060336

0.4077155036867005 0.5050099809994471 0.5575993960158077

0.3684870650877226 0.3638034509329089 0.5673668926758112

0.5975303615169760 0.4974351512213457 0.2436169938682932

0.5768340309354766 0.3252835996797552 0.3186386458266925

0.6522789064597477 0.3716763313274573 0.2074636694035030

0.6540558769646907 0.6208338755184771 0.2028354643572443

0.3700619590830970 0.6469594460991538 0.5616338553475100

0.5047174557195265 0.2338297781796201 0.3980988917289133

0.6810902252166779 0.5664006284122077 0.4706121527947933

0.6802889877877043 0.4364152783881364 0.4732750129409581

0.7738970958170510 0.4988394372294699 0.3818399985502274

0.6311332533500791 0.6458225086175955 0.5725018213688520

0.5928940435789299 0.5039129084347844 0.5656154045379175

0.6288912482735802 0.3618943366605476 0.5782463945186715

0.5068622290001625 0.5008584762384086 0.3900168998512988

0.4247412653573802 0.5916154132732716 0.2542199312789541

0.3228050918017338 0.5018200754347066 0.3813600908038391

0.4234062321139080 0.4054021985088324 0.2578602695591995

0.5082666170607992 0.6845765453198622 0.3733599090438575

0.4015372280512837 0.4113497486434137 0.5050009805079386
0.5973927534750400 0.4035033674672024 0.2639183981863573
0.5988619940561103 0.5917958951756709 0.2604074496454106
0.4025879208564307 0.5965331932905936 0.5012615381333797
0.5057452483859490 0.3169397024991391 0.3808795400437008
0.6897907883620794 0.4996474750996479 0.3937193314237275
0.6035873467708283 0.5956354860559284 0.5093745140596091
0.6022690588868140 0.4098388993985334 0.5130169101740102
0.4991201071285344 0.5050755479739165 0.5928129928198482

PMA-4H@Tc

PMA4HTc

1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Tc

40 1 12 1

Direct

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0.4419560439563316 0.3264968084258429 0.3129217183329543
0.4441691380666590 0.6729035271671160 0.3062548167323166
0.5131592688544192 0.3916969487698804 0.2214172956803229
0.5091612464698934 0.5634389961997838 0.3450732827029031
0.4416197652702992 0.5022207345749606 0.4334013833965941
0.5083155651256507 0.4366163039621764 0.3475855476045751
0.5686497530739175 0.5014593922703617 0.4385454176620053
0.4375877294548284 0.3538834116011412 0.4463404504866041
0.5782972609889917 0.6721291388846840 0.3117860956743690
0.3603477394124103 0.5665068981238385 0.3218541023068122
0.3595087499990234 0.4347141217919849 0.3243830033202932
0.4297555248706429 0.4983289813953005 0.2358584204517706
0.6594500803429836 0.5647416679664264 0.3341309167787767
0.5012494871509887 0.5872537933960021 0.5422192589193043
0.5698139107747828 0.3531004340383748 0.4517809808241842
0.5717231735865448 0.6502765715958915 0.4460021209062522
0.5001465030542394 0.4208731103739954 0.5455100732912885
0.6584380585691000 0.4329075268103856 0.3366197536323148
0.3767805413943188 0.6225052986724530 0.1915809464722222
0.3258562814794267 0.5688094216383136 0.4544629741792073
0.3250350997139792 0.4381195102953969 0.4569586581873543
0.2399994146643573 0.5021452796248391 0.3589981851767746
0.3750679600253372 0.3731058345980987 0.1964639870539594
0.4395531028734420 0.6511057395720653 0.4406454649357618
0.5084525969052610 0.7664119785009373 0.3895184446262980
0.4021272799020063 0.5050308734656972 0.5583289509170334
0.3670970316197782 0.3636521144462864 0.5667172487043315
0.5964600019304017 0.4974073899423547 0.2427386073700862
0.5759684946892818 0.3257673372310287 0.3183798984395385
0.6526257318157084 0.3716027897170106 0.2077560510241982
0.6544067164200832 0.6209720493397322 0.2031078926322990
0.3687830270315339 0.6471312052535492 0.5610781948223870
0.5050509635196500 0.2357292433825402 0.4002748457308835
0.6830023837018614 0.5666779001212170 0.4690687911015967
0.6820760626955055 0.4359680066783065 0.4716358482001958
0.7755133476777155 0.4988334223317429 0.3808749009308621

0.6324030432253489 0.6455516078828031 0.5718093655286037
0.5977876428831800 0.5038628443504806 0.5663842898093557
0.6302949972176638 0.3620733649233031 0.5775537441721493
0.5069741993862249 0.5009132242497135 0.3902622517248689
0.4260802552610554 0.5925767521094698 0.2538758604643159
0.3225158864956160 0.5019337954302493 0.3787093188384853
0.4247693610817107 0.4047234491691125 0.2575705135555647
0.5085238935422185 0.6827355683840635 0.3753421220584254
0.3989806412310267 0.4130984241380906 0.5052415568334797
0.5984183901902980 0.4037896263593898 0.2645830535513759
0.5997747556613071 0.5916431586405041 0.2610879471646416
0.4000858837077437 0.5947996501590485 0.5017262341740328
0.5062227036404811 0.3187148941302939 0.3826127634421544
0.6916729089839529 0.4996477745235954 0.3938044557253588
0.6054541879594315 0.5935847398017301 0.5100501445448551
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PMA-4H@Ru

PMA4HRu

1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Ru

40 1 12 1

Direct

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0.4417127490922721 0.3261818620992297 0.3132113858727891
0.4440183155359569 0.6732119705072562 0.3063634911253406
0.5131305659097278 0.3909552625486589 0.2208663921469874
0.5092636577307523 0.5634098521581967 0.3429863862314715
0.4415169536367735 0.5021480890121778 0.4308135467783600
0.5084051675794884 0.4365121376949694 0.3454455996144949
0.5688873608243075 0.5013885544377356 0.4360176950820826
0.4384241514473511 0.3535104793866336 0.4463954035557512
0.5784482901712501 0.6724745043659764 0.3118568347673461
0.3610112190898361 0.5666280085433182 0.3224709816286594
0.3600896925857124 0.4343469094826259 0.3251531317240164
0.4291313313402769 0.4983041121236023 0.2358132124898864
0.6587188771861768 0.5649267986924699 0.3346324806405871
0.5013342679816291 0.5865469160344257 0.5397654511637228
0.5690284329300174 0.3527100702008189 0.4517035622426199
0.5709735290845882 0.6508121128717773 0.4458561295530390
0.5003168456706449 0.4216160314092670 0.5430780829116478
0.6577502972652144 0.4325897380215999 0.3372487953294738
0.3769339052489629 0.6226989449125058 0.1918514223720995
0.3277724926364147 0.5686542939085204 0.4553213549838155
0.3269199607683448 0.4382698824324839 0.4579966514618687
0.2418287482736882 0.5020881383994397 0.3608049456427667
0.3750879021468525 0.3731031542557788 0.1968070463075228
0.4402864039233969 0.6515786364336250 0.4405788435226651
0.5084461518892505 0.7669092018638034 0.3892678092078851
0.4028938720935261 0.5050221723621263 0.5561845208713883
0.3688413424632531 0.3632767091619796 0.5674932757379763
0.5970095488827092 0.4973719984369193 0.2426848784735449

0.5761869489103287 0.3254264402634005 0.3186612594558480
0.6524571629916694 0.3715972698424695 0.2080757595614026
0.6542669957856764 0.6210920275525730 0.2033907216010324
0.3703833740475838 0.6474112203342312 0.5618027946033654
0.5050143347076307 0.2352564913824363 0.3999880848957793
0.6809953148279460 0.5665972343444184 0.4697097395364545
0.6802148209537211 0.4361792291586591 0.4724797688884024
0.7736042821072650 0.4988104809393085 0.3825574896273073
0.6307765259498800 0.6458723329745989 0.5723694318210174
0.5971570757494372 0.5038290679180629 0.5641172369203605
0.6286044188059433 0.3616623951995239 0.5781049726462830
0.5070218695110524 0.5008795375813232 0.3885858235511585
0.4265144524887495 0.5926379537618058 0.2538669505297342
0.3245635582407823 0.5019176997974508 0.3798255751325314
0.4250957921497595 0.4048538521780501 0.2576003771421336
0.5085536467818086 0.6832014006926703 0.3751280709246553
0.4011886810002612 0.4130598132879830 0.5064980268196495
0.5980222155094627 0.4039305801404290 0.2646034697997491
0.5994094822432366 0.5916615415552844 0.2611000449160423
0.4022703969231478 0.5948765148599855 0.5029123104488333
0.5062244858178623 0.3182607359397533 0.3822732966874974
0.6895882139237555 0.4996456884583112 0.3947298289913702
0.6031632793772480 0.5937154055058578 0.5110337741962503
0.6019180376774677 0.4117715390806863 0.5146886221984512
0.4988740881289142 0.5050460058636908 0.5890930133800507

PMA-4H@Rh

PMA4HRh

1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Rh
40 1 12 1

Direct

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0.4441138035619731 0.6728196632398284 0.3067504869694361
0.5131366571669926 0.3909289188382111 0.2209478191172618
0.5092525015112870 0.5633326923672225 0.3431844126159496
0.4413561081595592 0.5021759232337001 0.4308831384790817
0.5083890052903409 0.4366799913783297 0.3456559272851080
0.5690929711901103 0.5014138678848847 0.4360466344504060
0.4381981213085563 0.3545175453052118 0.4466124502172239
0.5782788510104009 0.6720477043073865 0.3122609596826111
0.3604671563338194 0.5666042665945946 0.3222465202620886
0.3595437723362291 0.4343948179110275 0.3249218102410286
0.4288180059929098 0.4983123391798812 0.2360131408406189
0.6592845591229102 0.5648634507584002 0.3344877685151170
0.5014208402952031 0.5845301942460490 0.5377565267651825
0.5692294015549422 0.3537602904753525 0.4519400192107174
0.5711912940286058 0.6497501796371419 0.4460868345062643
0.5003625909469734 0.4234847645408600 0.5410233012507106
0.6583387052049675 0.4326259269561090 0.3371091812766989
0.3771161931510139 0.6229769070592637 0.1919582323547239
0.3264732653296470 0.5684942206825270 0.4550561268937767

0.3256252638219170 0.4384472002396845 0.4577360692810923
0.2410039314657672 0.5021008285092570 0.3595663874630062
0.3752743680200887 0.3728794031377356 0.1968604338679918
0.4401035477491939 0.6505273442522836 0.4407880117062978
0.5084068643331675 0.7659842663732217 0.3901034332607032
0.3996661928658909 0.5050226270017230 0.5568595093627626
0.3692943935280419 0.3641854500246697 0.5678847467133288
0.5972949632915762 0.4973729433961928 0.2429622766158185
0.5759544144898878 0.3258723468923101 0.3190322052775303
0.6522414819119733 0.3713524521862319 0.2081428883053843
0.6540306277568446 0.6213998622977652 0.2034575414035789
0.3708546378693183 0.6465157212642111 0.5621504077431881
0.5049524362347440 0.2361865061961351 0.4008600914939837
0.6823592890332113 0.5663516398107727 0.4695334131766987
0.6814915189623888 0.4363761244156223 0.4722990793438259
0.7745041178437472 0.4988103102356527 0.3813353717464953
0.6303399713687921 0.6450030696981247 0.5726042639188181
0.6004196946445989 0.5038338990423383 0.5650353576027496
0.6281337836196800 0.3625824656259797 0.5784066698634388
0.5070219163996622 0.5008888973900089 0.3888770046826731
0.4265863374920577 0.5927203674189097 0.2539443823657261
0.3236300828486280 0.5019006363529459 0.3789993872156759
0.4251834427279541 0.4047472187639667 0.2576402317413019
0.5084959550501610 0.6822241462468176 0.3761458419112859
0.3999681560483649 0.4144680658838716 0.5064466080901470
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0.5993119859673286 0.5917523734614348 0.2611738365577979
0.4010735586646650 0.5934395686582746 0.5028796988048255
0.5061292011511682 0.3192555701437008 0.3832907466526334
0.6905602849900738 0.4996213522128814 0.3940060741686927
0.6044011695440850 0.5922416427574513 0.5110663044833001
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0.4989691324319630 0.5050028900765613 0.5877946547243595

PMA-4H@Pd

PMA4HPd

1.0000000000000000

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0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Pd

40 1 12 1

Direct

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0.4443222350184842 0.6731140491409385 0.3059767395256079
0.5131561875491615 0.3913251205116315 0.2206891002527648
0.5092567347218221 0.5634460635637916 0.3432163751218759
0.4418984678573001 0.5020636296323563 0.4315016953951240
0.5084015203278217 0.4364510871080446 0.3456143630504488
0.5685791822651625 0.5013094653942405 0.4365857381500315
0.4378982590088903 0.3535081884147356 0.4458323611806646
0.5780895833563431 0.6723686057124056 0.3114904244136778
0.3611597447830420 0.5665583190926896 0.3227983408098009
0.3601707548139556 0.4343362167567270 0.3254828500381207
0.4286229502481975 0.4983145765265878 0.2361818949783707

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 0.5013107008855953 0.5938492327911338 0.5421242098292989
 0.5696162214763132 0.3527758252434147 0.4511974941473785
 0.5715356314405221 0.6507780030277630 0.4453848665526134
 0.5001376782037682 0.4145305456276708 0.5455927632039029
 0.6576429858100384 0.4325994189800886 0.3376433534009932
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 0.3279106910887678 0.5687218617385917 0.4556527757278614
 0.3269464431533369 0.4382206713770865 0.4584107525035299
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 0.3750519221576655 0.3733279710016923 0.1967233620413168
 0.4398232008827964 0.6515311007042509 0.4400318370223260
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 0.4002168888094023 0.5050244625224587 0.5561651003634526
 0.3680417279126389 0.3625153929330777 0.5675019169811599
 0.5974462288084603 0.4973911361815733 0.2431866095032775
 0.5758335622171822 0.3254990058368326 0.3182365481939602
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 0.6318145587976061 0.6466467222592418 0.5722689892451353
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PMA-4H@Ag

PMA4HAg

1.0000000000000000
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 0.0000000000000000 20.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Ag

40 1 12 1

Direct

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 0.4438651163605272 0.6730276901438917 0.3065078980924396
 0.5131151899075178 0.3902311067495262 0.2208908901128688
 0.5092977140739933 0.5634156521952197 0.3422103036068093

0.4414383219580378 0.5021458793588700 0.4298223240056521
0.5084381052931516 0.4365866701015209 0.3447149601973696
0.5691728765967414 0.5013836556272033 0.4349763752355741
0.4386212113183793 0.3544411766816172 0.4463846272108783
0.5784690155964868 0.6723128170461091 0.3120481204502307
0.3607898327307581 0.5664128198382183 0.3216837458496882
0.3598464672650274 0.4345295636117775 0.3243659806612120
0.4292601008946139 0.4982926238470060 0.2352131935080483
0.6589611367382681 0.5646771531649458 0.3339543615574061
0.5015609185285423 0.5869935637384118 0.5361398257079398
0.5689194229109864 0.3536569056203208 0.4515469678163351
0.5708127218993605 0.6499084344846711 0.4457332345463157
0.5004621850441890 0.4209924739071754 0.5394572765585138
0.6580407801100425 0.4327904525802157 0.3365671510573735
0.3770152327061744 0.6227854963205747 0.1916442046130778
0.3277307962666696 0.5686571676883262 0.4544959445603874
0.3268602148888378 0.4382277544691938 0.4572048210157559
0.2414643351709670 0.5020978139783184 0.3603629004052384
0.3751661935555344 0.3730444659602567 0.1965735872875853
0.4405085593271397 0.6506348144050857 0.4405501667114994
0.5082976244530465 0.7664354094312200 0.3895659046517024
0.3983792156920861 0.5049830723407126 0.5551815903610591
0.3701698237904958 0.3655067317796769 0.5685648190843738
0.5968381636038140 0.4973661810626573 0.2421716130322402
0.5761895941426596 0.3255846305019605 0.3188133507332949
0.6523877338585038 0.3715064260955850 0.2078896590398853
0.6541826853802039 0.6212284026311050 0.2032497159466709
0.3716918577020141 0.6451397598269395 0.5628760317599423
0.5048861117500567 0.2357654252580509 0.4004440093370540
0.6811825424662069 0.5665653878442448 0.4689159485918382
0.6803419338084279 0.4361935732547125 0.4717203849101730
0.7739889836098076 0.4988091266646884 0.3821720817589380
0.6295030606658325 0.6437241751848515 0.5732046228347154
0.6018084333616975 0.5037916036571930 0.5634701516220599
0.6272620370489594 0.3638545433833980 0.5789187957839472
0.5070842075488832 0.5008560086566338 0.3879553717928401
0.4264801889743183 0.5925912382332881 0.2536709880924858
0.3242142281795984 0.5018978592373361 0.3794388968786632
0.4250697884232890 0.4048497577920956 0.2573872169928743
0.5084538897487610 0.6827006053946129 0.3755200660107277
0.4015979165163539 0.4150153592839064 0.5068717393345518
0.5980382240846255 0.4038898712323864 0.2644531004537393
0.5994350723563852 0.5916543435755649 0.2609766591222837
0.4027084282822458 0.5928855800870799 0.5032746488432341
0.5061265572333230 0.3187793151285249 0.3827146346888964
0.6899669339287382 0.4996093875310519 0.3944428660148701
0.6027452479211017 0.5918261621234125 0.5112721878453433
0.6014477426697744 0.4137106892424092 0.5149449323164053
0.4983777420393986 0.5053610937038708 0.6054117019874389

PMA-4H@Cd

PMA4HCd

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Cd
40 1 12 1

Direct

0.5146917242342613 0.6035175725614228 0.2161461075591492
0.4418491363307556 0.3259060732930685 0.3121384364135057
0.4441336234609528 0.6734321189694901 0.3053505519597999
0.5131555861310763 0.3912542840925209 0.2201749200414587
0.5093072175052926 0.5634377583666212 0.3419265721919920
0.4418220253709867 0.5020845802717546 0.4299076393221338
0.5084383466986936 0.4364576535438300 0.3444052328080969
0.5686958285589520 0.5013174649123361 0.4350532171850507
0.4386962201268122 0.3525264570424762 0.4453498275700367
0.5783202812688366 0.6726884403533004 0.3108808139176434
0.3612606259850625 0.5665180974556320 0.3219916567913655
0.3603471657071584 0.4343587144566923 0.3246782835692130
0.4287614190502969 0.4982743933449247 0.2351465423730457
0.6585369638591083 0.5647973180779098 0.3341869778662719
0.5015033924009608 0.5897999007300813 0.5374118596941956
0.5689213072825301 0.3517138587181862 0.4505889004366985
0.5708446629927465 0.6517734765151533 0.4446753534938495
0.5003800976178672 0.4183815369939042 0.5408753583707523
0.6575771621596153 0.4326251512930598 0.3367751177041031
0.3769575378441866 0.6228110835308819 0.1914162238034062
0.3299717732718579 0.5686468427860993 0.4551339523290919
0.3291411449512310 0.4382249890257816 0.4578504228518047
0.2424940090522304 0.5020538438667326 0.3625844498376198
0.3750707882131830 0.3730455924554766 0.1962709417959349
0.4405343657805895 0.6524702209154881 0.4394362534617411
0.5084247902831227 0.7677151116111322 0.3878426023970075
0.4006534195904278 0.5050468659945152 0.5557299629283253
0.3712434462775856 0.3651354394065289 0.5689718320952577
0.5973983492669699 0.4973504487038226 0.2420977611692945
0.5760796771119122 0.3251764797547771 0.3175940612240064
0.6524604755991176 0.3715141518131017 0.2074959461325926
0.6542838554696548 0.6212873836157061 0.2029981470519579
0.3727405539787537 0.6456144365573423 0.5632525761851342
0.5050510441944889 0.2344332758009801 0.3984664583373896
0.6788335697411951 0.5665689276540027 0.4693200007937142
0.6779797681821804 0.4362521569366001 0.4721688672870991
0.7727998297850245 0.4987349987800219 0.3842777853224906
0.6284039803243401 0.6441967999546875 0.5735046755737133
0.5994660596492797 0.5039201424080364 0.5638212013846328
0.6261122817958895 0.3635749318130870 0.5793033114120691
0.5070779350125261 0.5007867491986286 0.3875184036447776
0.4263807911761447 0.5926974653378211 0.2535365489545230
0.3255060550872223 0.5018548949244030 0.3805560089501001
0.4249725158246860 0.4047493758710087 0.2572063502241008
0.5085084916963751 0.6838375753421929 0.3746478443512374
0.4042255472769412 0.4133426001494607 0.5069259343321023
0.5981639977892762 0.4038146348471602 0.2642004739070824
0.5996118615687326 0.5917598900596436 0.2608583461561730
0.4052506633722670 0.5945036857105644 0.5033210043291791
0.5062226938766140 0.3176557006202166 0.3817286370620326
0.6886065849826666 0.4995310363475942 0.3954355526932030
0.6002000368639545 0.5934585442449398 0.5111313164131451
0.5987648533413694 0.4121192359117227 0.5148299321354510

0.4980742710260201 0.5055596750574846 0.6095028352042650

PMA-4H-5d_TM

PMA-4H@Hf

PMA4HHf

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Hf

40 1 12 1

Direct

0.5146042717287319 0.6035817509797952 0.2176097245810627

0.4419536604932562 0.3261190720561478 0.3121151661153999

0.4440110581256875 0.6732382466189222 0.3057820652572961

0.5131341657116821 0.3921559199686991 0.2211933620350895

0.5091506976320681 0.5634353325006785 0.3452404664207188

0.4415780888878211 0.5021844108397946 0.4334729915146767

0.5082984691634578 0.4364181789428637 0.3478563713196323

0.5686454029820807 0.5014300276931436 0.4386440559557025

0.4374902871237422 0.3527726274106601 0.4456806609825678

0.5784931553408883 0.6725062087722372 0.3113090645054546

0.3607998643848694 0.5665150239745964 0.3220258252776595

0.3598552737127234 0.4348759763902825 0.3241938595982092

0.4302435567719509 0.4983774814625941 0.2353993192500786

0.6589600787718619 0.5647483366196220 0.3342101006275388

0.5013799126431469 0.5851611770704894 0.5399656338095649

0.5699592160049837 0.3519941361269653 0.4511024598003606

0.5717082688351027 0.6513125367888462 0.4454524924683384

0.5003008001573825 0.4231058982738640 0.5428483137472409

0.6580500281156949 0.4330907919294743 0.3363747874524737

0.3765146207892854 0.6220068930459334 0.1912922889552662

0.3272400452569236 0.5688915514531161 0.4547747444275985

0.3263342209845929 0.4381210296277965 0.4571979438258166

0.2403896334897450 0.5021109960328070 0.3600834114595761

0.3748126730775007 0.3733137264956815 0.1961295852970031

0.4396708914410896 0.6521030259153878 0.4400960919100330

0.5084785274225252 0.7674034153722099 0.3883271764561830

0.4039791923889306 0.5050939121120420 0.5595906577668827

0.3697871193712216 0.3650333491418714 0.5680998719209605

0.5959224704827477 0.4974709470336866 0.2421788472545160

0.5759793599723256 0.3253451509536979 0.3175318102891074

0.6528046240748049 0.3718223980908783 0.2074214761034255

0.6546415862748965 0.6204703778601027 0.2028044541179593

0.3713703765202440 0.6458540734257852 0.5625014533339081

0.5050414152572534 0.2347846609104351 0.3994002298962609

0.6816455000799124 0.5668056126975827 0.4692273971748340

0.6808055206823019 0.4359626146575316 0.4717185561707843

0.7750619610904947 0.4988216666990920 0.3819335117776056

0.6297834621925616 0.6443625563801655 0.5729943422199919

0.5958344430217712 0.5039436663390101 0.5674257627186678

0.6275875331732662 0.3634220527473208 0.5786503270299963

0.5069878771972463 0.5008461795938435 0.3902375672435123

0.4259036635092441 0.5922343374287882 0.2536841759787743

0.3230232442407899 0.5018783601278906 0.3793708423401631

0.4245788499368034 0.4045780721809393 0.2574343434202621
0.5085961340650957 0.6836724282899451 0.3740757738060835
0.4009695492393408 0.4128062429774911 0.5047203829823165
0.5985503169384409 0.4036688315886791 0.2644649637815726
0.5999417441931616 0.5912904217602709 0.2608807935442914
0.4020767879591938 0.5951133950783202 0.5012141089073758
0.5062459817026378 0.3177701222222272 0.3818465012210399
0.6911382255817152 0.4996225456079416 0.3944104385958145
0.6035801296098470 0.5939771156690864 0.5093681833643370
0.6022510801085291 0.4115475118802169 0.5129787486725185
0.4987647880864144 0.5051376621825576 0.5940565063165150

PMA-4H@Ta

PMA4HTa

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Ta

40 1 12 1

Direct

0.5146517759192376 0.6037123259680801 0.2178414740269333
0.4420695834473576 0.3259199474887601 0.3117092588951840
0.4440399287949481 0.6734149836659055 0.3056349796831330
0.5131897134332304 0.3923569508015753 0.2211941532209457
0.5091084128721396 0.5634644298472125 0.3458770612462380
0.4419586867802798 0.5021870452393763 0.4346764704639662
0.5082206686959762 0.4363367212446852 0.3485196037945963
0.5682906539593304 0.5014153898394171 0.4397049728249197
0.4375101499781420 0.3517340477587269 0.4457017085300901
0.5786250934275700 0.6726351775067761 0.3113550253925146
0.3610658554053376 0.5664081742979578 0.3220623903419255
0.3600757715238030 0.4350699622026039 0.3239956411687472
0.4305456615531219 0.4983845026492605 0.2352688909206732
0.6587364878097781 0.5647645225753221 0.3344746833867172
0.5012136199515828 0.5899865162443156 0.5447812334185876
0.5700266270212212 0.3509635902655282 0.4511549612636352
0.5717257271074888 0.6522749018325020 0.4456030101972873
0.5000777757454683 0.4186467293925537 0.5476667182200312
0.6578461538619181 0.4331770692226042 0.3364633334382980
0.3763677456305537 0.6216985334833776 0.1913856842414278
0.3274404130975304 0.5691736946117411 0.4547595476638354
0.3265977944869213 0.4378856862352281 0.4570569070660752
0.2404901142809864 0.5020900414597901 0.3603627412321231
0.3747035517521065 0.3734625038062733 0.1961006993225372
0.4397740293702716 0.6530567978389443 0.4402420849217160
0.5084898632145711 0.7679958893380251 0.3873637999612883
0.4056649350384814 0.5051071605480453 0.5593350781400109
0.3670455261628535 0.3629234635995476 0.5664869069289792
0.5960112736807368 0.4974825727848333 0.2424095590600614
0.5760123190427341 0.3252467568584246 0.3173553328647287
0.6528210394041351 0.3719183961109204 0.2074155057172775
0.6546987538133815 0.6202332454386034 0.2028811348153914
0.3685933300593179 0.6479977796533624 0.5608337933604133
0.5049947255679399 0.2341392562232852 0.3985225599297885
0.6814744670013152 0.5669681927209159 0.4693852615270384

0.6805911291592117 0.4358722904588985 0.4717900703478576
0.7747741703001984 0.4988219688042422 0.3820123972598881
0.6326620486340867 0.6464764616816469 0.5716306379232312
0.5943127219584906 0.5039651090913795 0.5670765593067879
0.6303552837532016 0.3612803453567380 0.5773353110161428
0.5069726526533632 0.5008122146123402 0.3907480720101330
0.4257235680144469 0.5919944473087140 0.2537490538121103
0.3230796803991937 0.5018302618348019 0.3797387887305857
0.4243941460755514 0.4045553864309711 0.2574942736702609
0.5085698045236768 0.6842648029312774 0.3735153075842060
0.4004960204784788 0.4109798930299425 0.5047967218804355
0.5984463071982248 0.4035496671058984 0.2644097150270096
0.5998666013911459 0.5912164558301209 0.2608363213716577
0.4014973661248435 0.5969841440796618 0.5012283157078160
0.5061566478380325 0.3172227781550196 0.3814879980759370
0.6908519680720303 0.4995982318948669 0.3944828155857045
0.6042472592764152 0.5958423706594014 0.5094323660617995
0.6027888936125162 0.4097023904731269 0.5130570730150131
0.4989653076451080 0.5051078595064751 0.5881960254263277

PMA-4H@W

PMA4HW

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo W

40 1 12 1

Direct

0.5149503258585124 0.6037917807694989 0.2184733918925021
0.4426895229784863 0.3259916031942179 0.3109011982270314
0.4444843504411673 0.6733967382212154 0.3051905813402929
0.5135207528194923 0.3929955742055285 0.2214413300133383
0.5089710895489001 0.5635375104506679 0.3471410169514045
0.4419566501792567 0.5023526326519202 0.4362230300854005
0.5079899715989157 0.4363181164978873 0.3499339283711227
0.5681793800516817 0.5015061653927259 0.4411025590690879
0.4375272269824034 0.3505674174638697 0.4456085799730208
0.5791301357580816 0.6724428242386975 0.3119908814233385
0.3609158252189966 0.5661461044341772 0.3213796192054491
0.3596994311074793 0.4356381384697003 0.3227657122571989
0.4320868912113559 0.4984276695468951 0.2342255792209330
0.6591620276718826 0.5650663787862201 0.3348818596314787
0.5010613926699018 0.5919549908356574 0.5481989904373765
0.5707529618749038 0.3498698629836886 0.4514998376868053
0.5723074772540885 0.6530409205325222 0.4459868611163925
0.4999683750859618 0.4172692866688734 0.5505441539602542
0.6583945528825182 0.4331105624401665 0.3365527382763904
0.3759961338799249 0.6213013193579808 0.1912199190747882
0.3272138048040878 0.5699236913134738 0.4537761789898726
0.3266236131571835 0.4372415718265897 0.4557877756907988
0.2394475458341273 0.5019619661850535 0.3612403897326266
0.3743636435298205 0.3734332077631399 0.1959359131920511
0.4399093475907283 0.6539718159660781 0.4402964932005800
0.5084003178725124 0.7684266544443790 0.3865366340670244
0.4069579634064907 0.5052038317314861 0.5608550410797246

0.3652357988956047 0.3620621591287772 0.5655773051843034
0.5966810557020504 0.4975808393417122 0.2431040555780941
0.5764372810598754 0.3256727024831443 0.3177802677867450
0.6524665660718749 0.3715263596524706 0.2069957864121611
0.6544064384938004 0.6203623117240771 0.2024752750821811
0.3669580254810806 0.6487433436151324 0.5600580215421790
0.5048103742288986 0.2335761348722683 0.3976859357355040
0.6818835857647043 0.5671056036126115 0.4695432874587653
0.6808550893218797 0.4359156880024025 0.4718091889905499
0.7751580508436322 0.4987534301101846 0.3815958823789734
0.6341319023634736 0.6471119716375570 0.5713804092470949
0.5928936869261298 0.5039954961386279 0.5684782251689875
0.6319000410106653 0.3606098903067469 0.5769530458379242
0.5068534194525668 0.5009200739414316 0.3917343394742636
0.4246953823256062 0.5913039649238523 0.2539462746718087
0.3219797689759540 0.5016955294973861 0.3803734223882939
0.4233639420258756 0.4046338946026723 0.2577812075197738
0.5083774883982694 0.6846254365220714 0.3730334654041602
0.3999272452623452 0.4098782029500762 0.5045554631537681
0.5979319240512709 0.4030594889540789 0.2638964928231844
0.5994997621647029 0.5912695534678152 0.2603218301918722
0.4007114427815280 0.5980155686734335 0.5007695251539251
0.5057767878149245 0.3168156400704802 0.3815447584614642
0.6910612439523957 0.4995166742453785 0.3933761739543853
0.6053457676555869 0.5968727330650881 0.5089956462549715
0.6037153675752855 0.4085474844280177 0.5125803381663532
0.4991916561311420 0.5052515256602006 0.5825641728120469

PMA-4H@Re

PMA4HRe

1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Re
40 1 12 1

Direct

0.5146056350349675 0.6041711414350110 0.2181705618065204
0.4421414140607191 0.3264947837674602 0.3124315392686513
0.4438400035352692 0.6729205251691588 0.3068799314615970
0.5131535897643914 0.3927282787208984 0.2209804968313816
0.5091402627300801 0.5632898552207090 0.3456043071991768
0.4415412537872227 0.5021813659246870 0.4340824849408183
0.5082938425244804 0.4364016677821815 0.3483433058496729
0.5686250685910521 0.5014249896682262 0.4392647801212755
0.4370130940951458 0.3535005903395111 0.4461241184746958
0.5785551293357120 0.6721616438947728 0.3123977228457505
0.3602386440484041 0.5668079238118440 0.3221635856295337
0.3592783141505704 0.4350289871020311 0.3236888968347961
0.4299574296812808 0.4984894228501673 0.2357578239220332
0.6595321329459866 0.5649856086331208 0.3343781711804478
0.5012162806350251 0.5865712769540263 0.5436189976292445
0.5703280805709391 0.3526866698197388 0.4515953061002106
0.5716550446717084 0.6503410389194010 0.4463910766915123
0.5001393956975666 0.4218134859201080 0.5460375274266170
0.6587214661383578 0.4332730797088671 0.3358762841873871

0.3767578003011608 0.6221467975515734 0.1915463894218432
0.3250615518120697 0.5689773481368918 0.4543698941288481
0.3243407066090059 0.4382675780836642 0.4564154150028251
0.2394243096477626 0.5020991456960132 0.3581758447078321
0.3751618110678566 0.3726312366481353 0.1962817278649600
0.4395464301650374 0.6511575452409269 0.4410496287881087
0.5084897899771006 0.7666231406071591 0.3889738679038997
0.4030006358752066 0.5051587614641661 0.5584815883981410
0.3666526055126170 0.3642683489215822 0.5668667968279580
0.5961529902786264 0.4975871654121173 0.2424940862648166
0.5757444666957798 0.3257713662332273 0.3178041002121802
0.6525564777930870 0.3711989480638598 0.2075625609034412
0.6544951015489048 0.6206058009171290 0.2030759842270399
0.3682651369028819 0.6469139351520000 0.5612727661691653
0.5050694016959122 0.2355996071364171 0.4003571569872082
0.6837973705050379 0.5668822770247164 0.4689579165571585
0.6827754878101983 0.4360604881817831 0.4710720855200803
0.7761985400737652 0.4987614445245322 0.3802479901434067
0.6329223308537898 0.6453569310671473 0.5720350162831490
0.5969355133204800 0.5039944176895219 0.5664351864756124
0.6307537062726336 0.3626337578815729 0.5777346557641784
0.5069495310449101 0.5008281761429622 0.3907456394878384
0.4259618242806234 0.5918660787472492 0.2537724810906088
0.3218453034862471 0.5017834176352146 0.3782704396754113
0.4247224357765556 0.4039942016431759 0.2576232899361746
0.5085703515150537 0.6829517475390579 0.3745326487523752
0.3982506011226192 0.4128790093060330 0.5045893522003149
0.5985122686122362 0.4031351048534187 0.2646782569760134
0.5999802140577799 0.5909381797274804 0.2610296369058772
0.3991188054190813 0.5952456977255050 0.5010573621409806
0.5062078866958980 0.3186356199856015 0.3832232946898135
0.6924166254156633 0.4994862741570773 0.3935142388532945
0.6064770825433512 0.5940266946544487 0.5094685517394058
0.6048917978163646 0.4115974234432738 0.5131255923505808
0.4989268314958099 0.5049740351634505 0.5879716292481523

PMA-4H@Os

PMA4HOs

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Os

40 1 12 1

Direct

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0.4419572704417811 0.3263109249556854 0.3126618945841982
0.4441643463759963 0.6730493663111168 0.3060470169796213
0.5131514544029661 0.3915671276263872 0.2213389959734672
0.5091505564936186 0.5635289957155962 0.3453275545576326
0.4415070036430207 0.5021983076445615 0.4336095872394141
0.5083115425391411 0.4365037944487268 0.3478135950392622
0.5686878847059192 0.5014526777381710 0.4388142479372032
0.4374358396892014 0.3532488158245380 0.4462684615394503
0.5782910064104309 0.6722916762620996 0.3115571275634812
0.3606547634230518 0.5664263967522020 0.3219073013064433

0.3598024813733751 0.4347561689014287 0.3243828021213754
 0.4301712581243118 0.4982954231656276 0.2355901539923664
 0.6591301827502560 0.5646325066129926 0.3340710062917902
 0.5011005167718290 0.5908757758431101 0.5473308869950785
 0.5699195702688334 0.3524999243799637 0.4516842969010529
 0.5718125600776123 0.6508392604347837 0.4459315442855737
 0.4999520300709942 0.4177292354800070 0.5504384885838556
 0.6581353220592278 0.4329824417380441 0.3365269728017041
 0.3766563026604370 0.6223862230728830 0.1915747899780516
 0.3257073678256573 0.5691077234113193 0.4545646043302227
 0.3248944710349038 0.4378859961432604 0.4570785857990819
 0.2401900441292470 0.5021054931630053 0.3593731691970850
 0.3748720538469831 0.3731824149231155 0.1964642550423100
 0.4394243373044684 0.6516332918810303 0.4406064888948234
 0.5084859097818635 0.7668141411470508 0.3888535847843206
 0.4035897007583507 0.5050907621884487 0.5583057460799168
 0.3658954472764752 0.3624706705825501 0.5662197751785499
 0.5959788128056090 0.4973845023547509 0.2423479713387171
 0.5759695497725767 0.3255590758445892 0.3180826795172967
 0.6528346464113177 0.3717309450988428 0.2077381886159301
 0.6545718237102741 0.6208078409058181 0.2030986330736594
 0.3674605966668668 0.6484163698191042 0.5605230716210631
 0.5051090773757053 0.2352165598012354 0.3995055776068366
 0.6830944862766198 0.5670141467505018 0.4691104449176050
 0.6821494403981342 0.4357191605761911 0.4716991117307711
 0.7752964598285923 0.4988160612239847 0.3813492563129333
 0.6337273075866914 0.6468215000336113 0.5714022895867330
 0.5965384955657009 0.5039678551761405 0.5662957980883379
 0.6315100404699854 0.3609001983308791 0.5771813488490477
 0.5069485378058606 0.5008923474376381 0.3904561894974483
 0.4260809901666673 0.5924389319236557 0.2537503454201060
 0.3227429451728647 0.5018845213329518 0.3788863669053288
 0.4247600518099344 0.4047273991032899 0.2574437292440488
 0.5085583374240774 0.6831714352284166 0.3747321005363453
 0.3984318029462302 0.4116804496828634 0.5050144556782027
 0.5984580487674049 0.4038156549817594 0.2644457813240049
 0.5998117833557933 0.5915090193086024 0.2609708661474086
 0.3994315947954679 0.5962389476959776 0.5015186421397199
 0.5062775398024044 0.3182385729907160 0.3820630238937591
 0.6914272141425131 0.4996025857599343 0.3939751231508503
 0.6061207157277907 0.5950505556197884 0.5098858822809685
 0.6046740186549294 0.4104608170429093 0.5135476154335158
 0.4992680572007620 0.5049469312186685 0.5817539460301653

PMA-4H@Ir

PMA4Hr

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Ir

40 1 12 1

Direct

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 0.4418259254486574 0.3266868126986754 0.3136131099497800
 0.4441597643839710 0.6726925272964230 0.3068467386559660

0.5131321927418877 0.3909546356850874 0.2208743894550198
0.5092211554894265 0.5632928587286703 0.3434191012727463
0.4414483270058948 0.5022163198059253 0.4315255578725183
0.5083498096440546 0.4366821213203732 0.3458915545845613
0.5689226352966845 0.5014216462622009 0.4366902807155555
0.4379417819641203 0.3546134695898214 0.4465990569686583
0.5782930572224374 0.6719524138201998 0.3123146902856236
0.3602821286843222 0.5667430202799429 0.3221528933801497
0.3594245241571272 0.4343303912000955 0.3248273684506489
0.4289507504560274 0.4983117803502441 0.2360279778200867
0.6594775648926939 0.5649674874326188 0.3344286078672867
0.5011348366353041 0.5885330901626449 0.5419641289227628
0.5695558236952217 0.3536981373572902 0.4519253363341693
0.5714703001593008 0.6496049067793987 0.4461031953329138
0.5003171642291973 0.4197424402546518 0.5453107253119232
0.6584932770635498 0.4325949500093532 0.3370144165679743
0.3771279446096559 0.6230781766752436 0.1919338143583678
0.3260389310562425 0.5685176386575481 0.4547457104152291
0.3253437400056967 0.4383628770787876 0.4573553438071709
0.2407876019334786 0.5021071802835396 0.3592132204873729
0.3752665285500218 0.3727176547418926 0.1968576920965359
0.4397280894450450 0.6504729140396807 0.4407717363035921
0.5084614830553605 0.7657145963440823 0.3903421644177649
0.3993559542076549 0.5051401298912451 0.5563941356379412
0.3672224618857316 0.3630965024874544 0.5669447655254977
0.5971696701202067 0.4973489432112782 0.2429056719396274
0.5759686618185954 0.3259557400241411 0.3191054324211935
0.6522763804082448 0.3711670541231313 0.2081295705614823
0.6540772830436833 0.6214750124536820 0.2034167530540200
0.3687244548075778 0.6478252907015207 0.5612111914854195
0.5049395465220575 0.2363537535219429 0.4008578105315163
0.6827111621856906 0.5664814699243849 0.4692705443034824
0.6818896458344353 0.4362842804770964 0.4719428618871825
0.7747708424294476 0.4988378983818173 0.3810060823925568
0.6323596555730568 0.6461448931102104 0.5719284008245021
0.6007043157535875 0.5037541042235433 0.5645677164024023
0.6303359656528399 0.3613555433941624 0.5776644687572819
0.5069935916578939 0.5009112730144202 0.3892426460619817
0.4266025169830884 0.5927696239293264 0.2538711997688519
0.3234309213565571 0.5019429961931849 0.3785867755674682
0.4251656943271149 0.4047269367419292 0.2575541721330681
0.5085562645539345 0.6820105773391740 0.3762405356488250
0.3989608119482680 0.4138002723844553 0.5064903402463035
0.5979571109976921 0.4037498616061106 0.2645792834910584
0.5993504787344450 0.5917765488277219 0.2610855569196157
0.3999109216601787 0.5943321686821786 0.5029129108324745
0.5061024990589233 0.3193783991413972 0.3832953815363893
0.6908362432237343 0.4996258301541184 0.3936434286546753
0.6054249902002006 0.5929525572336467 0.5112785868359064
0.6041947768198613 0.4123361769307015 0.5148099522138626
0.4990926162473271 0.5049661412414668 0.5841502417321163

PMA-4H@Pt

PMA4HPt

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Pt
40 1 12 1

Direct

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0.4418601601676899 0.3261991200752795 0.3130289904654703
0.4441373383903301 0.6731135783787977 0.3062981545712062
0.5131635768818275 0.3908298845966844 0.2205677236195189
0.5092533194343514 0.5633403899479773 0.3426366384778992
0.4417381823343073 0.5021009244756741 0.4308190181613001
0.5084025736221469 0.4365825878009433 0.3450425366538759
0.5686866579711731 0.5013419496870719 0.4359624821427227
0.4380556800062737 0.3537155708679006 0.4461790624134733
0.5782826963870356 0.6723554364746027 0.3118189060379083
0.3610251625788149 0.5666752469371343 0.3225467044230864
0.3601420826158045 0.4343411681628654 0.3251965983996791
0.4288623997442186 0.4982754781936284 0.2358626342794221
0.6587282475883660 0.5649387098068467 0.3347513972930228
0.5011528174294336 0.5968610802205631 0.5459088663712124
0.5694194153429686 0.3529245230767033 0.4515383647138061
0.5713725025172005 0.6505132390608634 0.4457675745963443
0.4999763560705324 0.4118156895518027 0.5493515715008354
0.6577334428601304 0.4326271924897164 0.3373556022269785
0.3769099610114819 0.6226895907412414 0.1920067902979644
0.3278084978400022 0.5686989586825991 0.4554785599449770
0.3269795155765644 0.4382818166550504 0.4581358640670916
0.2420727727116510 0.5021517951463087 0.3609414235736413
0.3750616742631797 0.3730981759593522 0.1968353299137945
0.4399169042254649 0.6512606378811052 0.4404328166617809
0.5084026774701796 0.7663894849226117 0.3894000558666649
0.3993804193221021 0.5050701261534565 0.5561546033882648
0.3659168392162372 0.3616713292424303 0.5667266759435703
0.5972599965874786 0.4973517548049781 0.2427940805474989
0.5760230209584832 0.3254481677376266 0.3184858398204073
0.6524959459478273 0.3715946005576125 0.2081124683645763
0.6542287849337186 0.6211368157089552 0.2035256257654705
0.3674015569104205 0.6490885064840952 0.5610194033285566
0.5050027328481980 0.2356381861384031 0.3999678365499610
0.6809557156568393 0.5666355190149986 0.4698663342286090
0.6801170328896629 0.4361819865872992 0.4725961739174289
0.7733488785891530 0.4989015715103969 0.3826479725323602
0.6338488530208003 0.6475761490932731 0.5717738826072654
0.6007471550438496 0.5038783830801593 0.5643596754630303
0.6315499639818037 0.3600261450655035 0.5775385280025273
0.5070336304647348 0.5008150074674246 0.3884348319149574
0.4266558982861736 0.5926727711207528 0.2537936110651504
0.3248743131142074 0.5018900362015123 0.3796497103089232
0.4252787285164921 0.4047638388381181 0.2574446327301559
0.5084826881138396 0.6826861791190156 0.3754820232914887
0.4001826998375720 0.4119439700615662 0.5074131807363582
0.5978963245469142 0.4038475192259783 0.2644766895151798
0.5992692064253117 0.5917325016918075 0.2610373481317001
0.4011741222772688 0.5960094769062032 0.5039199475857704
0.5061943957404559 0.3186491891510486 0.3824585397852722
0.6893104332443027 0.4996598598064943 0.3945995799666386

0.6041864110630699 0.5948695731821542 0.5121075661668764
0.6028124514573356 0.4106898566070368 0.5156840246826874
0.4994671509912679 0.5048839290052241 0.5761515186667602

PMA-4H@Au

PMA4HAu

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Au

40 1 12 1

Direct

0.5146464396801644 0.6039544455927340 0.2168178936026184
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0.4439503460693404 0.6735656555963678 0.3061607370961015
0.5131465306365668 0.3907863533692922 0.2208466106907647
0.5092611309459415 0.5634236201915302 0.3423537108449465
0.4420312453769498 0.5020607599588980 0.4307250000411219
0.5084075340804733 0.4364198386429882 0.3447524487120865
0.5683994709917678 0.5013095209125951 0.4358626448713308
0.4381157670407092 0.3514457057061350 0.4463786184700882
0.5784595356037114 0.6728342649045761 0.3116791429564494
0.3615703475036036 0.5666052140806727 0.3227290806980347
0.3606861465251679 0.4344085627287020 0.3253602532152417
0.4288812505669595 0.4982845887495401 0.2354174455552275
0.6581487714572873 0.5648805541295877 0.3349042792447154
0.5011779821485134 0.6013566157445588 0.5467557786902293
0.5693094791399252 0.3506923357168475 0.4516994025460083
0.5712656529559855 0.6527710392615860 0.4458148078380587
0.4999188687373095 0.4071515360971892 0.5504474798226464
0.6571686009014748 0.4327176829167367 0.3374737086836663
0.3768081429419205 0.6225591829731966 0.1920230527120802
0.3295790269904139 0.5689857941282060 0.4558714465597378
0.3286997542459954 0.4379396992533434 0.4584906228484654
0.2430143680561120 0.5021211315587675 0.3628365313989795
0.3749713206405794 0.3732053450704775 0.1968707445169088
0.4400342997629251 0.6535431790957782 0.4405219602282968
0.5084573642141936 0.7679535365437595 0.3876138351232737
0.4003420085794440 0.5050622550883307 0.5560245885653685
0.3649123170838374 0.3606039338403709 0.5665267346817632
0.5972451880187033 0.4973545833454758 0.2423620402678531
0.5762122390469246 0.3250028433661040 0.3183941864361976
0.6525932717084071 0.3716891983785281 0.2081656418555738
0.6543281716135461 0.6209937522394218 0.2035749304596963
0.3665152202216345 0.6502474607702809 0.5607388977455520
0.5050631277631802 0.2340770253083543 0.3981816781195315
0.6791894050578603 0.5669837216449821 0.4700736796901729
0.6783663651971552 0.4358608845839118 0.4727825837528609
0.7722617185848794 0.4988795762055866 0.3844579874559940
0.6347885621501372 0.6487941832909557 0.5715478881667346
0.5998678211783470 0.5039068496719687 0.5641424865650934
0.6325314506049501 0.3589227520425259 0.5774139430646694
0.5070429009598667 0.5007812575472261 0.3880294241213421
0.4265361647705907 0.5924917369285150 0.2538427327586363
0.3260058538693688 0.5018982199154212 0.3809084373375338

0.4251668740048655 0.4049576119247750 0.2574955709652880
0.5085472246407180 0.6841857283272206 0.3743467973906298
0.4016028969292014 0.4097811608546647 0.5078023357085893
0.5979976098345274 0.4040221638720234 0.2645402305380588
0.5993717323746703 0.5915182933350479 0.2611013180868322
0.4026636795061183 0.5982198712394401 0.5042069625406908
0.5062189264601089 0.3172313045716513 0.3814428954359623
0.6880900670859598 0.4996686423352091 0.3957884554299984
0.6027434819032699 0.5971311031195471 0.5122663364106832
0.6013174535699387 0.4085336441596125 0.5159652665032064
0.4996075547091193 0.5047660710614905 0.5731416646842979

PMA-4H@Hg

PMA4HHg

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Hg

40 1 12 1

Direct

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0.4419110495161780 0.3258215835157473 0.3118137548951366
0.4441066365094002 0.6734487489337122 0.3053397115506225
0.5131501543038937 0.3913509358802068 0.2200542700341793
0.5092993022912823 0.5634294741891100 0.3422864061484895
0.4417608132431067 0.5020900494089565 0.4302640329172754
0.5084268813359902 0.4364362814427990 0.3447654834876780
0.5687480804076386 0.5013171534517092 0.4354100402162495
0.4384171976035982 0.3519882041950829 0.4449536183987068
0.5783353057281962 0.6727179639574513 0.3108652025639941
0.3611926893287119 0.5665630017745288 0.3222462564324309
0.3603283873359161 0.4341943782120956 0.3248536135236792
0.4286894655473819 0.4982963032149112 0.2354080126827949
0.6585725941170681 0.5648332706572445 0.3344518570325700
0.5016065804362688 0.5910269843782837 0.5354538077263634
0.5692284322204426 0.3511630501583002 0.4501899287844038
0.5711808545381281 0.6521547960298284 0.4444397612221853
0.5004508933150339 0.4174064944360502 0.5389153182509419
0.6575639766009623 0.4324588043808382 0.3369463365425598
0.3769581972675544 0.6227093337814323 0.1915150913266113
0.3296776920619571 0.5685076468907970 0.4554911635373066
0.3291788252525452 0.4384606132068855 0.4582619344567744
0.2425289265220578 0.5018375867806020 0.3625135201672016
0.3750974243748129 0.3731459260227320 0.1961819114289748
0.4402472191426168 0.6528409088317655 0.4392074094667058
0.5084100316486427 0.7679348806715214 0.3876029494002978
0.4001856261933545 0.5052844745968825 0.5567159742854328
0.3713560349057599 0.3646994321184379 0.5687117051070189
0.5974317540706048 0.4973672764475219 0.2423605351424719
0.5760148545916330 0.3250848565577845 0.3172670554265788
0.6524362073565406 0.3716107259714441 0.2074155937806075
0.6542976038747900 0.6211875533007275 0.2031240819853385
0.3724269380928479 0.6462187927549405 0.5628595260863283
0.5050414026814680 0.2340730821345772 0.3979804969009474
0.6791121844485958 0.5664334394797478 0.4696839827150402

0.6779037707680503 0.4364846810935404 0.4725741019241907
0.7727729886101671 0.4984877931395565 0.3841965417073194
0.6287936779527353 0.6448181661095694 0.5731028851553157
0.5998844572955219 0.5041658910985811 0.5648611412220056
0.6260126713924149 0.3631358457875740 0.5790102074131884
0.5070730074816332 0.5008029611799630 0.3878905864562636
0.4264063954133726 0.5926623522125655 0.2536035880386547
0.3255532103279337 0.5016994371746468 0.3804063521057920
0.4250531567263784 0.4047096576576200 0.2571256069641052
0.5085105045132187 0.6840414585363809 0.3745596418461579
0.4042956657253543 0.4128753836906608 0.5066869505076367
0.5980596026647225 0.4037621999438402 0.2641050052986805
0.5995750167746300 0.5917211724052979 0.2609322320914453
0.4048041464722920 0.5949269647902509 0.5030841384074720
0.5062077784397002 0.3173584883980539 0.3814930396151128
0.6885758910010685 0.4993598241266291 0.3952796145921874
0.6006915493383731 0.5938975725335920 0.5109058793402971
0.5986929799476927 0.4116358424589323 0.5145621002979199
0.4979877939266639 0.5060531863384120 0.6123722106171565

Fractional coordinates of adsorption geometries of one CO molecule on Rh, one O₂ molecule adsorbed end-on(η^1) or side-on(η^2), two CO molecules or the co-adsorption of one CO and one O₂(η^1) molecule

PMA@Rh-CO

1.0000000000000000		
20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000
O	P	Mo Rh C
41	1	12 1 1
Direct		
0.5148618957439525	0.6023220323785079	0.2146748742847399
0.4446263371494969	0.3252080011769761	0.3139451996068857
0.4414950169463304	0.6716569160444722	0.3017591904159835
0.5168218213085117	0.3895210826499898	0.2221685752470129
0.5073710786738230	0.5635806340407968	0.3412835760868639
0.4383608306127629	0.5019942336964159	0.4277374879709089
0.5087381827012688	0.4367367455293362	0.3452987753730898
0.5664518578882700	0.5036396586495057	0.4358371832697394
0.4375521506394208	0.3539467500049900	0.4460819394869364
0.5752710570357876	0.6733684238911306	0.3102933400356974
0.3590097997615743	0.5642709688200883	0.3174735659735794
0.3600006756025327	0.4319595836672154	0.3219428618462367
0.4302707695445554	0.4957417774000584	0.2336595470123629
0.6575800955176087	0.5677893388736754	0.3361273407180410
0.4951689204312344	0.5830957167656665	0.5313801191060920
0.5683923905195366	0.3558350434051487	0.4545122703868532
0.5656462958324023	0.6530225555050969	0.4440253394798470
0.4965278609982757	0.4255547374219091	0.5374866519200422
0.6589482861541032	0.4354547577668460	0.3405924573250790
0.3775570079012803	0.6189026982942220	0.1866734041305048
0.3238264639007879	0.5669636095324755	0.4501713627598208
0.3238077575102611	0.4370334127148513	0.4541173498629615
0.2400621844385107	0.4987479863119940	0.3545688352330955
0.3797828818205997	0.3688343053647912	0.1953752338053384
0.4346293693662350	0.6516290866490337	0.4358356393006122
0.5020702572471459	0.7673836912872156	0.3854355511509698
0.3948230315246360	0.5054193796208188	0.5548621238038023
0.3667542694882695	0.3656620533194183	0.5666139643143681
0.5987873547572599	0.4979487254490206	0.2441935208660078
0.5790514803853097	0.3268099693622869	0.3221516546356870
0.6565522839582680	0.3726041367649904	0.2122012573556800
0.6541012048179050	0.6225454456908049	0.2041261405002702
0.3659823809174508	0.6463367824510160	0.5576727932317750
0.5079747146849830	0.2363985528531589	0.4027616859348139
0.6757291903858819	0.5707822769395180	0.4722474797755996
0.6781958460769311	0.4412240655890762	0.4764438500649638
0.7723208366745201	0.5046564368216375	0.3875768644864532
0.6188887586666288	0.6490539026010649	0.5733112536305879
0.5930034646939589	0.5076397707861920	0.5677356098990248
0.6234946044668934	0.3688447801309032	0.5828894381404892
0.4770793593459819	0.4261477550594952	0.7205456858895454
0.5052364249757885	0.5015203207393366	0.3876139637468443
0.4261017306560951	0.5905088361556572	0.2502003805143676
0.3224941344267148	0.4997842713083953	0.3748186233699588
0.4277384821558559	0.4025807041988296	0.2567310104580309
0.5039146720469214	0.6834957754296026	0.3727522107000351

0.3978300958520891	0.4143341719545593	0.5040074601630550
0.6005487534565871	0.4049799548744838	0.2671349452081865
0.5986757870826530	0.5929010043010211	0.2610988333302625
0.3976963590772483	0.5938462927543839	0.4986239306968506
0.5080314741683720	0.3192933373423669	0.3844069492862086
0.6880268007240291	0.5039407696236128	0.3975000269620140
0.5957667993869427	0.5959359739328112	0.5110013903592207
0.5992038759864196	0.4171687650458739	0.5171104720520032
0.4915687515316576	0.5056698768203759	0.5921972998792424
0.4839258483814824	0.4528220942368701	0.6700115439553458

PMA@Rh- η^1 O₂

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Rh

42 1 12 1

Direct

0.5151623009617810	0.6040746769167481	0.2179764801975551
0.4420768932996236	0.3265195096824008	0.3143493981847679
0.4442895203669456	0.6727540495846757	0.3074503071235152
0.5137823591798258	0.3907272529336912	0.2222203520816583
0.5089930871699547	0.5632685753574592	0.3440798258841382
0.4408954763193778	0.5020766321396432	0.4317507883320241
0.5082082369904589	0.4365260643721790	0.3466197169546874
0.5681764131132357	0.5013769793113578	0.4374755271226299
0.4371154345149095	0.3536922313499437	0.4469914023926906
0.5785859703426930	0.6719347285958348	0.3136464236630372
0.3601467738940387	0.5664294622397343	0.3222509446880954
0.3593380609119765	0.4344876133924308	0.3249183499742510
0.4296110794051303	0.4982585582298471	0.2365588327073746
0.6592856176692384	0.5649047604207577	0.3361162383466173
0.4996835352361758	0.5876155139709457	0.5400819794581803
0.5682548808399591	0.3533666350213884	0.4536199583709739
0.5702162745596659	0.6499332426529377	0.4476267720171667
0.4985912311247482	0.4205244423716414	0.5435002102210363
0.6583589819446699	0.4326801550102328	0.3387725251767460
0.3776792552102330	0.6228744976313947	0.1923968574220281
0.3262628480262541	0.5685980538164284	0.4547954938501962
0.3254137982175780	0.4381135294843952	0.4574266295564788
0.2405672774194443	0.5019393026758074	0.3598245352358315
0.3760532001892522	0.3726639844270181	0.1974198347143521
0.4389909182715682	0.6511864256329040	0.4410515385599305
0.5086524695279646	0.7661354920555974	0.3907469987334881
0.3979767214894278	0.5050024747169806	0.5565183425372809
0.3671296437196989	0.3640481979854976	0.5681815484519600
0.5978164533593318	0.4973054788454299	0.2440694353932123
0.5763232066882001	0.3258104919263594	0.3205504401520517
0.6528504174876925	0.3711101387373222	0.2097091133180014
0.6545034607551570	0.6212610570508058	0.2047131902370628
0.3687964754609809	0.6466507877218060	0.5624889656089036
0.5051594844270290	0.2357928344918621	0.4014904531868476
0.6805209331506646	0.5664678753577983	0.4717432675309601
0.6795973204451112	0.4363122413774146	0.4743636267075466
0.7736987827760411	0.4989395509505551	0.3846377709954212
0.6288685912075556	0.6445353310569043	0.5752851422003021

0.5980397508453489	0.5038621923404419	0.5661267010023865
0.6269002636237321	0.3632364338346425	0.5810086162163359
0.4935662352390994	0.5074042629111576	0.6827282264273485
0.5446599828802218	0.5078402261550605	0.7199679106281451
0.5065676667681559	0.5008073557752353	0.3897786853219776
0.4266466848594845	0.5926144995387307	0.2547300671447897
0.3231860896780279	0.5018194341369631	0.3793326472734163
0.4254352065520426	0.4047385838611604	0.2584982050802693
0.5085761478614163	0.6824033584554520	0.3768733057296606
0.3992923569868038	0.4134592167690397	0.5069012054585745
0.5983281749973085	0.4037309876856865	0.2659464082284227
0.5995534094568030	0.5916217048315752	0.2621653453734899
0.4003869214551232	0.5943971176701504	0.5033054643750762
0.5062081886504842	0.3188687652540946	0.3841713947140304
0.6896061862787788	0.4997683329406685	0.3960588682879796
0.6026563270131656	0.5926690236565243	0.5132038371647710
0.6013896894953430	0.4128614474518729	0.5168415974911682
0.4961771086850535	0.5050781102354091	0.5893422517931768

PMA@Rh- η^2 O₂

1.0000000000000000		
20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

O P Mo Rh
42 1 12 1

Direct

0.5144060826079511	0.6036123329246357	0.2169308286758008
0.4427341756675452	0.3263029619129817	0.3131225299575541
0.4443687627742837	0.6724388495947230	0.3069063509591745
0.5133690962388791	0.3909432895368719	0.2202390466962386
0.5095454667908424	0.5631915461920898	0.3430807445083245
0.4413892867082311	0.5014648382066766	0.4301496570964162
0.5089523390081994	0.4364854089916353	0.3449314740747375
0.5696316885204864	0.5008973221673817	0.4354411245357410
0.4391164438312012	0.3540416300139047	0.4456102634451621
0.5784447594580275	0.6721676527050331	0.3121274576300679
0.3601354537234031	0.5660921263866362	0.3225921686656478
0.3594299125547873	0.4336463770818127	0.3247833205576246
0.4289429160601104	0.4979676763650092	0.2364202280368744
0.6596289574486222	0.5648502119350898	0.3336554631199220
0.5017892071646187	0.5816342504058742	0.5336704559223772
0.5704046995990099	0.3532228169091648	0.4515265687638352
0.5717602839508577	0.6498654521622573	0.4458431155225726
0.5012500246219589	0.4257521180234249	0.5369589763991286
0.6590235601400627	0.4324574724672079	0.3360205492210100
0.3766742820120715	0.6223398697433216	0.1924921290938194
0.3270283112220226	0.5674803120143241	0.4555554537031402
0.3263780643538816	0.4377101467432638	0.4580948269391895
0.2410003721375921	0.5008038785339838	0.3603380269095340
0.3757095206080381	0.3724139813446494	0.1965760092954730
0.4398628938331531	0.6501661517844670	0.4403521884233386
0.5083524951289269	0.7657354855357724	0.3908042165348852
0.4003001353204264	0.5044233782945247	0.5579734949638481
0.3720536453382720	0.3640567051572066	0.5681885009481904
0.5975307514655628	0.4976715327858424	0.2421096639906224
0.5770521610199119	0.3261694150014728	0.3179596563086680
0.6522418407746482	0.3722921453953611	0.2059855630062916

0.6533478615900413	0.6222393491553305	0.2026121882101555
0.3724583871179635	0.6450563860273851	0.5630011487190631
0.5072225267101393	0.2359902573385188	0.3998142579045736
0.6819001934266329	0.5659717970752897	0.4692070785117516
0.6815421136653784	0.4364237864923425	0.4721159996697507
0.7745300799589832	0.4985200060813392	0.3811852016851291
0.6291315767588075	0.6437930404791521	0.5733448958572270
0.6006148016588990	0.5037183909723195	0.5662389047929576
0.6270214457987823	0.3636065001871900	0.5792921509554733
0.4929368936595940	0.5416114177483691	0.6877328045745698
0.4931247977700844	0.4758747993324904	0.6900084182124571
0.5073314723983958	0.5004947100874241	0.3884300209987920
0.4262462524134614	0.5923302160747013	0.2544423563439008
0.3237661811979258	0.5008159039246083	0.3792621130401210
0.4254798485686784	0.4041933905420977	0.2575087247043444
0.5087609628139629	0.6820743847498547	0.3764975515668270
0.4016363066164441	0.4138030668143780	0.5057920579099285
0.5983092955292489	0.4043729436203031	0.2631053968312742
0.5991675216335118	0.5924069790436476	0.2606652325058404
0.4018766334640977	0.5927288855894430	0.5026997149521188
0.5078979595487991	0.3190883020733736	0.3824595714002740
0.6904895602656198	0.4993523019805539	0.3930979925853778
0.6040802045522102	0.5917360144458731	0.5108761251749416
0.6031512915840600	0.4133672819613498	0.5144956754901636
0.4988983702146665	0.5048724598860731	0.5916543804977746

PMA@Rh-2CO

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Rh C

42 1 12 1 2

Direct

0.5111553655698100	0.6027694838606367	0.2149242694701615
0.44691571105862590	0.3242054022331459	0.3135462229513138
0.4393218293601917	0.6709387036615384	0.3047734896265730
0.5158760282752178	0.3904327102688283	0.2206583970100339
0.5077273230163606	0.5632905261215301	0.3409013470108611
0.4412956209003012	0.5007265623395616	0.4283308429402933
0.5103416021530698	0.4363604380522655	0.3443398279638401
0.5703877797038983	0.5035545512185138	0.4329328359666683
0.4432710039139202	0.3522250082295301	0.4467789693596776
0.5734660406183590	0.6738093570700543	0.3089938944239810
0.3586504300225079	0.5622287466865988	0.3218923464213472
0.3617803405885380	0.4297009526570545	0.3257006248181518
0.4280671815956328	0.4955071273974032	0.2355703672738988
0.6572453208587342	0.5692987860563121	0.3326832773775353
0.5004921539282827	0.5793322567575441	0.5292726396932268
0.5740872918394982	0.3551625573664190	0.4510089326397068
0.5673391996459587	0.6527135364334326	0.4435190701460625
0.5038854191256219	0.4301675408671626	0.5330791884905123
0.6603613001572994	0.4367669053387987	0.3360366088449092
0.3729518058187907	0.6185968402397708	0.1911438184869748
0.3272971371868573	0.5634093021413897	0.4561867786643335
0.3302422100352810	0.4338840989257636	0.4596686844163240

0.2422354881624707	0.4944089314695175	0.3628773105192164
0.3782720507132384	0.3687408813956988	0.1973539155978588
0.4366133609016560	0.6498043457387477	0.4383890654835034
0.5021815626795227	0.7667584131106705	0.3868055790033139
0.4020510402352098	0.5031264459061231	0.5598340460443434
0.3795890708945688	0.3634859245259504	0.5712781162308785
0.5974758162825718	0.4987429769010014	0.2415572931765065
0.5809914795348505	0.3270924881547779	0.3188084463005784
0.6553690611883080	0.3736110620225440	0.2076773374839291
0.6500964022487381	0.6234184244031327	0.2004248788836638
0.3734624044961651	0.6422001268389789	0.5634708565053307
0.5122979713609622	0.2355362129380156	0.4010491490276655
0.6789651105747384	0.5720807547334696	0.4686852865692536
0.6819674579630050	0.4425836606237036	0.4721200267488425
0.7736426167765291	0.5069042846851349	0.3817370580866529
0.6219248118835199	0.6480622654925953	0.5726967843182901
0.5999646209315262	0.5079697682770387	0.5669153254254959
0.6280216096036610	0.3694413723363488	0.5797795440557164
0.4897807860376623	0.6167579956506367	0.7047132281959664
0.5009106589418069	0.4004760685447691	0.7095522031750870
0.5074253398516509	0.5009828552755429	0.3869539810219340
0.4235988632511444	0.5902360615262997	0.2530786347685775
0.3253353271105257	0.4968617869644235	0.3802542965669785
0.4275956174667419	0.4023341300495671	0.2577345526625059
0.5045561939558385	0.6829445076957766	0.3733970142294061
0.4064194117903259	0.4128098431608417	0.5070869090273245
0.6004887131985390	0.4050296745016089	0.2642956932256432
0.5965189260277903	0.5928948700686457	0.2587706834213065
0.4028375308743612	0.5912174192107120	0.5016564223737903
0.5110186725401665	0.3185296123789915	0.3831551581270896
0.6894914813845201	0.5051870850056546	0.3931580607356056
0.5996198385659111	0.5954295544339174	0.5094225071787024
0.6033278538643998	0.4170977504385047	0.5134341022383216
0.4996602107761757	0.5064015914811009	0.5987467143541672
0.4941229005556093	0.5763705269440350	0.6643663836875457
0.4999517964751783	0.4393789311922751	0.6675610525525946

PMA@Rh-CO-O₂

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Rh C

43 1 12 1 1

Direct

0.5169119967185413	0.6041151679247559	0.2157854696729059
0.4394898191967496	0.3270244412003433	0.3107586944206184
0.4463844395981120	0.6735524705738715	0.3053797776881768
0.5124354278668776	0.3911553745821975	0.2193246832581821
0.5099573936530433	0.5629905034200038	0.3413927627848015
0.4397730203638134	0.5020594922547660	0.4270678763288139
0.5073786851205347	0.4360051957294653	0.3432293079443629
0.5685879994528809	0.4995792269212124	0.4337363348194256
0.4354763818648797	0.3537997870394922	0.4436401088680526
0.5805148526645123	0.6712791433878011	0.3118244398559419
0.3612482799318529	0.5685556827304450	0.3198716156299283

0.3585295924689428 0.4361522730171845 0.3221721598219160
0.4294482070262026 0.4995328781693629 0.2338758953571662
0.6600309160693090 0.5629910582824756 0.3348662961803727
0.5008898897668408 0.5774248033407482 0.5312416493611646
0.5662688627079009 0.3510374679233817 0.4500493600334304
0.5718699335951432 0.6488297003521915 0.4456454387973287
0.4980736364859974 0.4261248708531777 0.5323158141261600
0.6573903871317077 0.4305193760975515 0.3368363956517018
0.3798696855201164 0.6248160092162831 0.1896403489915642
0.3283931977258315 0.5694200971761765 0.4537827031808046
0.3247064676363725 0.4398730384421468 0.4553450979872724
0.2413039504403098 0.5058976116955414 0.3583469166101188
0.3744825764355541 0.3749668749557205 0.1939917186774021
0.4413769348387491 0.6512686564420203 0.4393316166613148
0.5110063144263715 0.7660430946290571 0.3892776635705628
0.3989265523058718 0.5041632818409230 0.5571132310062507
0.3689839112767838 0.3660059078334075 0.5665541183305762
0.5979172121390851 0.4964136878955503 0.2424597452188062
0.5737477345349762 0.3243651869178759 0.3172212633457174
0.6513531437423373 0.3698354849388436 0.2074731623422336
0.6566057211446473 0.6196974541147476 0.2037414500629958
0.3748588813376389 0.6450611806731967 0.5624266515080562
0.5007645885627218 0.2346990594695976 0.3973446899712593
0.6796514604473158 0.5627167645421877 0.4710131018024238
0.6782095073193524 0.4331417966995657 0.4727965152334092
0.7732449560010186 0.4954333033738381 0.3842738266885134
0.6258854549440928 0.6403207042329133 0.5745772700058974
0.5963952316703675 0.5004403223361171 0.5670822466667143
0.6207503131310188 0.3608736719828756 0.5788056866614812
0.4863084175687625 0.3993717113540535 0.7094275919642292
0.4713419498164715 0.5776302273228234 0.6693287294208293
0.5253075549428133 0.5987706516198795 0.6938788492169278
0.5064043755527503 0.5001639007367658 0.3866182880776224
0.4283681398394321 0.5938193085234000 0.2520437280449137
0.3241388224363235 0.5042720147124441 0.3769383428700429
0.4242119037965046 0.4058908924482109 0.2554402200086691
0.5103652949147321 0.6823470971050867 0.3750650110354575
0.3991031226713057 0.4148167521208783 0.5034676442692133
0.5970559702258306 0.4027223413673510 0.2638184325416988
0.6010098565157678 0.5906506130539927 0.2609252072974526
0.4040572715809954 0.5933073417815852 0.5013941719498751
0.5032914370982884 0.3178914887715073 0.3806000637722901
0.6889966762081903 0.4970709809857553 0.3948961420026009
0.6006759692799177 0.5895550749765608 0.5109259183308674
0.5985815614530060 0.4107337067182193 0.5133002551048477
0.4957979218176157 0.5015738931217362 0.5959915371070170
0.4903302750169127 0.4364798110707257 0.6659067978616202

Optimized fractional coordinates of the Rh@PMA Catalytic cycle (MvK Mechanism).

IS1

PMA4H-Rh

```
1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
```

O P Mo Rh

40 1 12 1

Direct

```
0.5146576386747326 0.6038971215294322 0.2168078878529396
0.4418202328774972 0.3265942622310100 0.3135598094022834
0.4441138035619731 0.6728196632398284 0.3067504869694361
0.5131366571669926 0.3909289188382111 0.2209478191172618
0.5092525015112870 0.5633326923672225 0.3431844126159496
0.4413561081595592 0.5021759232337001 0.4308831384790817
0.5083890052903409 0.4366799913783297 0.3456559272851080
0.5690929711901103 0.5014138678848847 0.4360466344504060
0.4381981213085563 0.3545175453052118 0.4466124502172239
0.5782788510104009 0.6720477043073865 0.3122609596826111
0.3604671563338194 0.5666042665945946 0.3222465202620886
0.3595437723362291 0.4343948179110275 0.3249218102410286
0.4288180059929098 0.4983123391798812 0.2360131408406189
0.6592845591229102 0.5648634507584002 0.3344877685151170
0.5014208402952031 0.5845301942460490 0.5377565267651825
0.5692294015549422 0.3537602904753525 0.4519400192107174
0.5711912940286058 0.6497501796371419 0.4460868345062643
0.5003625909469734 0.4234847645408600 0.5410233012507106
0.6583387052049675 0.4326259269561090 0.3371091812766989
0.3771161931510139 0.6229769070592637 0.1919582323547239
0.3264732653296470 0.5684942206825270 0.4550561268937767
0.3256252638219170 0.4384472002396845 0.4577360692810923
0.2410039314657672 0.5021008285092570 0.3595663874630062
0.3752743680200887 0.3728794031377356 0.1968604338679918
0.4401035477491939 0.6505273442522836 0.4407880117062978
0.5084068643331675 0.7659842663732217 0.3901034332607032
0.3996661928658909 0.5050226270017230 0.5568595093627626
0.3692943935280419 0.3641854500246697 0.5678847467133288
0.5972949632915762 0.4973729433961928 0.2429622766158185
0.5759544144898878 0.3258723468923101 0.3190322052775303
0.6522414819119733 0.3713524521862319 0.2081428883053843
0.6540306277568446 0.6213998622977652 0.2034575414035789
0.3708546378693183 0.6465157212642111 0.5621504077431881
0.5049524362347440 0.2361865061961351 0.4008600914939837
0.6823592890332113 0.5663516398107727 0.4695334131766987
0.6814915189623888 0.4363761244156223 0.4722990793438259
0.7745041178437472 0.4988103102356527 0.3813353717464953
0.6303399713687921 0.6450030696981247 0.5726042639188181
0.6004196946445989 0.5038338990423383 0.5650353576027496
0.6281337836196800 0.3625824656259797 0.5784066698634388
0.5070219163996622 0.5008888973900089 0.3888770046826731
0.4265863374920577 0.5927203674189097 0.2539443823657261
0.3236300828486280 0.5019006363529459 0.3789993872156759
0.4251834427279541 0.4047472187639667 0.2576402317413019
0.5084959550501610 0.6822241462468176 0.3761458419112859
0.3999681560483649 0.4144680658838716 0.5064466080901470
0.5979587804096643 0.4038040954114515 0.2646693428189065
```

0.5993119859673286	0.5917523734614348	0.2611738365577979
0.4010735586646650	0.5934395686582746	0.5028796988048255
0.5061292011511682	0.3192555701437008	0.3832907466526334
0.6905602849900738	0.4996213522128814	0.3940060741686927
0.6044011695440850	0.5922416427574513	0.5110663044833001
0.6031266284147088	0.4132337042653964	0.5147387304467712
0.4989691324319630	0.5050028900765613	0.5877946547243595

IM1

PMA4H-Rh-2CO

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Rh C

42 1 12 1 2

Direct

0.5111788283558338	0.6026369041446452	0.2148635838190386
0.4468944382186245	0.3242077910875182	0.3135469552009651
0.4393705443385034	0.6709453615742312	0.3047970812558723
0.5158555710295217	0.3905623455413108	0.2205972983260546
0.5077362925927311	0.5632569800012637	0.3409357524141000
0.4412727393329898	0.5007287463631743	0.4283972503331819
0.5103363734637909	0.4364092826253271	0.3443763497568152
0.5704119144831062	0.5035689534643876	0.4330004717464528
0.4432183956187065	0.3522190385784377	0.4467802493887694
0.5734960077919405	0.6737926244411788	0.3089853082039564
0.3586911866764339	0.5622602453559974	0.3219559369801920
0.3618084476643249	0.4297260156079703	0.3257758661811460
0.4280280581472022	0.4955126515007037	0.2356391088733561
0.6572114954767889	0.5692922696084944	0.3327443742797727
0.5004926469154437	0.5792610031569602	0.5290914231304976
0.5741191238557679	0.3551373727168262	0.4510375608328629
0.5673940806680291	0.6527386033690830	0.4435266169760825
0.5039066917613043	0.4302397368411486	0.5328800986180063
0.6603148851433771	0.4367514538504886	0.3361016184079811
0.3729432378787745	0.6186152051003988	0.1911756087545503
0.3273166905904082	0.5634435881393067	0.4561397474846586
0.3302198417149184	0.4339120055107725	0.4596522989918668
0.2422622952339722	0.4944531264372058	0.3629358787156861
0.3782644419359012	0.3687828613400935	0.1973796358481010
0.4365912162271610	0.6498356087121427	0.4384047145371034
0.5022204077250563	0.7667516164500150	0.3869177393315745
0.4020375341297030	0.5031171011929910	0.5598806229734500
0.3794641399798735	0.3635245140006601	0.5712823205876607
0.5975123864137439	0.4987512677493737	0.2416261202507084
0.5809339546759605	0.3270678623933990	0.3188335534490577
0.6553594731100629	0.3735953673475243	0.2077107759705659
0.6500970307496841	0.6233677116171402	0.2004348666425867
0.3734505291022467	0.6421784861549847	0.5634579194605775
0.5122654453604818	0.2355559066023316	0.4011721586732933
0.6789890724476091	0.5720696240759350	0.4686680199951696
0.6819617539330567	0.4425637832257371	0.4720730246713252
0.7736117905796697	0.5068756257429119	0.3817916405438564
0.6220474785021813	0.6480452547508611	0.5727173183578886
0.5999802527516468	0.5079937098383753	0.5669593257892849
0.6280525782853990	0.3694802619438027	0.5797766616927962

0.4891195239895459	0.6165028480103153	0.7047138824257960
0.5015232603671658	0.4006052265989063	0.7094912959523342
0.5074283832526754	0.5009796121811729	0.3869842120355061
0.4236348929357297	0.5902652568312011	0.2530808098396301
0.3253665108775457	0.4968630233270883	0.3802445292807547
0.4276200103589848	0.4023714776569403	0.2577159706286065
0.5046336128376298	0.6829686172095134	0.3733977745618562
0.4064195842070708	0.4128489955208894	0.5070884636603026
0.6004433588794279	0.4049902103093538	0.2642996314677288
0.5964855700497593	0.5928462866560718	0.2587362463268191
0.4028626046059492	0.5912149897409033	0.5016492377460327
0.5109531659408783	0.3185079464749372	0.3831647731169791
0.6894694823574972	0.5051898542982614	0.3931434697459167
0.5996295627843642	0.5953996123215866	0.5094306772251391
0.6033225103741633	0.4171073285923964	0.5134245862863170
0.4996717071046053	0.5064192111053870	0.5985492100707125
0.4938873337769055	0.5763134167324879	0.6642230940174075
0.5001597034381653	0.4393881422774649	0.6673793771652858

TS1

O P Mo Rh C

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Rh C

42 1 12 1 2

Direct

0.5108654620269119	0.6058685700443003	0.2208723144397284
0.4463864497727643	0.3256070975550891	0.3095798831500076
0.4395404275150228	0.6716048838434242	0.3127873312109943
0.5147751150503568	0.3941537851609019	0.2184692751813353
0.5077997591535196	0.5633530698265207	0.3454821497835595
0.4424963116110863	0.5000171145947117	0.4334466762389605
0.5101063935539507	0.4368193975210437	0.3464188756158784
0.5698718742009296	0.5023986976726253	0.4374598006451509
0.4430609116544209	0.3484691155879616	0.4436397189837952
0.5734928613097900	0.6743224619942113	0.3168371298266718
0.3588019621336169	0.5616881679819878	0.3270180102169865
0.3608764198890603	0.4291824299043880	0.3251623527309825
0.4275247501640881	0.4982900642309737	0.2379530709680654
0.6574940671915934	0.5677256875303613	0.3364453892593582
0.5007739311333393	0.5932352449741883	0.5486722955645575
0.5751342636430111	0.3506832776179607	0.4475186996481982
0.5692120620858252	0.6470835688507477	0.4492968960172121
0.5050608085300921	0.4182604690479697	0.5343590912196429
0.6605575862242126	0.4353262541973354	0.3343578299428657
0.3723758562346231	0.6229097834999229	0.1981874922264074
0.3238901661587705	0.5605151431391844	0.4592884979300942
0.3322734625357141	0.4315745013467565	0.4598017523418799
0.2414219323762375	0.4910812208361592	0.3635259972484639
0.3772014095368819	0.3729536336308199	0.1944885106065401
0.4366164697021770	0.6443105765010960	0.4451031682522054
0.5021769238976690	0.7633151028050978	0.3994940287824991
0.4042869261106499	0.4997608071015379	0.5609600637711470
0.3793798368042710	0.3580460717058849	0.5693190122975225
0.5967929160185749	0.5016126141666314	0.2432054672399754
0.5801361350121429	0.3283031007682223	0.3138650581144892

0.6540856496368457	0.3781169609321353	0.2030842418195994
0.6500033585325781	0.6280864140673722	0.2069787138506388
0.3662322996728589	0.6375930251857056	0.5666094865569495
0.5123747908673136	0.2339300899592171	0.3932397995985074
0.6841138602275709	0.5680883522419058	0.4704188274250408
0.6811361142301644	0.4385986423098709	0.4705972265959630
0.7750599926516070	0.5013688684017039	0.3803091579265352
0.6320768163761403	0.6430581469173817	0.5750652066520873
0.6007112095462424	0.5038734209835399	0.5669590529050201
0.6303245384479590	0.3625878997551419	0.5768135413372952
0.4952290392487276	0.6394119228497144	0.6629198584877047
0.5045308173566890	0.4260497641234193	0.7309493686976466
0.5076072474000992	0.5003241495378877	0.3903866152678284
0.4233331698028755	0.5924022388154833	0.2587915004750031
0.3243266222604921	0.4935585049309181	0.3816288939574294
0.4267873260566379	0.4042442325635075	0.2558082932518565
0.5044330671715532	0.6802533984605348	0.3821776763642168
0.4090848579458084	0.4078786936991084	0.5070009348117844
0.5997617931514636	0.4075458371313839	0.2612250198519585
0.5965397556338849	0.5956501228884344	0.2643395814300590
0.3974736086660029	0.5864118681149987	0.5062227713839030
0.5111572935100068	0.3175455214842642	0.3789473934969662
0.6911515588040213	0.5005723172359983	0.3932007119688766
0.6069478658290000	0.5906899632388154	0.5128608721425770
0.6023316201396500	0.4110493389668504	0.5126077177767707
0.5018093220989519	0.5007575064180706	0.6001504750269711
0.4983759714161125	0.5924452566928449	0.6281304931495381
0.5029368550875255	0.4507858974558914	0.6789708563361994

IM2

PMA4H-Rh-CO+CO₂

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Rh C

42 1 12 1 2

Direct

0.5108257968745403 0.6127820295492519 0.2319384794953987

0.4459711886312325 0.3236698227472751 0.2943296173724280

0.4401366898948482 0.6671450991012420 0.3318410470677294

0.5138781635734542 0.3995623638023568 0.2081300091070280

0.5090832042151854 0.5573218209521329 0.3499166510963871

0.4435097529494262 0.4853669075003244 0.4297056431989910

0.5109976623896016 0.4310027126054579 0.3374466080562554

0.5726897860465580 0.4871539983387773 0.4326887581990616

0.4454039613411405 0.3358715257984151 0.4304375418021763

0.5752937895471890 0.6694248206034737 0.3348424146639574

0.3584393106462372 0.5574297946714902 0.3319419461592520

0.3610223121976177 0.4259935467600689 0.3187818008760714

0.4280002330805271 0.5028426592145000 0.2376989876368279

0.6602483871736895 0.5617277148672565 0.3386072079259244

0.4511153403421034 0.7456875585335978 0.7248477135437449

0.5749671091710207 0.3376401248592608 0.4334954816869349

0.5690627490086045 0.6295657043199984 0.4659155275899855

0.5068532541157261 0.4063109271203242 0.5269846954440838

0.6613488420292559 0.4302311168821570 0.3253920793743264

0.3727999530681479 0.6315846532404307 0.2116860132323537

0.3216109153731867	0.5468319296600270	0.4625309779239493
0.3330249226285532	0.4174016446772048	0.4535397977585392
0.2411752051722850	0.4833581660042139	0.3623231608969642
0.3761154165451018	0.3817293224184056	0.1844214384876408
0.4414302729213989	0.6278922227268902	0.4632892960227500
0.5043668120324771	0.7508406918514794	0.4245745453828997
0.4051094645043751	0.4795984253883266	0.5569392965823388
0.3830107826408056	0.3365866332113901	0.5558694037052857
0.5959739373851910	0.5054927527895137	0.2414971507413555
0.5805825467477265	0.3257315268281059	0.2971753646025403
0.6525383020212477	0.3859690875781213	0.1900318304279749
0.6487821033763000	0.6359855518410930	0.2179277839058077
0.3648045784276893	0.6138074185145551	0.5798235485859664
0.5131244504165506	0.2252938954767055	0.3686110213541705
0.6907829687279842	0.5520394707304641	0.4708191113794146
0.6834424114990049	0.4223201928797937	0.4618885195000598
0.7775978778873528	0.4902715321935037	0.3754270241425365
0.6403413321492717	0.6179586124999749	0.5858916470938846
0.6048047451075178	0.4825630555259564	0.5616441771773301
0.6308968693478065	0.3399486022405279	0.5620041915672023
0.4593161991476519	0.6757796496232178	0.8190139749100961
0.4989638446015017	0.6024134988674621	0.6797587863879363
0.5090349798048039	0.4899103600068164	0.3878631876588520
0.4236802862902424	0.5943771529297093	0.2684810050818652
0.3240112829988291	0.4849942823411549	0.3809035076278131
0.4264971513299518	0.4076082315501622	0.2475773746830770
0.5061083620540512	0.6695526244679232	0.4001555506693686
0.4114690351785463	0.3904755092076581	0.4965796333097431
0.5990726066946757	0.4105064110312507	0.2511435579071192
0.5969551471623716	0.5972208740589532	0.2727978929295782
0.3937730200108926	0.5673795048206381	0.5144385606488384
0.5122209407009261	0.3097609330214474	0.3605009902167495
0.6938405217335172	0.4896735104436086	0.3893716161737385
0.6159251449335844	0.5704383653953352	0.5194703732714936
0.6038122857330073	0.3930953884112559	0.5013284045914448
0.5043194638256375	0.4980884554226287	0.5720365500098789
0.4552221411508884	0.7107470243528460	0.7719344258876522
0.5011842624409942	0.5658224305439034	0.6350671662671954

IM3

PMA4H-Rh-Ov-2CO

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Rh C

41 1 12 1 2

Direct

0.5097624082666697	0.6088287428045556	0.2241063087102686
0.4463739690733334	0.3234087508108351	0.3024327903646067
0.4372284230096888	0.6683681099449825	0.3200928701090522
0.5149751409163148	0.3934767068659650	0.2112612740773110
0.5067015916837339	0.5602930726480178	0.3435662715707526
0.4408167426294543	0.4916544799686485	0.4253628088205745
0.5097467450467255	0.4332694462491827	0.3374027023899496
0.5698539328360076	0.4945365138850507	0.4297612340985335
0.4426691417729411	0.3440776261835748	0.4382494854132361

0.5725849370816511	0.6715277334704860	0.3247701124188145
0.3568961492503580	0.5580174212517995	0.3246131824280448
0.3602702771285398	0.4258772938085092	0.3190032539215466
0.4278948136375622	0.4981811023031599	0.2341505110532839
0.6574572228809378	0.5648721886314932	0.3349982475255172
0.5738167055651583	0.3470548167250360	0.4427913105207249
0.5638199124245368	0.6386926012999825	0.4591319158807307
0.5035113905441844	0.4128866257169644	0.5322117211708248
0.6603328169598581	0.4327242567402845	0.3293420088035261
0.3723110200292704	0.6250499056072778	0.2005860024110383
0.3144978108295219	0.5589734285552866	0.4533073686383532
0.3325009137559830	0.4303548616212706	0.4562951387898581
0.2398074344994777	0.4831766788632514	0.3588113754425826
0.3778527450343603	0.3733252133190629	0.1877878403893492
0.4383398445768178	0.6357964488233547	0.4549289212467061
0.4998468691233936	0.7572261676773044	0.4080012185763360
0.4165374711649801	0.5051601558086986	0.5509997418578835
0.3794681808210526	0.3608144749919328	0.5654181726558245
0.5955603969872597	0.5020969235053069	0.2399331741592299
0.5803056597808230	0.3265402341894695	0.3070299481877182
0.6541630803052546	0.3797680574075397	0.1972603814948810
0.6477188569853454	0.6314149284966121	0.2101856810146529
0.3534906184814651	0.6326141820831149	0.5673850830631537
0.5127787892245327	0.2309357886659588	0.3847427009836675
0.6907976064562663	0.5675096095270941	0.4662668681121628
0.6784178127260920	0.4382091912118232	0.4682801424677815
0.7751170479797972	0.4951426324163631	0.3774048773295879
0.6406860372775928	0.6391993004188746	0.5772617288592233
0.5846696507311554	0.5090981143051725	0.5566907823865053
0.6271898425365690	0.3665473323713380	0.5740349876687565
0.3886930644833588	0.5404601556606208	0.7228698130026157
0.5996164250013394	0.5455250382777116	0.7295021073733340
0.5067528876370946	0.4947867329496115	0.3847719728261100
0.4220261598840052	0.5910079008848736	0.2603649629726370
0.3225534702056628	0.4871891118099644	0.3776605142887889
0.4274496405517555	0.4034887984833337	0.2497291348693272
0.5024989491138747	0.6748535419924792	0.3876173158769878
0.4130536133973413	0.4055784836679289	0.5011927557054144
0.5990827739512321	0.4075758562014524	0.2555652736502726
0.5955717161090252	0.5951217057067097	0.2664672142300223
0.3842668195454073	0.5820880055070271	0.5056952792033665
0.5113546151895133	0.3147218216516114	0.3713942780086770
0.6911788977545453	0.4954611095450004	0.3904075363913808
0.6166006018895893	0.5874469613559971	0.5136315618477045
0.5961284751271979	0.4097809167335289	0.5075362570938712
0.4980013272057073	0.5183034926740011	0.6223713139491934
0.4305436658768440	0.5322011702623872	0.6841025196626421
0.5606267310618390	0.5353182244611568	0.6882497790350934

IM4

PMA4H-Rh-O₂-2CO

1.0000000000000000		
20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

O	P	Mo	Rh	C
43	1	12	1	2

Direct

0.5100075881136011 0.6036775796051053 0.2147688364326319
0.4456198868666628 0.3237148027147622 0.3141726424715597
0.4378321698724635 0.6713817961798344 0.3046431836194461
0.5151673292470613 0.3886784481098688 0.2200084173842850
0.5066291784145873 0.5634763870457865 0.3386773867855348
0.4416260996904002 0.5008553298573714 0.4268680318126441
0.5094424299519964 0.4361273860305517 0.3420706838711413
0.5682382373699728 0.5037329549307427 0.4313071526148343
0.4427263890864441 0.3517323910144732 0.4481854134049404
0.5723779234136391 0.6745377428108897 0.3096565497034856
0.3587417873561674 0.5617088098746161 0.3216942358589286
0.3615012305516137 0.4292992037306281 0.3252383602717548
0.4277424560824450 0.4947741416654471 0.2343875780994107
0.6551847150482376 0.5687125560421651 0.3325641795678113
0.4984636313329480 0.6106780218386560 0.5496529912036587
0.5721472302354971 0.3547858114189907 0.4525991008168055
0.5659078627334162 0.6541673160131771 0.4438821044105877
0.5027126528768348 0.4164128156714518 0.5483061953399017
0.6587258908270113 0.4364413622974079 0.3359500976596257
0.3713526128492566 0.6178050256794680 0.1912091932667087
0.3264342160463469 0.5650020130446066 0.4553751936104780
0.3325756415563841 0.4368855207246996 0.4608015657745020
0.2426878497734992 0.4932606206415583 0.3641054992921633
0.3776137590583281 0.3675684994747446 0.1973452679461963
0.4363636841244282 0.6508657818246318 0.4394298396282635
0.4997760831693588 0.7679723857387363 0.3851763742513310
0.4133963533530206 0.5090801708262245 0.5511059345020731
0.3745893644061985 0.3682800783995984 0.5726257203106694
0.5958966221670371 0.4986919238498042 0.2405804130329046
0.5801130693022953 0.3269858139962507 0.3191285078134192
0.6550585862060604 0.3740363442602788 0.2079193286741678
0.6490086663447527 0.6243322920613453 0.2013954423936628
0.3621534459076154 0.6468781772055682 0.5608657055592977
0.5119111538663716 0.2349687071401188 0.3999881839682657
0.6783629167635493 0.5732042830047174 0.4679320902147851
0.6775801152676770 0.4446230390928171 0.4726408346460745
0.7714780394906582 0.5058337023788569 0.3830738507819911
0.6319059905490152 0.6539258767615606 0.5698616126598016
0.5877835783771356 0.5132949608726862 0.5567895148250422
0.6306927967654716 0.3742580066995658 0.5813405590834259
0.3862501090312392 0.4799891369174009 0.7150102908981066
0.6078955731517985 0.4819644275938790 0.7194927137689459
0.4964378798960603 0.5996431795771221 0.6194804272826365
0.5065289497482169 0.5010538623318425 0.3846628243526175
0.4223881544940177 0.5893624971213133 0.2528271442559046
0.3259550689231101 0.4957731048567661 0.3808955470378628
0.4273106923028440 0.4016882732210247 0.2571476197222561
0.5023911868757439 0.6841106155430979 0.3724756376790541
0.4090259773894435 0.4129869641613931 0.5086739169233406
0.5995872676102794 0.4056754028904999 0.2638790563666771
0.5951427429649851 0.5933093318722666 0.2592211275441522
0.3982536118805070 0.5957380721466382 0.5032418536369447
0.5105504402022517 0.3180050484896749 0.3824921820762078
0.6872586718054136 0.5045456950626744 0.3939998676569359
0.6019351257897643 0.6010982761817562 0.5103056234241521
0.5989104833424067 0.4175287146074099 0.5150242766314214
0.4989165814495957 0.4997742559627401 0.6153027970477346

0.4285043338849511 0.4855422731190209 0.6767321304253801
0.5668678778418949 0.4874626768137226 0.6799010377054409

TS2

O P Mo Rh C

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Rh C

43 1 12 1 2

Direct

0.5089023359069228 0.6042926009512301 0.2159347365326472
0.4459803923222152 0.3239674143291532 0.3150419613257039
0.4374723587991925 0.6716099829747121 0.3053512307872523
0.5154584721581092 0.3883058484711701 0.2208221163924726
0.5061541020245136 0.5635807706835504 0.3396913530702970
0.4424637672511502 0.5014213480914224 0.4290767924499454
0.5094719769824005 0.4366054059419206 0.3432007706147031
0.5692264637947074 0.5040607153362061 0.4318648576223107
0.4446018104920212 0.3533087770278137 0.4501202817025033
0.5727652484381379 0.6736361599464749 0.3116552038955823
0.3579974409584971 0.5606387204548504 0.3224543494338517
0.3622682382319181 0.4290174019080221 0.3255208215780163
0.4280049784875751 0.4949770352470860 0.2344946672293292
0.6556312159499185 0.5689195791360013 0.3307346918857755
0.4933771956482924 0.6144655744640968 0.5485371505941837
0.5732598089986262 0.3564600309613785 0.4531684774608588
0.5599374271605757 0.6505468737922915 0.4479035694303629
0.5044893790926444 0.4183864501221812 0.5510194630481483
0.6598002731679671 0.4372615261142054 0.3351103195780646
0.3699218674585205 0.6178381071940880 0.1929460266438034
0.3251081456037468 0.5631502699895217 0.4549460716623920
0.3333759130163304 0.4347087266740000 0.4607251484275589
0.2421287811458925 0.4899658893246712 0.3646111473231592
0.3780740705523255 0.3677763699874858 0.1974223463104797
0.4314719330601793 0.6526145653179283 0.4378000837411091
0.5013722533807993 0.7673241551893876 0.3866746643417739
0.4113428027721289 0.5099687062845321 0.5517273016197752
0.3753638156770624 0.3684590852453523 0.5737876198317269
0.5951504153559890 0.4985319848622418 0.2401096148354873
0.5806660359567368 0.3276134213057624 0.3205390010089664
0.6549188869053588 0.3733841532992333 0.2081769138791700
0.6470774104351072 0.6244856217885996 0.2000347990396363
0.3572783924954313 0.6472239758070303 0.5588056272285392
0.5118599231924715 0.2361978505415376 0.4020155815395111
0.6795658920945225 0.5768934474950811 0.4648234820738211
0.6807263371276708 0.4456891592556931 0.4707920669386090
0.7728118494294400 0.5077404958397160 0.3802545812211697
0.6314251242676130 0.6501674632851812 0.5720324212178974
0.5965477480688574 0.5120151121674771 0.5558482980099035
0.6344270138420603 0.3735513228477039 0.5797925618322879
0.3855433219436353 0.5612050545072261 0.6990839470374102
0.5917689412998746 0.4629132165171897 0.7265623119624744
0.4820396858480565 0.5955348258898044 0.6337511611696131
0.5067881762168103 0.5013769373892368 0.3859455275815637
0.4208054133418299 0.5894035275786038 0.2546632700467417

0.3251879344144114	0.4938884501498437	0.3820778749374835
0.4276849845660969	0.4021864458410379	0.2571176120281268
0.5025226709173457	0.6835261528008292	0.3731803070067455
0.4098201119329903	0.4142192463728768	0.5108741698995001
0.6000333757812699	0.4053062606436133	0.2645084782304459
0.5940402777786340	0.5927212084439193	0.2582305532335252
0.3965327503421805	0.5971361860968645	0.5021828705253396
0.5100829243729198	0.3190113736042480	0.3835254276270369
0.6887583953582386	0.5060903169681485	0.3922661797908388
0.6034583151582307	0.5974090083285372	0.5113613632659701
0.6029251959257088	0.4181724856324754	0.5143102375995063
0.4974602636931089	0.4985875930849821	0.6129534026547876
0.4315243698202539	0.5509884123467864	0.6643245496660852
0.5571952745849482	0.4743312781479913	0.6821723193781524

IM5

PMA4H-Rh_CO_CO2

1.0000000000000000		
20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

O	P	Mo	Rh	C
43	1	12	1	2

Direct

0.5107197101514931	0.6049630577404378	0.2175861112446886
0.4466786312545311	0.3248441057890816	0.3146143253637433
0.4388241403273025	0.6711974286241713	0.3084649610103422
0.5155828471826046	0.3917251402194117	0.2219681963602057
0.5075157129818980	0.5636112964196163	0.3434627660776233
0.4414862445525632	0.5002288608807781	0.4306412781102316
0.5103223325548619	0.4367469310443224	0.3457752577429911
0.5705610833608581	0.5031112322536399	0.4348386824873801
0.4434297684716705	0.3518576381238426	0.4474409646751388
0.5731322406383174	0.6744360406799105	0.3128947651371546
0.3584477110803687	0.5630341868889727	0.3244373063759990
0.3614536484451005	0.4307541826139575	0.3269334512056214
0.4283381797015500	0.4966660480035442	0.2374927616423687
0.6573709470911596	0.5699404869895757	0.3343748696691550
0.5009892733184891	0.5770290765146210	0.5333620358664181
0.5742492551040469	0.3549650260454365	0.4517534203460434
0.5672494527901749	0.6516575175730333	0.4469394001995975
0.5043432283753927	0.4274905430755669	0.5346087923206745
0.6603414312158767	0.4377058182148709	0.3369113485865275
0.3726583502396164	0.6194473967202375	0.1935951559102085
0.3278549553867962	0.5627239322355861	0.4591797565689602
0.3293155720228234	0.4331125044412777	0.4605971411391748
0.2419469456803654	0.4955378011668538	0.3646766024573815
0.3782164717870464	0.3696916881801909	0.1987095193843901
0.4369564083921680	0.6486853297104409	0.4428819076381022
0.5009517459660605	0.7660840181019043	0.3916168705732020
0.4023364275699762	0.5002209452273272	0.5615216813852246
0.3782973079872597	0.3609828377686519	0.5711380380272234
0.5964983700842525	0.5006217180958278	0.2431308195694525
0.5810601769111222	0.3279607033810211	0.3190286911415950
0.6551826265163663	0.3762303751469919	0.2080615152371321
0.6492982345236771	0.6260029408258676	0.2029949774117830
0.3745609668403851	0.6393452900377219	0.5683203496519542

0.5131769500805077	0.2356348095968799	0.4007595402204521
0.6791399146763222	0.5708747654391039	0.4706823053781888
0.6835106187401844	0.4412219268635720	0.4722902095450118
0.7740269108087553	0.5079025890132208	0.3824199655812218
0.6225055350783683	0.6460343844633678	0.5754761130417485
0.6010400993206146	0.5050029367414997	0.5679194553745218
0.6305413694388164	0.3668899725302219	0.5794938062423753
0.4971616512043926	0.5824499769951137	0.6771331986300116
0.4982999259160775	0.4015672227075670	0.7140028965057402
0.4550447530695820	0.6870330454328859	0.7098423179549916
0.5074835056688883	0.5009004899067383	0.3890040634764501
0.4233187681674073	0.5907507249174172	0.2553980094514867
0.3250315502565594	0.4973696946188288	0.3821571643752910
0.4275169211429544	0.4028541722154628	0.2593459162359300
0.5035293831774795	0.6824303699849268	0.3772085982504470
0.4053144136150562	0.4112524349444491	0.5078419141151957
0.6004489078479022	0.4069908994045207	0.2651979436161710
0.5960152309746453	0.5948355990973068	0.2613034426481459
0.4034678637816410	0.5889828128765193	0.5055344423064833
0.5118750413315440	0.3187797255939148	0.3836263873107986
0.6899895918743223	0.5058861761849771	0.3944400542848054
0.5995109456890713	0.5937913203139307	0.5120517953682858
0.6055612427001485	0.4160563229975184	0.5144650038962745
0.5005523256054151	0.5008289315016972	0.5985697184440077
0.4752436495228476	0.6353786411199707	0.6922546642820725
0.4994126258043285	0.4372979108037048	0.6690274279461930

FS

PMA4H-Rh_CO

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Rh C

41 1 12 1 1

Direct

0.5148618957439525	0.6023220323785079	0.2146748742847399
0.4446263371494969	0.3252080011769761	0.3139451996068857
0.4414950169463304	0.6716569160444722	0.3017591904159835
0.5168218213085117	0.3895210826499898	0.2221685752470129
0.5073710786738230	0.5635806340407968	0.3412835760868639
0.4383608306127629	0.5019942336964159	0.4277374879709089
0.5087381827012688	0.4367367455293362	0.3452987753730898
0.5664518578882700	0.5036396586495057	0.4358371832697394
0.4375521506394208	0.3539467500049900	0.4460819394869364
0.5752710570357876	0.6733684238911306	0.3102933400356974
0.3590097997615743	0.5642709688200883	0.3174735659735794
0.3600006756025327	0.4319595836672154	0.3219428618462367
0.4302707695445554	0.4957417774000584	0.2336595470123629
0.6575800955176087	0.5677893388736754	0.3361273407180410
0.4951689204312344	0.5830957167656665	0.5313801191060920
0.5683923905195366	0.3558350434051487	0.4545122703868532
0.5656462958324023	0.6530225555050969	0.4440253394798470
0.4965278609982757	0.4255547374219091	0.5374866519200422
0.6589482861541032	0.4354547577668460	0.3405924573250790
0.3775570079012803	0.6189026982942220	0.1866734041305048
0.3238264639007879	0.5669636095324755	0.4501713627598208
0.3238077575102611	0.4370334127148513	0.4541173498629615

0.2400621844385107 0.4987479863119940 0.3545688352330955
0.3797828818205997 0.3688343053647912 0.1953752338053384
0.4346293693662350 0.6516290866490337 0.4358356393006122
0.5020702572471459 0.7673836912872156 0.3854355511509698
0.3948230315246360 0.5054193796208188 0.5548621238038023
0.3667542694882695 0.3656620533194183 0.5666139643143681
0.5987873547572599 0.4979487254490206 0.2441935208660078
0.5790514803853097 0.3268099693622869 0.3221516546356870
0.6565522839582680 0.3726041367649904 0.2122012573556800
0.6541012048179050 0.6225454456908049 0.2041261405002702
0.3659823809174508 0.6463367824510160 0.5576727932317750
0.5079747146849830 0.2363985528531589 0.4027616859348139
0.6757291903858819 0.5707822769395180 0.4722474797755996
0.6781958460769311 0.4412240655890762 0.4764438500649638
0.7723208366745201 0.5046564368216375 0.3875768644864532
0.6188887586666288 0.6490539026010649 0.5733112536305879
0.5930034646939589 0.5076397707861920 0.5677356098990248
0.6234946044668934 0.3688447801309032 0.5828894381404892
0.4770793593459819 0.4261477550594952 0.7205456858895454
0.5052364249757885 0.5015203207393366 0.3876139637468443
0.4261017306560951 0.5905088361556572 0.2502003805143676
0.3224941344267148 0.4997842713083953 0.3748186233699588
0.4277384821558559 0.4025807041988296 0.2567310104580309
0.5039146720469214 0.6834957754296026 0.3727522107000351
0.3978300958520891 0.4143341719545593 0.5040074601630550
0.6005487534565871 0.4049799548744838 0.2671349452081865
0.5986757870826530 0.5929010043010211 0.2610988333302625
0.3976963590772483 0.5938462927543839 0.4986239306968506
0.5080314741683720 0.3192933373423669 0.3844069492862086
0.6880268007240291 0.5039407696236128 0.3975000269620140
0.5957667993869427 0.5959359739328112 0.5110013903592207
0.5992038759864196 0.4171687650458739 0.5171104720520032
0.4915687515316576 0.5056698768203759 0.5921972998792424
0.4839258483814824 0.4528220942368701 0.6700115439553458

Optimized fractional coordinates of the Rh@PMA Catalytic cycle (TER Mechanism).

IS/FS

PMA4H-Rh

```
1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
```

O P Mo Rh

40 1 12 1

Direct

```
0.5146576386747326 0.6038971215294322 0.2168078878529396
0.4418202328774972 0.3265942622310100 0.3135598094022834
0.4441138035619731 0.6728196632398284 0.3067504869694361
0.5131366571669926 0.3909289188382111 0.2209478191172618
0.5092525015112870 0.5633326923672225 0.3431844126159496
0.4413561081595592 0.5021759232337001 0.4308831384790817
0.5083890052903409 0.4366799913783297 0.3456559272851080
0.5690929711901103 0.5014138678848847 0.4360466344504060
0.4381981213085563 0.3545175453052118 0.4466124502172239
0.5782788510104009 0.6720477043073865 0.3122609596826111
0.3604671563338194 0.5666042665945946 0.3222465202620886
0.3595437723362291 0.4343948179110275 0.3249218102410286
0.4288180059929098 0.4983123391798812 0.2360131408406189
0.6592845591229102 0.5648634507584002 0.3344877685151170
0.5014208402952031 0.5845301942460490 0.5377565267651825
0.5692294015549422 0.3537602904753525 0.4519400192107174
0.5711912940286058 0.6497501796371419 0.4460868345062643
0.5003625909469734 0.4234847645408600 0.5410233012507106
0.6583387052049675 0.4326259269561090 0.3371091812766989
0.3771161931510139 0.6229769070592637 0.1919582323547239
0.3264732653296470 0.5684942206825270 0.4550561268937767
0.3256252638219170 0.4384472002396845 0.4577360692810923
0.2410039314657672 0.5021008285092570 0.3595663874630062
0.3752743680200887 0.3728794031377356 0.1968604338679918
0.4401035477491939 0.6505273442522836 0.4407880117062978
0.5084068643331675 0.7659842663732217 0.3901034332607032
0.3996661928658909 0.5050226270017230 0.5568595093627626
0.3692943935280419 0.3641854500246697 0.5678847467133288
0.5972949632915762 0.4973729433961928 0.2429622766158185
0.5759544144898878 0.3258723468923101 0.3190322052775303
0.6522414819119733 0.3713524521862319 0.2081428883053843
0.6540306277568446 0.6213998622977652 0.2034575414035789
0.3708546378693183 0.6465157212642111 0.5621504077431881
0.5049524362347440 0.2361865061961351 0.4008600914939837
0.6823592890332113 0.5663516398107727 0.4695334131766987
0.6814915189623888 0.4363761244156223 0.4722990793438259
0.7745041178437472 0.4988103102356527 0.3813353717464953
0.6303399713687921 0.6450030696981247 0.5726042639188181
0.6004196946445989 0.5038338990423383 0.5650353576027496
0.6281337836196800 0.3625824656259797 0.5784066698634388
0.5070219163996622 0.5008888973900089 0.3888770046826731
0.4265863374920577 0.5927203674189097 0.2539443823657261
0.3236300828486280 0.5019006363529459 0.3789993872156759
0.4251834427279541 0.4047472187639667 0.2576402317413019
0.5084959550501610 0.6822241462468176 0.3761458419112859
0.3999681560483649 0.4144680658838716 0.5064466080901470
0.5979587804096643 0.4038040954114515 0.2646693428189065
```

0.5993119859673286	0.5917523734614348	0.2611738365577979
0.4010735586646650	0.5934395686582746	0.5028796988048255
0.5061292011511682	0.3192555701437008	0.3832907466526334
0.6905602849900738	0.4996213522128814	0.3940060741686927
0.6044011695440850	0.5922416427574513	0.5110663044833001
0.6031266284147088	0.4132337042653964	0.5147387304467712
0.4989691324319630	0.5050028900765613	0.5877946547243595

IM1

PMA4H-Rh_2CO + O₂

1.0000000000000000		
20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

O	P	Mo	Rh	C
44	1	12	1	2

Selective dynamics

Direct

0.5110083817632266	0.6029952064100720	0.2135509055231094
0.4472767082553500	0.3240489550139803	0.3117939161780799
0.4389650102183187	0.6709243487881660	0.3030923100786929
0.5165607052592384	0.3903425545915569	0.2190237461306496
0.5075247642239459	0.5633090417498414	0.3393530285103315
0.4410692546844411	0.5003734691711045	0.4264185872870274
0.5105494868403697	0.4362866908431631	0.3425935387471323
0.5702573060353981	0.5035575846599096	0.4312940794648210
0.4430648741731246	0.3516495952398682	0.4445202073217054
0.5732041694929716	0.6740320419846643	0.3078918191625690
0.3584159547081510	0.5619868561811555	0.3200797914053799
0.3618143186591908	0.4295962173584395	0.3234128040197626
0.4285829139189168	0.4952946501580878	0.2338423863808420
0.6572345038382602	0.5693211976544431	0.3312190145724428
0.5001332346422382	0.5789528820496262	0.5271661331897558
0.5738667339792474	0.3549579197984305	0.4494687521634471
0.5671144209001890	0.6529176634568975	0.4418700104701396
0.5034933139765204	0.4299067712656394	0.5308480785048445
0.6607009543858130	0.4369131024784657	0.3346465001324936
0.3726400912808144	0.6180813338858564	0.1894992474619114
0.3269485226822511	0.5632854032649286	0.4539456687798403
0.3298167122040653	0.4336827245294125	0.4574481190520683
0.2419614117561861	0.4936595759542515	0.3604622248072968
0.3793384827289805	0.3681690419933955	0.1953221750671992
0.4363812249298736	0.6497469860145634	0.4368839873104363
0.5011445620588126	0.7669595507194096	0.3852422924797475
0.4015082615299218	0.5027735764568243	0.5575733781244135
0.3793506299991686	0.3630777879819687	0.5688796941312053
0.5974126177888442	0.4991135222199362	0.2401490283494249
0.5815437283327126	0.3271393188368801	0.3170079635511261
0.6562927825972956	0.3744225903361588	0.2061922055374846
0.6496673576083429	0.6243102280706386	0.1992590595837911
0.3730906595208159	0.6416687782787772	0.5616742946937630
0.5131552052929494	0.2351791572500273	0.3988384788228495
0.6788564730295301	0.5718856303931221	0.4673502244984259
0.6818519038384684	0.4423287266333339	0.4704981051792241
0.7737998847079899	0.5073765621856747	0.3804188028495509
0.6212343843555408	0.6478521294170456	0.5710760496055515
0.5995434368443093	0.5076945906917717	0.5651256938455663

0.6276238781584770	0.3693356265615946	0.5781534699674981
0.4907756689867020	0.6178522632170103	0.7012193528011612
0.4968885162239103	0.3983953932161893	0.7058512563562758
0.5339378962080575	0.5257009652773549	0.8322039451764300
0.4781613561408367	0.4991186754441014	0.8330663025959200
0.5073350184971940	0.5008967066678423	0.3852534778863206
0.4232632735719009	0.5898112811429571	0.2515153100746289
0.3249994542128853	0.4961820560647004	0.3781350157712864
0.4283447629973235	0.4018945535530491	0.2558877082384648
0.5036675500659974	0.6831477720299705	0.3718501319741317
0.4063407676296143	0.4121797457339830	0.5045264810669379
0.6011881658899110	0.4056295286426860	0.2627332718699918
0.5961331846430837	0.5935226439593161	0.2575048071341982
0.4022876413348853	0.5907133992770671	0.4998039033902243
0.5118351997292677	0.3182236702396961	0.3811637704515580
0.6896419695475511	0.5055562567448891	0.3917654472110036
0.5990657438210201	0.5954740628563376	0.5074953148546349
0.6032156863278680	0.4171314894297802	0.5118311126934905
0.4990233088050216	0.5060360239323747	0.5965750251652198
0.4941206865104930	0.5766146861999984	0.6616514914566007
0.4977349906562111	0.4382491798416013	0.6647512028899092

TS1

O P Mo Rh C

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Rh C

44 1 12 1 2

Direct

0.5114047982019551	0.6026176644531229	0.2147472035197532
0.4463173286702612	0.3244193080543046	0.3135825737847305
0.4397365909723079	0.6710756357023656	0.3040787582888875
0.5157871398496192	0.3902956295993998	0.2208821182567619
0.5079601373101066	0.5633937567641113	0.3414089007291558
0.4414619502080029	0.5011722107067972	0.4293759753375767
0.5102676934580682	0.4365071785571602	0.3450901158859315
0.5695061550837791	0.5037406244346907	0.4345937886505502
0.4424950473242223	0.3523299158856458	0.4465839143265177
0.5738254014263418	0.6737588514499402	0.3085268846569120
0.3587582538552243	0.5626136999216094	0.3215469463967348
0.3615136834797910	0.4301718142097739	0.3253039745284521
0.4283849550025736	0.4955173431643639	0.2354972785153506
0.6573899407956456	0.5689123084518432	0.3325511846076384
0.5005613445485655	0.5838767274698379	0.5311953208817488
0.5742004675827911	0.3545424093999299	0.4508602161720367
0.5682985948592083	0.6537349977894420	0.4427675772613714
0.5037634588252157	0.4261100583160797	0.5354128305013457
0.6601568679007946	0.4365591994533379	0.3363888749722869
0.3731265193026208	0.6184168652557620	0.1905801125376971
0.3269039333860960	0.5641652548997952	0.4550769712493871
0.3293971973866605	0.4344786962936933	0.4588946143567416
0.2417824083858027	0.4950149052532135	0.3614792969824331
0.3782913577054958	0.3686908473580686	0.1970443474580418
0.4368035532697649	0.6503820098808215	0.4377072559517671
0.5022899680833530	0.7672723833549362	0.3855911126247747

0.4022782347022246	0.5035199518728591	0.5579309089756209
0.3763845992126024	0.3634156390046923	0.5701753899221705
0.5972026265576390	0.4985161032925848	0.2417645612990766
0.5803274885472959	0.3269153878717456	0.3189006654269821
0.6554928606352617	0.3733953713267310	0.2082066117873911
0.6504145467281425	0.6230463047796836	0.2002661010925223
0.3708313412671944	0.6437074175996713	0.5612649645136061
0.5112827481153608	0.2353892623046477	0.4008922161751577
0.6795040314551921	0.5719779152529014	0.4680792371677535
0.6821771017603880	0.4424455654429042	0.4715214634804446
0.7741721343261505	0.5065482443591444	0.3809888875940146
0.6248864323248632	0.6494272212585674	0.5711071461763646
0.5992944240034841	0.5082058196382812	0.5654763974852952
0.6314363523193386	0.3681372500739703	0.5779108518066857
0.4799759635676710	0.6337566511758629	0.6732077478198450
0.5192454371584779	0.3827791683361191	0.6782118408407386
0.4640957940094376	0.5372540656875722	0.7420969231777761
0.4857393498229891	0.4758240844228530	0.7467126308056665
0.5072693459686483	0.5011958077886244	0.3874626785736381
0.4237204862122054	0.5902296385303858	0.2525949686409948
0.3247546708286024	0.4971980346782237	0.3793360828173552
0.4276086837931425	0.4022139191628339	0.2574142215524309
0.5047209387511071	0.6834099883394325	0.3727599951482119
0.4049376824117253	0.4126766877976120	0.5068679432989315
0.6005030813546794	0.4048745131088625	0.2646428335800262
0.5966506870798892	0.5928131608023828	0.2585428545092756
0.4018528402076848	0.5922871500715509	0.5009175817885029
0.5103901320610620	0.3184103447278167	0.3832948866454307
0.6901238642662666	0.5051606300511370	0.3928881596558131
0.6005598752609218	0.5967681783373869	0.5087996690148060
0.6041200202694630	0.4161543099429333	0.5131839726650648
0.4998576154072800	0.5066709103424714	0.5944036058412764
0.4842289001113962	0.5758247407712297	0.6666898931177800
0.5048212000451570	0.4386614542653829	0.6692669263456648

IM2

PMA4H-Rh_2CO_2

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Rh C

44 1 12 1 2

Direct

0.5113762108975977	0.6028910520015796	0.2150845446550622
0.4459716672606649	0.3246950847732336	0.3144473613431273
0.4400891070255191	0.6712537008944222	0.3047798470233528
0.5155895652703386	0.3897573094449197	0.2213505636420885
0.5079928401531505	0.5634132218729061	0.3416815068090448
0.4420209534433751	0.5012003212593543	0.4303465052782914
0.5101209961008571	0.4366149192977713	0.3452469154377697
0.5693670344938222	0.5037102681196332	0.4350866979272339
0.4420177556969263	0.3525066123056788	0.4474358208054647
0.5743014469602956	0.6736282782728095	0.3088470512083363
0.3589647346619957	0.5626979062666861	0.3218983395012172
0.3613960811317445	0.4303964686925729	0.3256080697128588
0.4285335453602965	0.4956481530269861	0.2357927389724607

0.6574600807161887	0.5687398674096111	0.3322727153139371
0.5010344634752396	0.5893967081023226	0.5358078365623968
0.5733554295263805	0.3552985551548853	0.4518082427173079
0.5688727505634728	0.6536675849072249	0.4432625875052763
0.5029952420464829	0.4213753396299314	0.5414387735466479
0.6600162511074520	0.4364182031030742	0.3363088005367328
0.3730678789061851	0.6188552443692086	0.1914102238827124
0.3269812404730084	0.5647980607931283	0.4548160013103804
0.3289430205712816	0.4348407373987789	0.4589822481745617
0.2416842463107709	0.4952669541595384	0.3615698076806457
0.3779988917538662	0.3689806504745384	0.1975668767908372
0.4373886666720425	0.6505225668040288	0.4381346929859676
0.5033252223019198	0.7672966845999295	0.3858702759390689
0.4021561792797368	0.5040095348270214	0.5570701260557347
0.3734084291870605	0.3629461733501348	0.5698595339625218
0.5970290173293636	0.4983439365216364	0.2416592664632969
0.5802993697128018	0.3269879944757537	0.3196922590799451
0.6551704512007944	0.3731573774855055	0.2083208156566657
0.6502802249897637	0.6228423868516538	0.2000026120616320
0.3682195814826638	0.6451165008125536	0.5598297137319759
0.5112898195543993	0.2356802711461131	0.4012332184865025
0.6799057618398530	0.5718875905205710	0.4676555983296548
0.6824431715940108	0.4419622446327691	0.4712041507458771
0.7741115949260381	0.5063996669328842	0.3805911579904803
0.6279895738951145	0.6498188340492888	0.5709284131386854
0.5999430790474775	0.5079743380207293	0.5644424625037677
0.6343642085835236	0.3673531704963918	0.5773687500836359
0.4727660972445752	0.6284613669679188	0.6656877596082670
0.5249493017464693	0.3877395334842965	0.6727589391102174
0.4662064200561296	0.5404769380043326	0.7307068050892140
0.4835124194422265	0.4687350938953093	0.7330676570981396
0.5073880817255358	0.5012329818883648	0.3878259294875924
0.4237233624188885	0.5905297179412486	0.2533040877273021
0.3245910539751373	0.4972945515956534	0.3797280370978167
0.4274621043402575	0.4025564455116437	0.2577853375456959
0.5054787883745093	0.6834162312527665	0.3731908574935268
0.4039580758799809	0.4121168925416047	0.5075451262011047
0.6003379314606805	0.4048461562195465	0.2647868193202949
0.5966440353271341	0.5926879465899425	0.2584305910242988
0.4014050036911350	0.5932286779488389	0.5012950018825189
0.5102997361406111	0.3186990264731339	0.3836551118533193
0.6901002469658674	0.5051129608650297	0.3927431283346656
0.6015911205162711	0.5972665657472256	0.5095227414245972
0.6051197631607883	0.4159318913745492	0.5141272873770414
0.5000816053426257	0.5067642578430981	0.5894104544480935
0.4784395155065970	0.5689118189788526	0.6707341806443902
0.5048796101810922	0.4443304916188759	0.6734811336787377

TS2

O	P	Mo	Rh	C
1.0000000000000000				
20.0000000000000000	0.0000000000000000	0.0000000000000000		
0.0000000000000000	20.0000000000000000	0.0000000000000000		
0.0000000000000000	0.0000000000000000	20.0000000000000000		

O	P	Mo	Rh	C
44	1	12	1	2

Direct

0.5116293235043149 0.5998869929593712 0.2132182651347536
0.4468185133352519 0.3249390864599910 0.3226583546374577
0.4402703610250566 0.6707284348118517 0.3006912070776986
0.5158472035254701 0.3875555717211401 0.2270323982689255
0.5080046189419644 0.5641795813825764 0.3413148793466915
0.4413881829177685 0.5040725223893012 0.4306516206964616
0.5105397713406664 0.4374911450106400 0.3486231343316624
0.5704359380071422 0.5068737059205272 0.4353145357841528
0.4422598823673011 0.3575253041962492 0.4534746319917736
0.5744231986881939 0.6735239699105223 0.3052516411008382
0.3585420145161454 0.5639146557507049 0.3213454043971669
0.3610179702722336 0.4316166746128318 0.3295640149521801
0.4287243878632507 0.4932094722122887 0.2381555113235881
0.6582497898550974 0.5702087106745048 0.3314320265200021
0.5007078167895522 0.5852570751811846 0.5272095130667280
0.5736612505336494 0.3608113617879517 0.4588171793653913
0.5681275289133244 0.6569001566690126 0.4401686647284831
0.5031232015799533 0.4353950264014049 0.5401295564933259
0.6608954885598469 0.4378628943457854 0.3397249385617447
0.3734268942444829 0.6142890454817278 0.1887200743001614
0.3276931649448905 0.5688357253197135 0.4552031849213517
0.3273967294851909 0.4395789231128771 0.4619863219862719
0.2411759534514039 0.4986834667275677 0.3630040652746761
0.3785293968226722 0.3643897021188105 0.2049533400683638
0.4372196772901333 0.6545753544371070 0.4351730554334778
0.5029165445632816 0.7692187074154203 0.3796988802195065
0.4009966779871057 0.5102726828013354 0.5607416485586924
0.3731003450079702 0.3714400017765490 0.5742836965104288
0.5974615448713979 0.4968206253114074 0.2434729560267405
0.5812120852778045 0.3277937278671615 0.3270602565146727
0.6551730607186945 0.3705808992873787 0.2137226267957351
0.6501473483116303 0.6202762550550549 0.1975003603394240
0.3736010676845158 0.6506183822738785 0.5596699530710063
0.5133457347318836 0.2395209292632112 0.4128830720439390
0.6791537013343366 0.5757989553451376 0.4677437577748759
0.6840519241399268 0.44692476074444083 0.4745168400128641
0.7747379098381608 0.5101582083019546 0.3815891939950189
0.6228598745448554 0.6550256526336665 0.5690280746403263
0.6001280441005076 0.5141745642527376 0.5683293954934737
0.6342976562236695 0.3771574627149346 0.5838449490623739
0.4891933433114836 0.6037826937379976 0.6674029635856926
0.5013142338057877 0.3716995540871995 0.6503877105515504
0.4708523346748294 0.5202611603548211 0.7467789010077283
0.4802119178266244 0.4345273717861536 0.7279889135968730
0.5075616475329123 0.5033106817681079 0.3892353490674166
0.4239517415804692 0.5880903525700397 0.2516606483118175
0.3240949569900270 0.5008426111070808 0.3811804643442744
0.4276150290636264 0.4003272706046466 0.2641154751232237
0.5049563643723859 0.6849930579945901 0.3691293981482049
0.4027104471400766 0.4190034706301908 0.5102319622577636
0.6006260431153972 0.4041642428845983 0.2693851578632514
0.5967237316022911 0.5917975765562637 0.2569580958506585
0.4035721451686766 0.5976392799679420 0.5000943928303737
0.5122097993183883 0.3217758529638941 0.3920216260283071
0.6906909834891560 0.5086899139930243 0.3936273842116340
0.5992512219532913 0.6009554955422531 0.5076307886647843
0.6069922427298540 0.4242277048343939 0.5184981134351148
0.4980825149019295 0.5123129313199961 0.5980448248743945

0.4822197089089773 0.5484971650127890 0.6922654181525369
0.4941869674035451 0.4314888925535961 0.6634575080904801

IM3

PMA4H-Rh_2CO₂

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O P Mo Rh C

44 1 12 1 2

Direct

0.5115832129619213 0.6029087064620117 0.2161473604987534
0.4459270653854233 0.3249139050286826 0.3153509352099219
0.4400406914963920 0.6708322822396704 0.3058172304357868
0.5151941103933438 0.3900879968978865 0.2220397207707971
0.5078232889285491 0.5632638637556321 0.3428167123322947
0.4419290673459051 0.5011237902964427 0.4313181353721632
0.5101004399317932 0.4365405982502444 0.3463064809420159
0.5697592769564169 0.5034833655661751 0.4357399996332790
0.4422167461925263 0.3533467625172609 0.4482526945135341
0.5742316663438333 0.6731569502705554 0.3104360805533589
0.3584483521374444 0.5629580641606287 0.3222003033611597
0.3607057151390396 0.4306332321300906 0.3258442673328578
0.4281791107781940 0.4955635329585340 0.2364525487783672
0.6583496709782815 0.5682350911149955 0.3325834967992702
0.5007909396700936 0.5857135077670860 0.5367264288499866
0.5735680234029872 0.3556414722718620 0.4527703188540188
0.5686391198803458 0.6520381482678334 0.4445336749877164
0.5035343084122791 0.4247147048170508 0.5413191818941642
0.6606386147837464 0.4359833808287034 0.3362652671650738
0.3735972329246303 0.6188615223643522 0.1915770101963000
0.3258416447704371 0.5648874183634455 0.4552718545209476
0.3280876184938914 0.4350340989769754 0.4589008834594897
0.2408944545543854 0.4957531218158532 0.3609820297599681
0.3777395879956670 0.3682849786862257 0.1984947434717882
0.4372064394288986 0.6497614310098070 0.4400535885741985
0.5027472650066367 0.7660797460962950 0.3884961218992216
0.4009934299530612 0.5040496254484136 0.5574305074129283
0.3736801819269581 0.3631177717637712 0.5697522640825067
0.5970845947667039 0.4985283620912046 0.2423482868372432
0.5801299141409937 0.3272364887591203 0.3200581509946592
0.6545470870442917 0.3732008405649645 0.2081192411050936
0.6504070587626668 0.6237048764345715 0.2012639747990229
0.3687536344649578 0.6444668995277976 0.5617506872437431
0.5115272207757818 0.2365063454703863 0.4031398298736714
0.6815991539626980 0.5712397196072572 0.4675592859782627
0.6838183573814153 0.4413387537227287 0.4712014930212630
0.7753538226542310 0.5053499567367590 0.3795410352468568
0.6285057607389317 0.6490271004357933 0.5708652804151212
0.6018304456174887 0.5075905563471674 0.5643366481721233
0.6331623077040782 0.3675739821332192 0.5785923810010780
0.4474758677266525 0.6566473205198454 0.8103165419563867
0.5247239516830904 0.3519285682646021 0.8066873810751168
0.4574440265689664 0.5879577110470310 0.9052574478329541
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0.3236975217352938 0.4976984152900818 0.3796773902246464
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0.6001137955821860 0.4050811073424553 0.2648969680162227
0.5969316808376182 0.5931098800234892 0.2596367733795931
0.4000426800825284 0.5919441748364380 0.5025744580710865
0.5107793437465066 0.3194070076689468 0.3848181832272604
0.6914418097609345 0.5042851215556318 0.3924853097647251
0.6033924966834230 0.5955396960994693 0.5096200680072055
0.6063299820900923 0.4167852847477933 0.5145813005802340
0.5004963985266205 0.5065844175803594 0.5874748580966491
0.4524378635371467 0.6224366876652709 0.8579408343329015
0.5011342592081728 0.3850337384716538 0.8491947948461900

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- 1 Hülsey, M. J. *et al.* In situ spectroscopy-guided engineering of rhodium single-atom catalysts for CO oxidation. *Nat. Commun.* **10**, 1330 (2019).