Supplementary Information (SI) for ChemComm.
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Supporting Information for:

Tuning CO_2 Uptake Capacity in Covalent Organic Frameworks via Metal Doping

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Experimental Methods

Instrumentation. Powder X-ray diffractions (XRD) patterns were collected on either a Bruker D8 with LYNXEYE XE-T detector and 40kV Cu Kα radiation (λ = 1.5418 Å) at room temperature or a Bruker D2 Phaser with LYNXEYE XE-T detector and 30 kV Cu Kα radiation (λ = 1.5406 Å) at room temperature. X-ray photoelectron spectroscopy measurements were taken on a Kratos AXIS Supra operated at a base pressure better than $5x10^{-9}$ Torr, using a monochromatic Al Kα X-ray source (1486.6 eV). Samples were packed densely onto conductive carbon tape. Surveys and high resolution for elements of interest were taken on each sample. Spectra were obtained using a large analyzer spot size and a pass energy of 160 eV for all surveys and 20 eV for the high-resolution elements, with a step size of 0.1 eV. Charge compensation was done using a charge neutralizer with a filament current of 0.42 A. Spectra were fit using CasaXPS with Shirley backgrounds and corrected to sp3 C at 285 eV. Both nitrogen (N_2) and carbon dioxide (CO_2) gas adsorption isotherms were obtained using a Micromeritics ASAP 2020, at 77 K and 273 K respectively. All COF samples were activated at 120°C for 8 h before analysis. The transmission electron microscopy (TEM) specimens were prepared by dispersing polymer powder onto carbon films supported by either Cu or Mo TEM grids. Structural and chemical analyses were performed using a FEI Titan™ G2 80-200 scanning transmission electron microscope (STEM) operating at 200 kV. This microscope is equipped with a spherical aberration (Cs) probe corrector and ChemiSTEM™ technology, which includes an X-FEG™ source and SuperX™ energy-dispersive X-ray spectroscopy (EDS) with four windowless silicon drift detectors. For STEM imaging, a high-angle annular dark-field (HAADF) detector with a collection range of 60-160 mrad was employed. Chemical mapping involved acquiring STEM EDS spectral images through multiple scans of the same region, which were spatially drift-corrected to compile the spectral data. Elemental maps were generated by selecting appropriate EDS energy windows for each element from the spectral images.

Materials. Benzene-1,3,5-tricarbaldehyde and 4,4'-diamino-[1,1-biphenyl]-3,3'-diol were purchased from Ambeed. Copper (II) acetate, manganese (II) acetate, zinc acetate dihydrate, and p-phenylenediamine, was purchased from Sigma Aldrich. Solvents were purchased from Sigma Aldrich. All materials were used without further purification.

*Synthesis of **1***. To a 50 mL round bottom flask, benzene-1,3,5-tricarbaldehyde (208 mg, 1.28 mmol) was added and dissolved in 8.75 M acetic acid (8 mL). In a 20 mL vial, p-phenylenediamine (208 mg, 1.92 mmol) was dissolved in 8 mL DI water. Both solutions were stirred for 30 minutes at room temperature before the p-phenylene diamine solution was added to the aldehyde mixture dropwise. The reaction was left stirring at room temperature for 4 days. The solid was then washed

with water, acetone, and dichloromethane (2x20 mL each) and dried under vacuum to yield a yellow powder (280.4 mg).

*Synthesis of **2**.* To a 100 mL round bottom flask, benzene-1,3,5-tricarbaldehyde (375 mg, 2.31 mmol) was added and dissolved in 8.75 M acetic acid (14.4 mL). In a 20 mL vial, 4,4'-diamino-[1,1-biphenyl]-3,3'-diol (500 mg, 2.31 mmol) was dissolved in 14.4 mL DI water. Both solutions were stirred for 30 minutes at room temperature before the 4,4'-diamino-[1,1-biphenyl]-3,3'-diol solution was added to the aldehyde suspension dropwise. The reaction was left stirring at room temperature for 4 days. The solid was then washed with water, acetone, and dichloromethane (2x20 mL each) and dried under vacuum to yield a yellow powder (678.4 mg).

Cation Complexation. COF (**1** or **2** 100 mg) and acetate salt (25 mg) were combined in a 50 mL round bottom flask. Ethanol (25 mL) was added to the round bottom and the suspension was stirred at 60°C overnight. The product was cooled to room temperature before being filtered and washed with ethanol (2x10 mL). The solid was dried under vacuum.

Computational Methods

Gas-phase electronic structure calculations were performed on molecules that represent the extended COF structure to evaluate the impact of metal adsorption on CO_2 uptake. Structural relaxations were performed at the density functional theory (DFT) level in the Gaussian16 code.[1] Carbon atoms were frozen to limit unphysical twisting. For the optimization, the hybrid B3LYP functional (Becke's three parameter hybrid exchange functional with the Lee–Yan–Parr correlation function) was used.[2-4] Metal cations Cu^{2+}, Mn^{2+}, and Zn^{2+} were simulated with the LAN2DZeffective core basis set[5,6] that includes scalar relativistic corrections and all other atoms were described using the 6-31G(d,p) basis set.[3,7,8] This level of theory has been successfully applied to previous investigations of cluster models including transition metals and *f*-electrons.[9,10] The lowest spin state was used for all calculations and all simulations were unpolarized due to the incorporation of adsorbed metal ions. A natural bond order (NBO) analysis was performed for calculation of partial atomic charges.[11-13]

Table S1. Cation loading in COFs as determined by ICP-OES analysis.

COF	Metal	Mass %
1	Mn	0.91%
1	Cu	0.56%
1	Zn	0.36%
2	Mn	3.50%
2	Cu	7.44%
2	Zn	6.04%

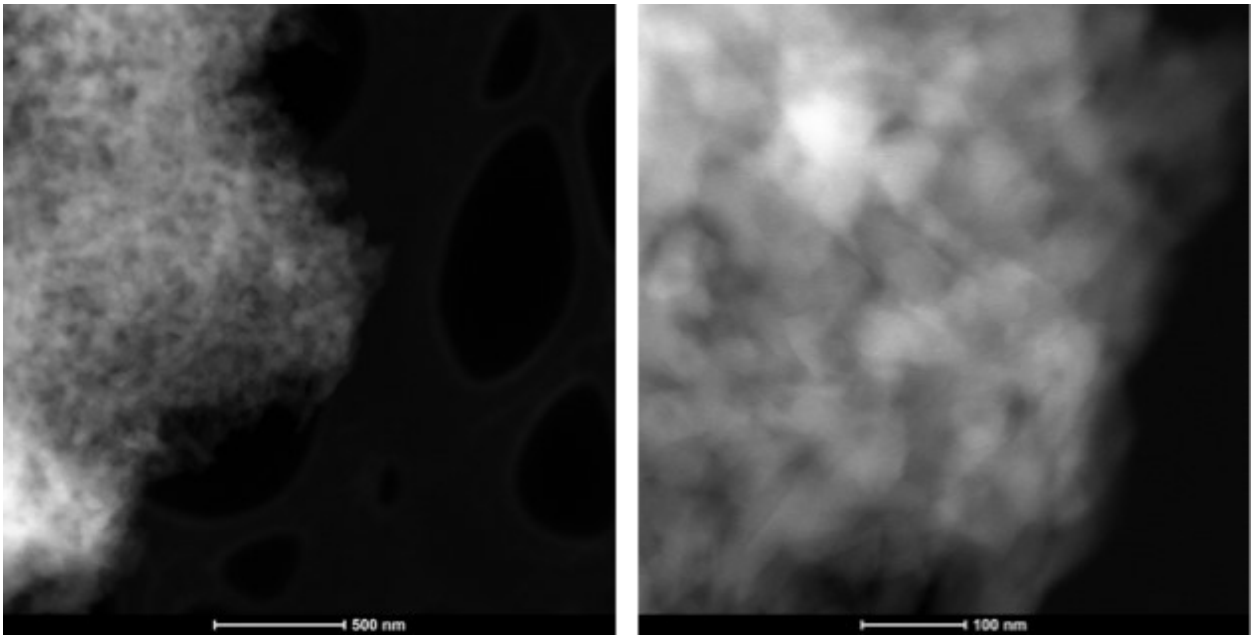


Figure S1. TEM imaging of 1 – Mn.

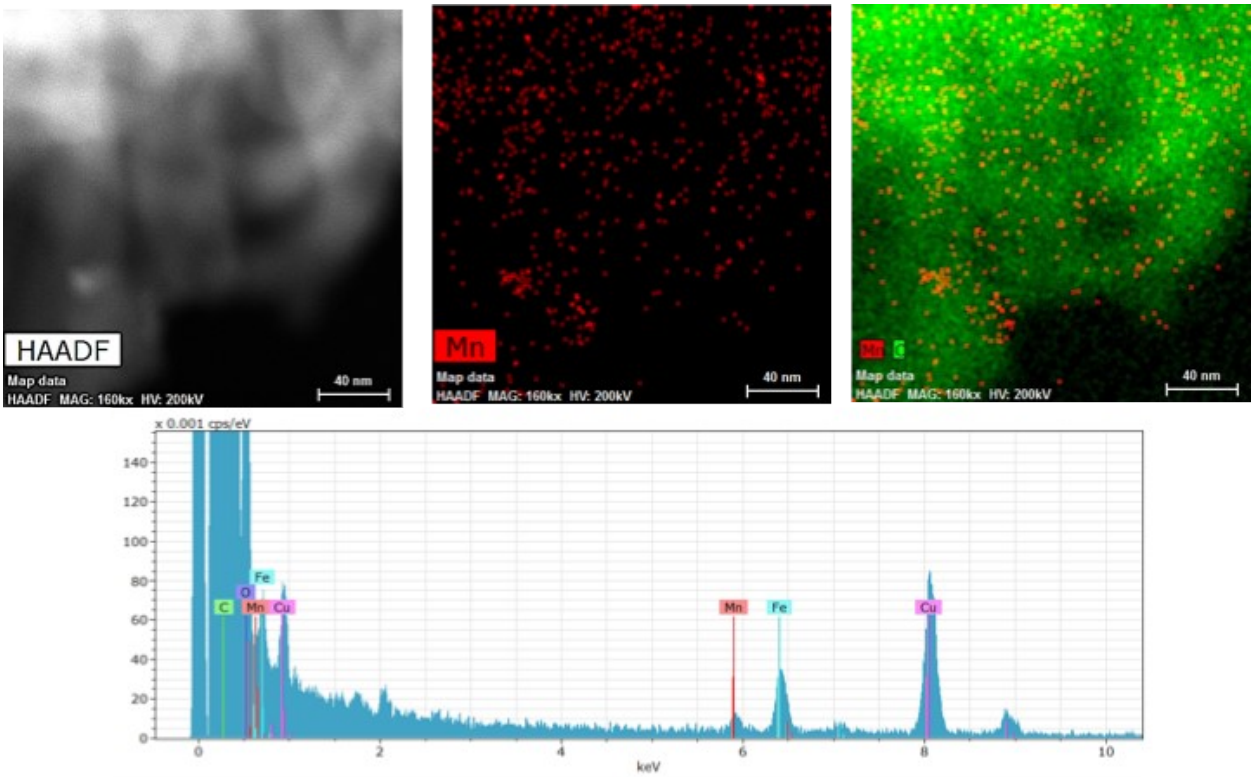


Figure S2. EDS mapping of 1 – Mn.

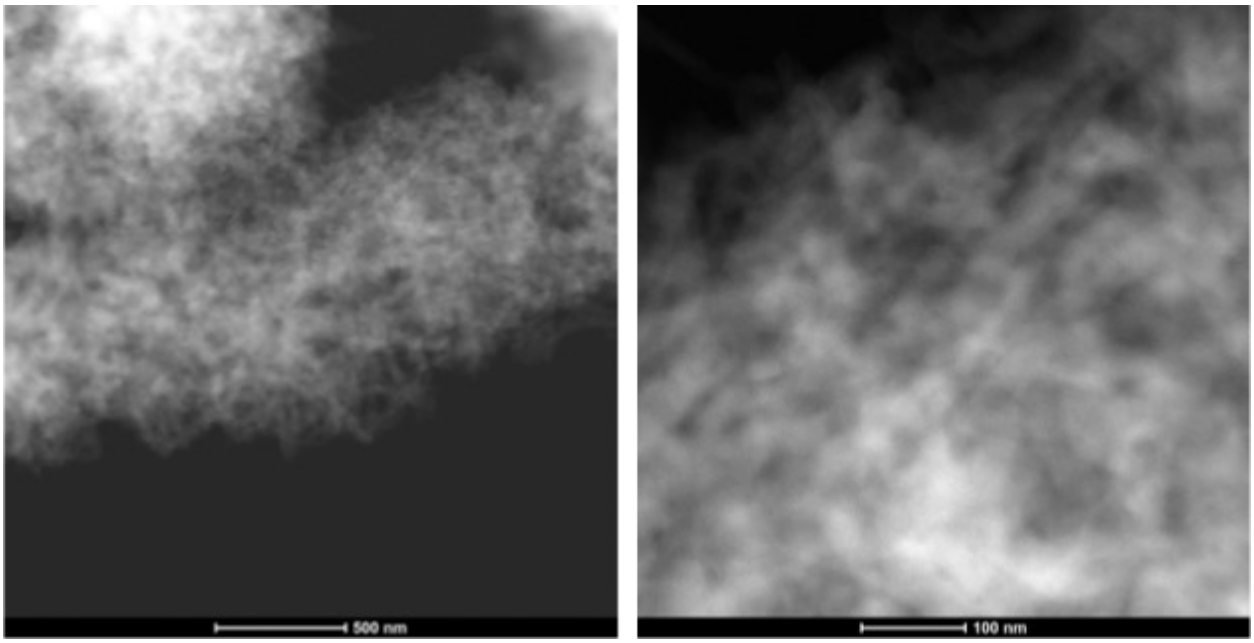


Figure S3. TEM imaging of 1 – Cu.

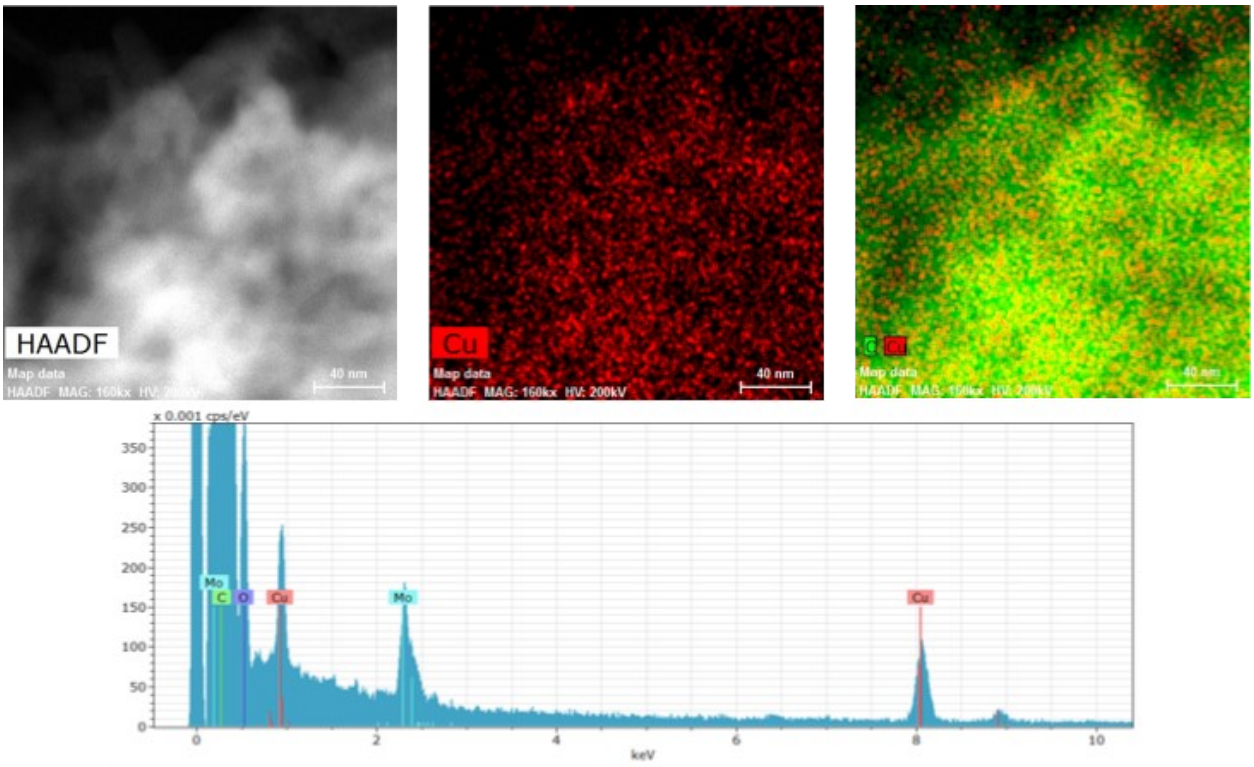


Figure S4. EDS mapping of 1 – Cu.

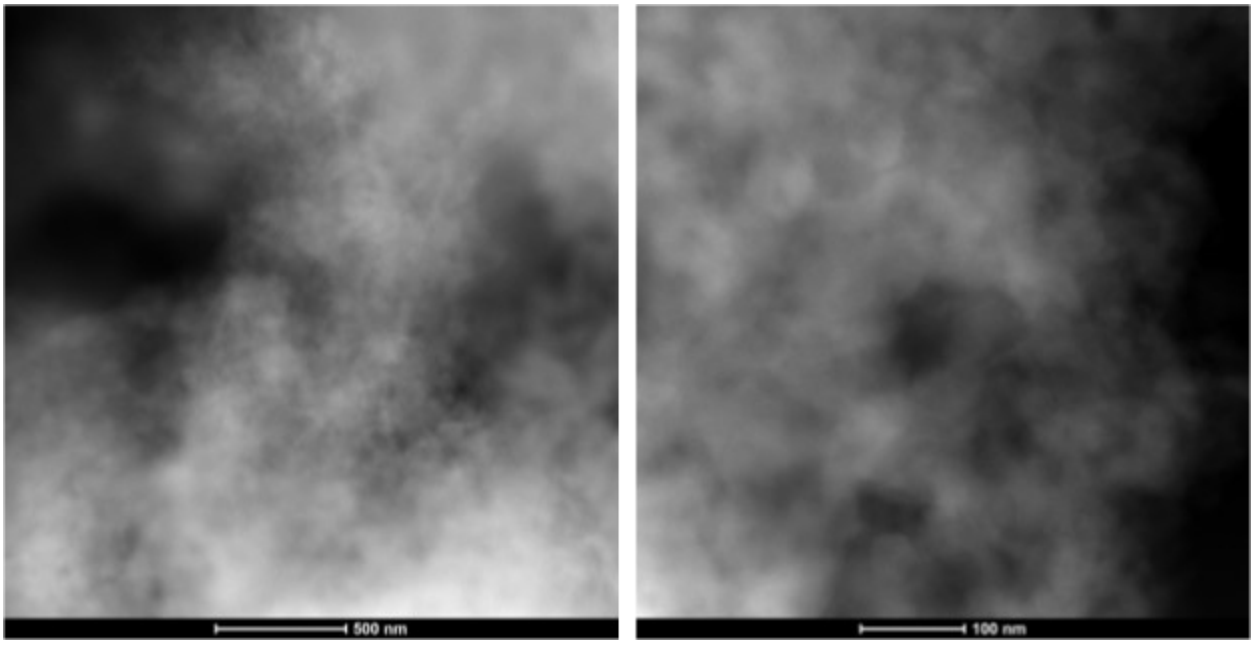


Figure S5. TEM imaging of 1 – Zn.

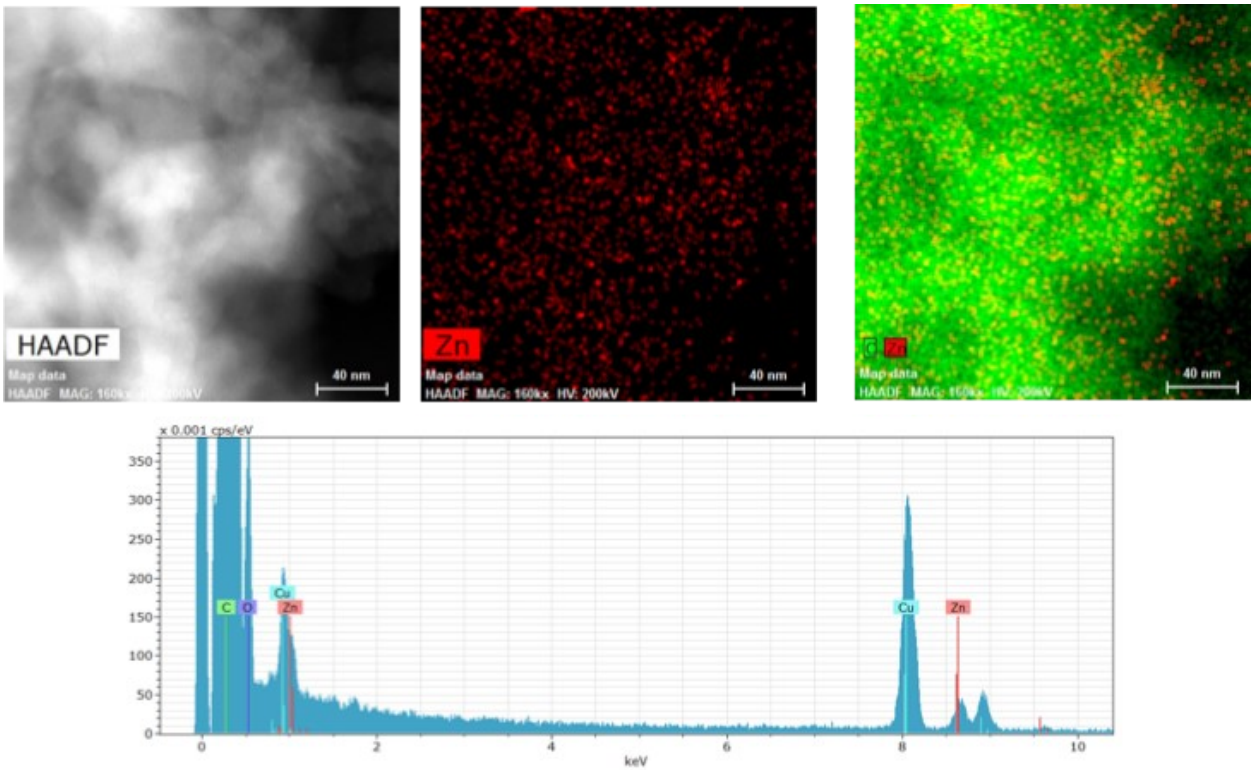


Figure S6. EDS mapping of 1 – Zn.

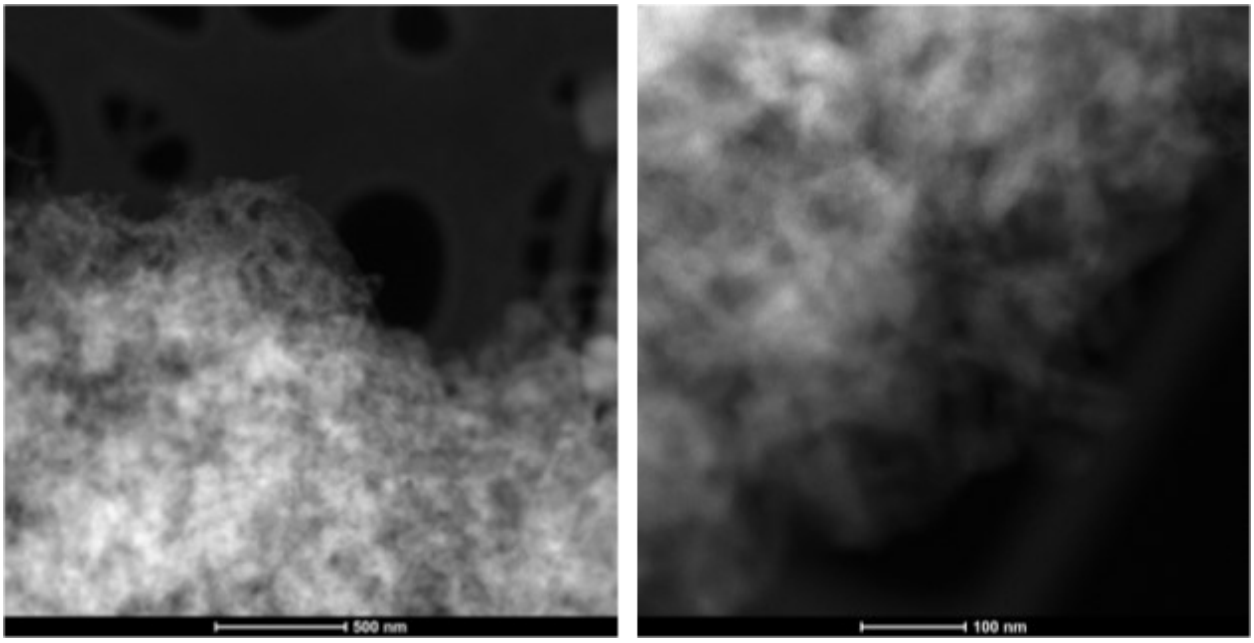


Figure S7. TEM imaging of 2 – Mn.

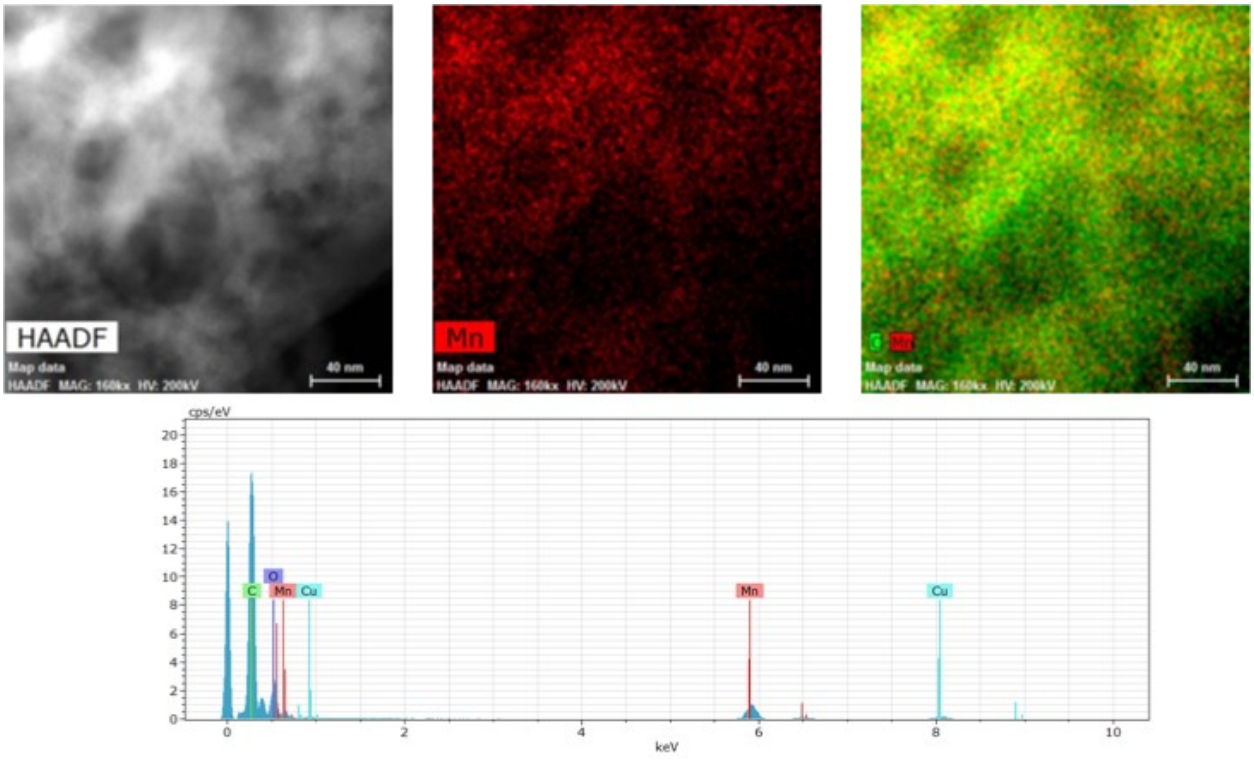


Figure S8. EDS mapping of 2 – Mn.

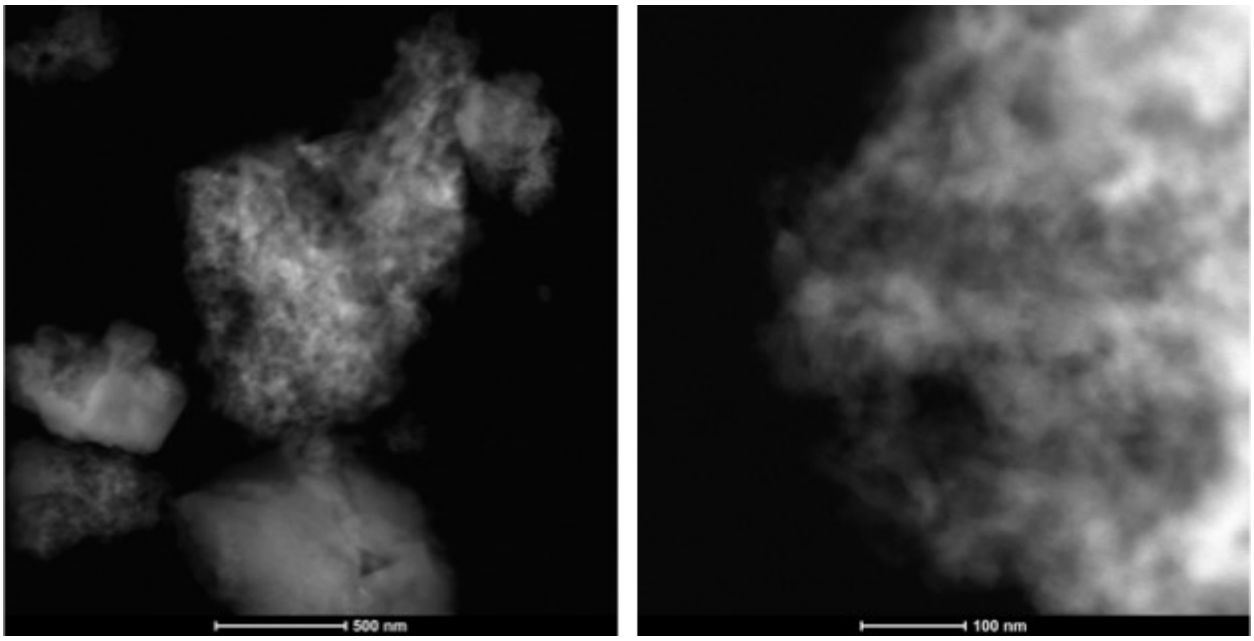


Figure S9. TEM imaging of 2 – Cu.

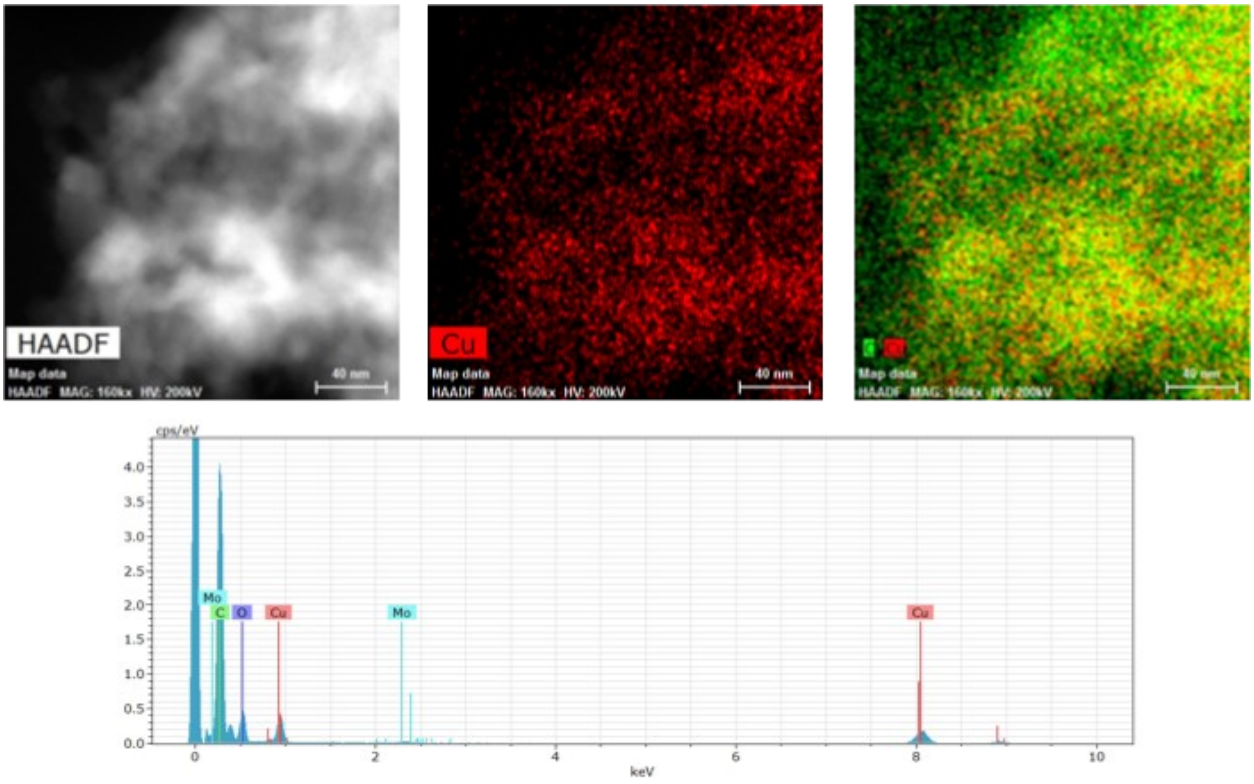


Figure S10. EDS mapping of 2 – Cu.

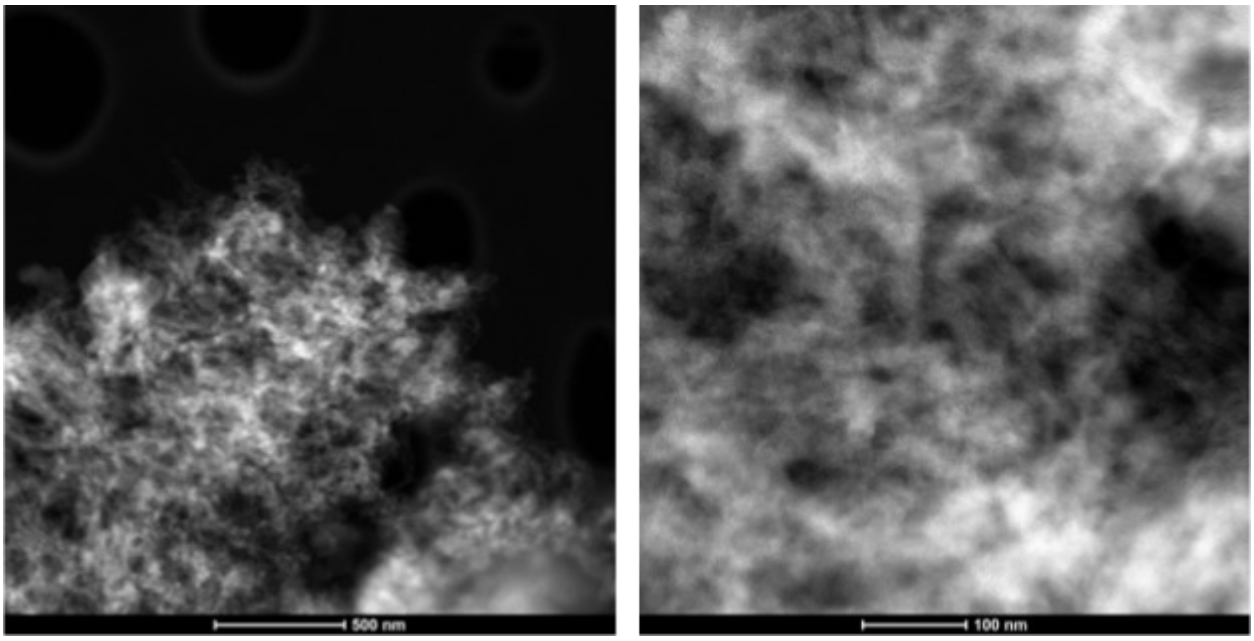


Figure S11. TEM imaging of 2 – Zn.

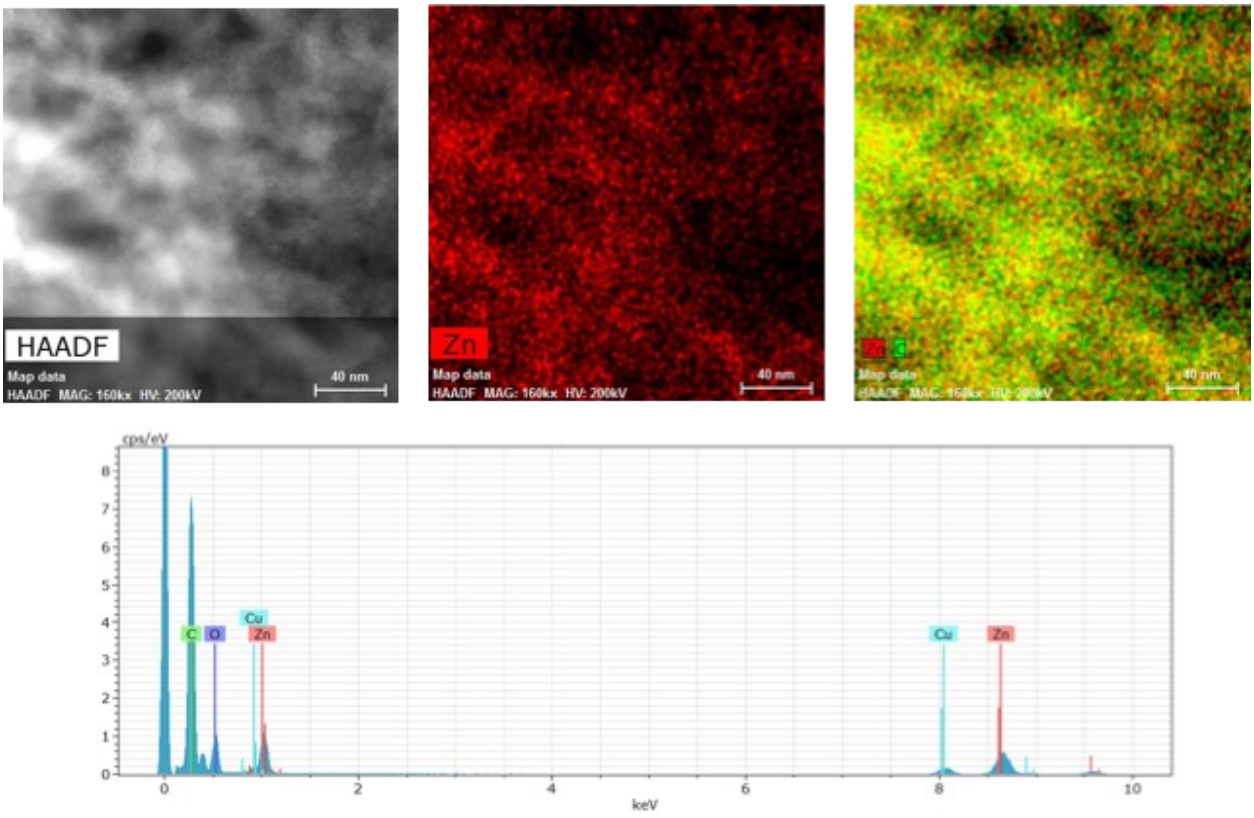


Figure S12. EDS mapping of 2 – Zn.

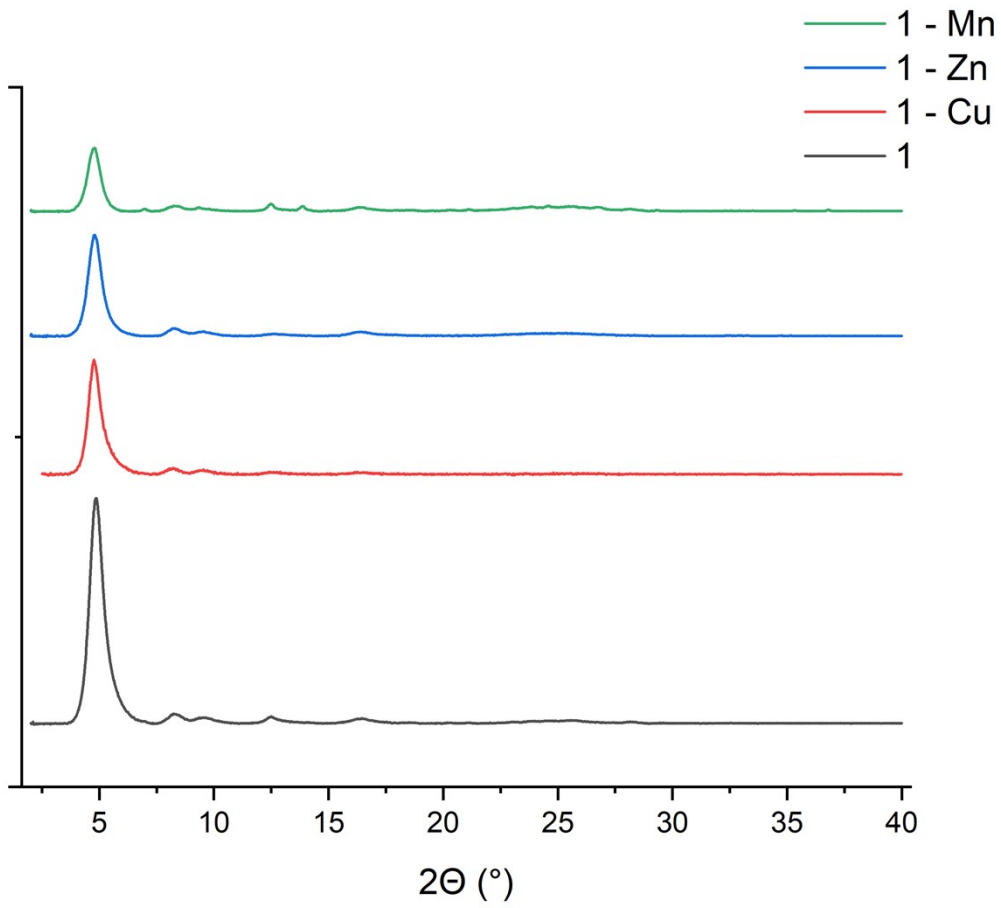


Figure S13: Powder X-Ray diffraction of **1** and metalated congeners.

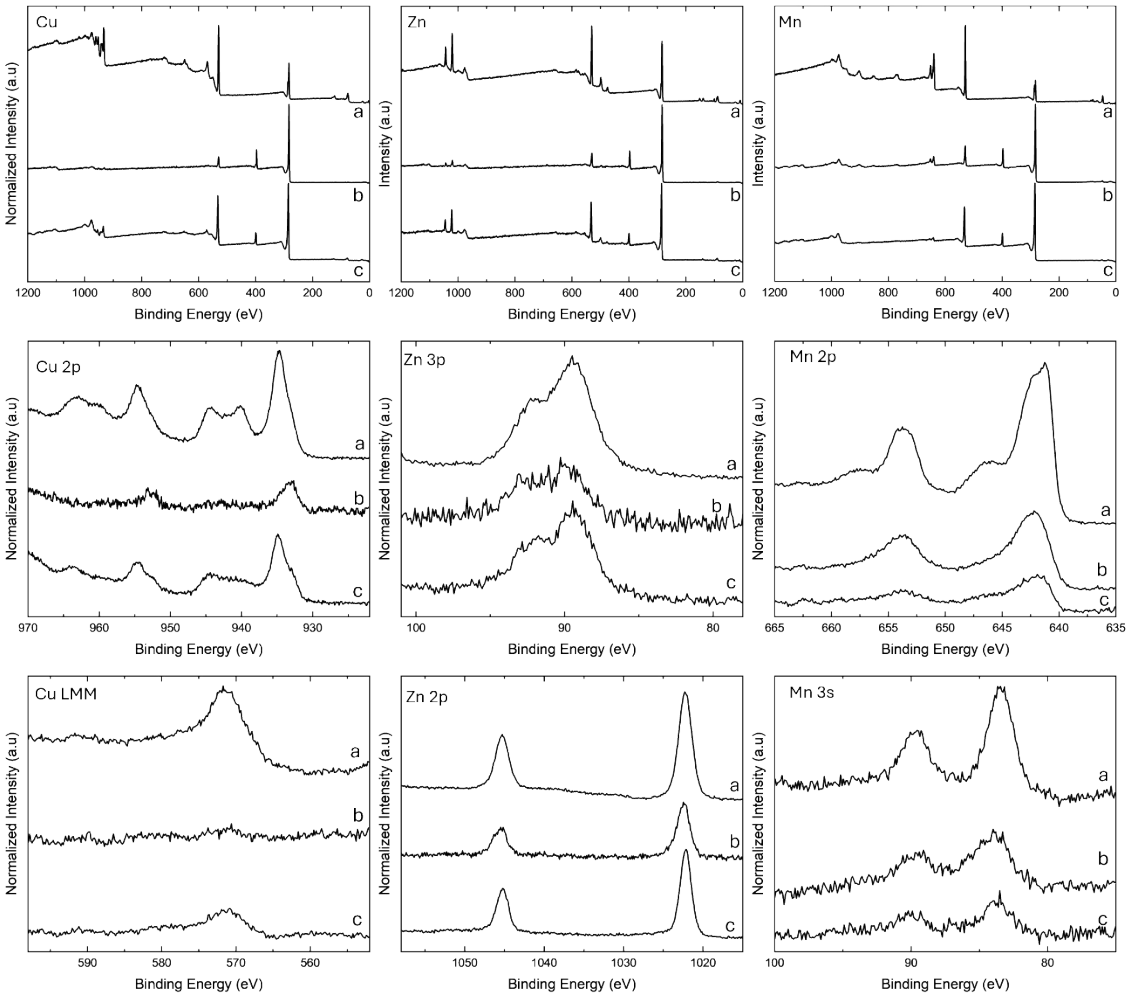


Figure S14. X-ray photoelectron surveys and high resolution spectra for a) Cu, Zn, or Mn acetate, b) Cu, Zn, or Mn complexed with 1, and c) Cu, Zn, or Mn complexed with 2.

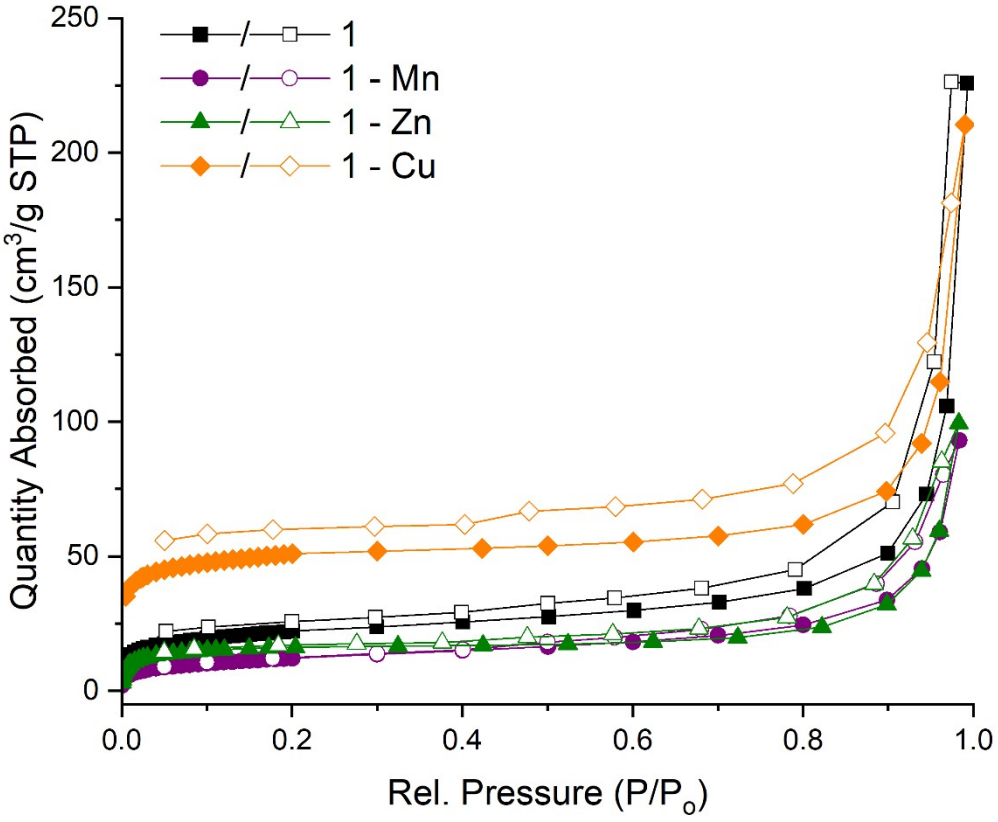


Figure S15. Nitrogen absorption isotherms of **1**.

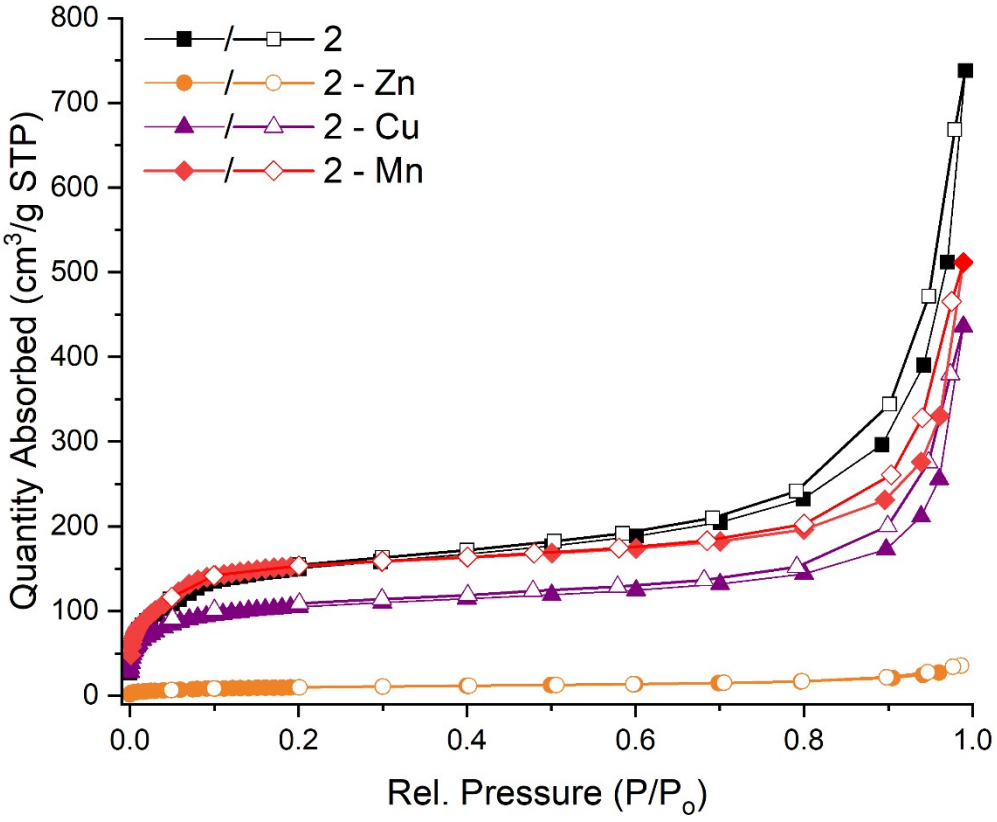
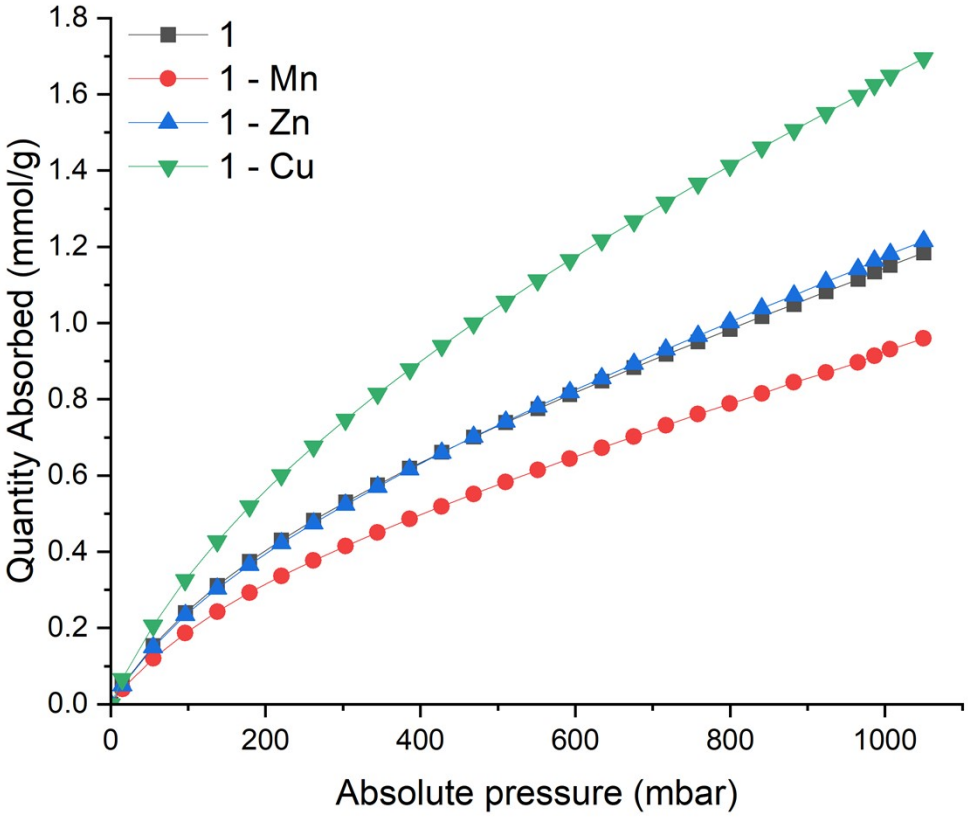


Figure S16. Nitrogen absorption isotherms of **2**.

Table S2. BET surface area analysis of **1**, **2**, and their cation – doped congeners.

COF	BET surface area (m^2/g)	Single point adsorption total pore volume of pores (cm^3/g)
1	79.1	0.16
2	549.0	0.63
1 – Zn	49.5	0.05
1 – Mn	43.0	0.05
1 – Cu	161.6	0.11
2 – Zn	26.1	0.03
2 – Mn	456.1	0.36
2 – Cu	342.5	0.27



S17. CO_2 uptake of **1** and its metal complexed species.

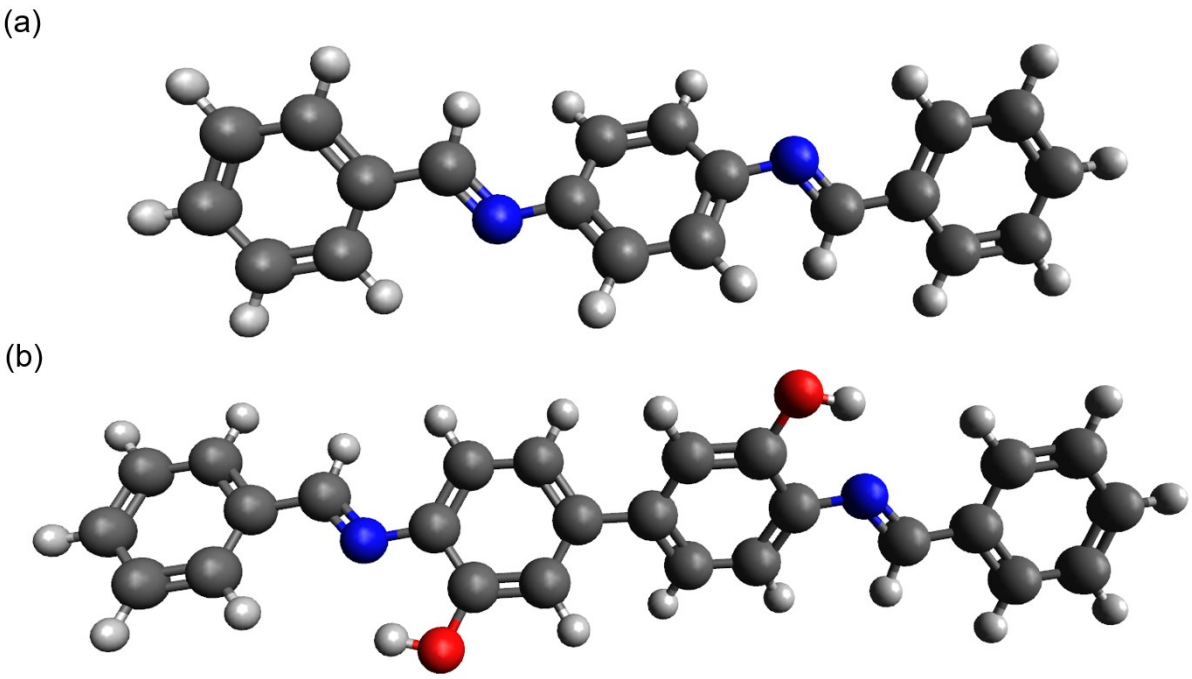


Figure S18: Snapshots of (a) **1** and (b) **2** linker molecules evaluated computationally. Atom colors: carbon (grey), nitrogen (blue), oxygen (red), hydrogen (white)

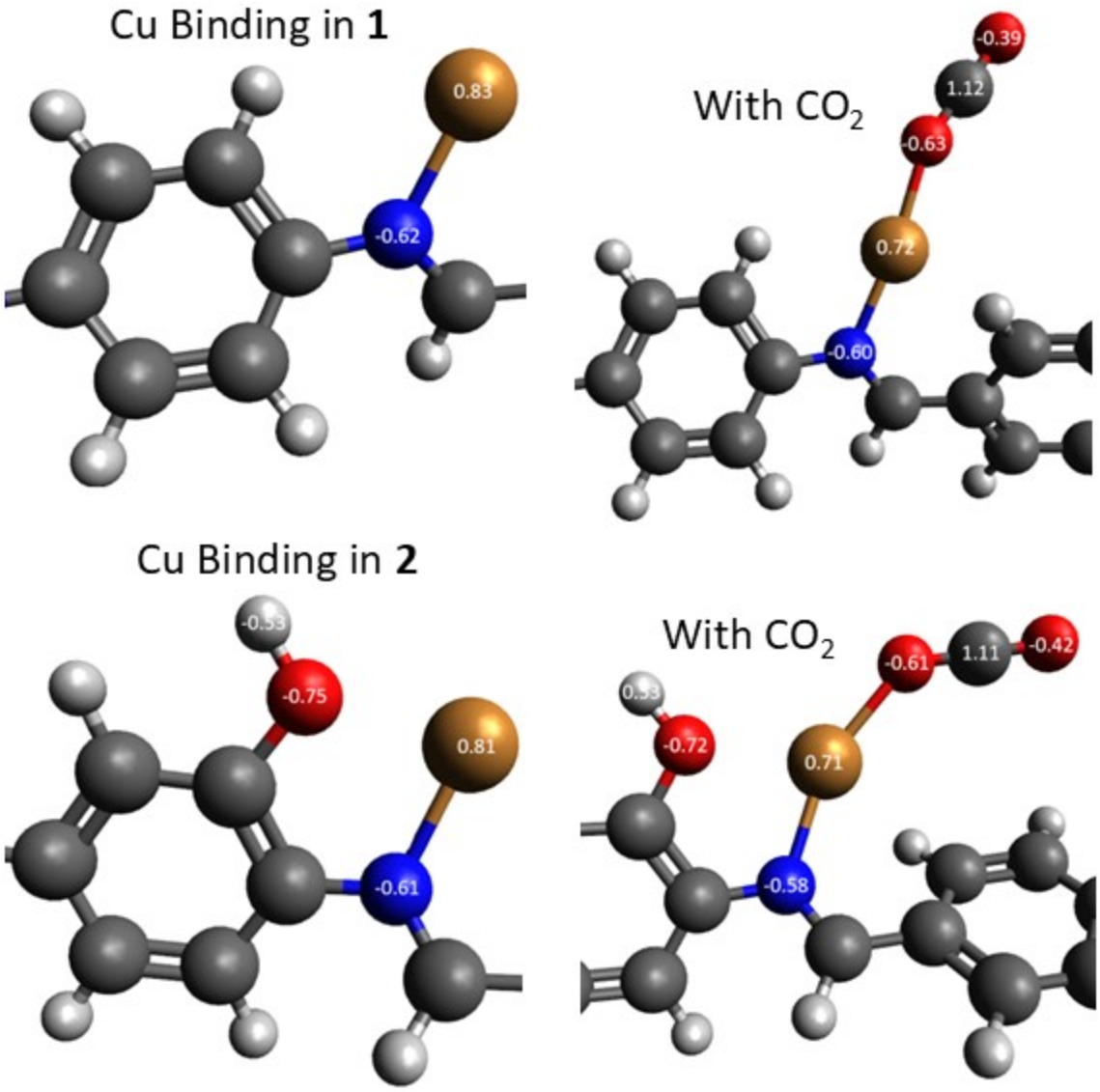


Figure S19. Snapshots of Cu2+ binding with 1 and 2 (left) and with bound CO2 (right). Mullikan partial charges are reported for nitrogen, copper, hydroxide, and carbon dioxide atoms. Atom colors: carbon (grey), hydrogen (white), nitrogen (blue), oxygen (red), and copper (gold).

Equation 2

$$B_M(\%) = \frac{E_M}{MW_M} \quad (2.a)$$

$$B_{\overline{OH}}(\%) = \frac{B_M}{I} \quad (2.b)$$

$$B(\%) = 100 - 2 \times B_M \quad (2.c)$$

Table S3. Distribution of CO_2 binding sites based on metal loading in COFs calculated via Equation 2 and the average ΔG (kJ/mol).

	1			
Metal	B_M	B_I	B	Average ΔG
Cu^{2+}	2.5	2.5	95.0	-24.47
Mn^{2+}	4.7	4.7	90.6	-24.29
Zn^{2+}	1.6	1.6	96.8	-23.84
No Metal	0.0	0.0	100.0	-23.00
	2			
	B_M	B_{OH}	B	Average ΔG
Cu^{2+}	45.9	45.9	8.2	-44.10
Mn^{2+}	24.9	24.9	50.2	-38.26
Zn^{2+}	36.4	36.4	27.2	-34.02
No Metal	0	0	100.0	-27.00

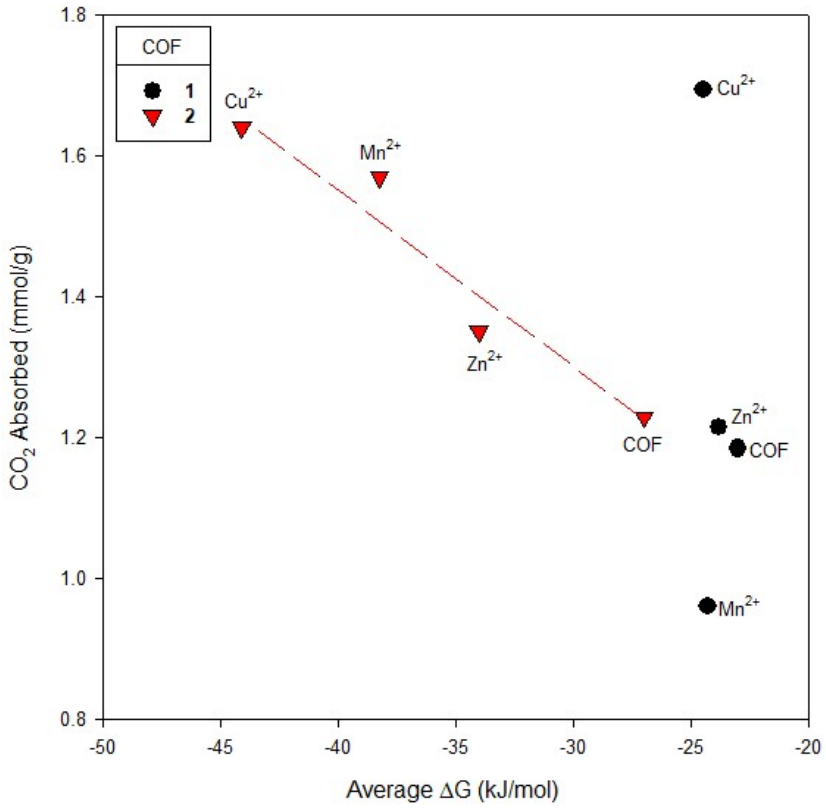


Figure S20. Trend between average reaction free energy for CO_2 absorption (calculated via density functional theory simulations) and experimental CO_2 absorption measurements for metalated COF **1** and **2** with Cu^{2+}, Zn^{2+}, or Mn^{2+}.

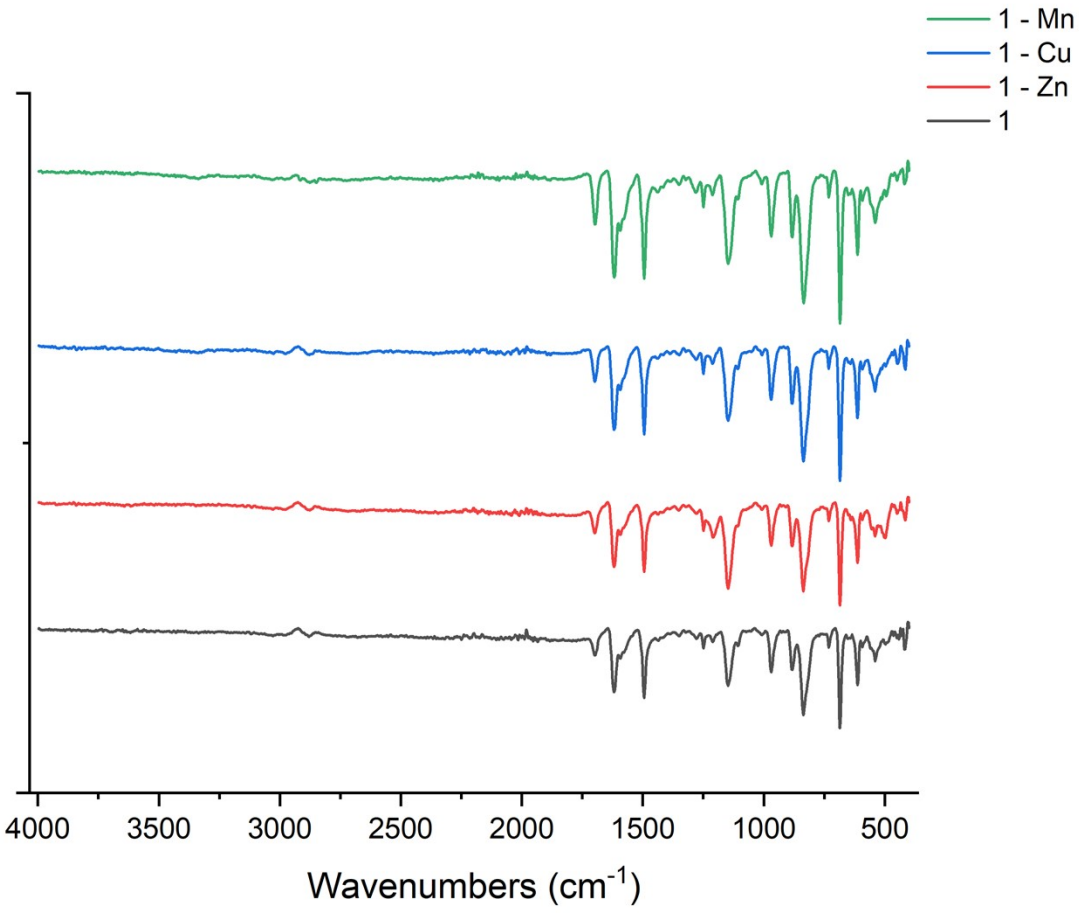


Figure S21: FTIR of **1** and metalated congeners.

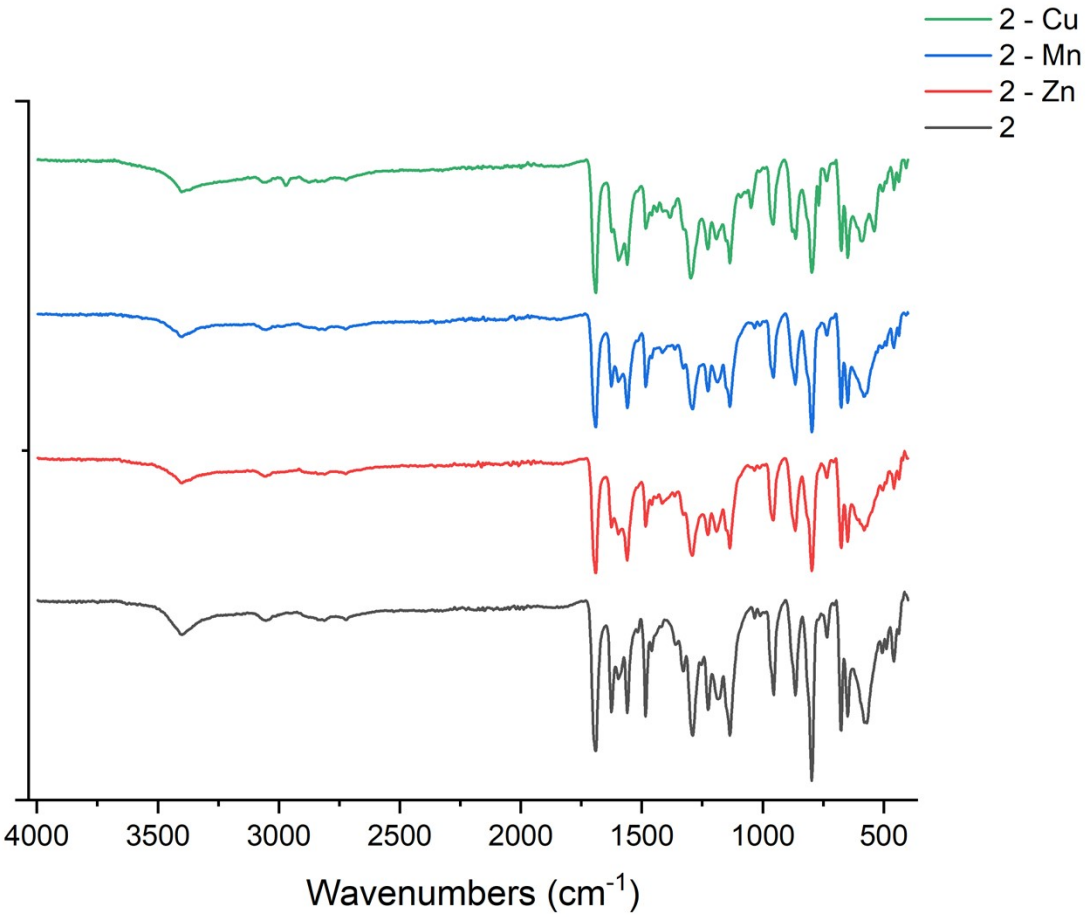


Figure S22: FTIR of **2** and metalated congeners.

Atomic Coordinates

Cu Structure 1 CO2 Bound to OH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.543697	-0.123132	0.072536
2	6	0	-0.836334	-1.357795	-0.076981
3	6	0	0.540890	-1.400403	-0.106215
4	6	0	-0.806939	1.103682	0.144903
5	6	0	0.562251	1.084829	0.134066
6	6	0	1.262922	-0.159522	0.031362
7	1	0	-1.357531	2.035518	0.210501
8	1	0	-1.412154	-2.273495	-0.178124
9	29	0	3.759175	-1.897457	-0.507738
10	7	0	2.645222	-0.312465	0.055990
11	7	0	-2.883638	-0.025222	0.104275
12	6	0	-3.714280	-0.866264	0.651011
13	6	0	-5.133663	-0.899564	0.378082
14	1	0	-3.342464	-1.564327	1.411053
15	6	0	-5.719718	-0.048552	-0.584829
16	6	0	-5.939880	-1.817439	1.082234
17	6	0	-7.304879	-1.888660	0.825632
18	6	0	-7.875010	-1.043617	-0.132373
19	6	0	-7.082063	-0.124583	-0.835501
20	6	0	3.427442	0.538145	0.663938
21	6	0	4.848382	0.618405	0.410425
22	1	0	2.994124	1.280986	1.337906
23	6	0	5.449898	-0.081199	-0.659265
24	6	0	5.642724	1.432607	1.244176
25	6	0	7.009598	1.547185	1.014004
26	6	0	7.594472	0.851003	-0.048892
27	6	0	6.813529	0.038029	-0.884215
28	1	0	-5.493922	-2.470637	1.827675
29	1	0	-7.924418	-2.592182	1.371780
30	1	0	-8.942538	-1.092368	-0.326535
31	1	0	-5.106464	0.674833	-1.108804
32	1	0	-7.534833	0.537559	-1.566102
33	1	0	4.848410	-0.463932	-1.495191
34	1	0	5.182793	1.964110	2.072770
35	1	0	7.617096	2.182594	1.650127
36	1	0	8.658000	0.952357	-0.242106
37	1	0	7.268805	-0.449501	-1.740572
38	1	0	1.120750	2.014710	0.173367
39	1	0	1.074819	-2.339750	-0.208057
40	6	0	-4.011083	3.397300	-0.433223
41	8	0	-5.058847	3.138900	-0.878913
42	8	0	-2.954277	3.634956	0.012367

Cu Structure 1 CO2 Bound to Metal

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.499023	-0.739403	-0.103659
2	6	0	1.769359	0.484885	0.021710
3	6	0	0.391398	0.504156	0.038255
4	6	0	1.783053	-1.970000	-0.264688
5	6	0	0.413975	-1.977720	-0.235085
6	6	0	-0.307748	-0.753280	-0.062165
7	1	0	2.350259	-2.885049	-0.393047
8	1	0	2.327721	1.414213	0.082513
9	29	0	-2.600175	1.114742	-0.137530
10	7	0	-1.687817	-0.629862	0.032120
11	7	0	3.838524	-0.806839	-0.128770
12	6	0	4.674882	-0.085537	0.557103
13	6	0	6.084767	0.032030	0.259364
14	1	0	4.319139	0.425908	1.460235
15	6	0	6.654016	-0.592058	-0.872598
16	6	0	6.898156	0.803180	1.114928
17	6	0	8.253617	0.953402	0.842357
18	6	0	8.807040	0.333888	-0.283189
19	6	0	8.006923	-0.438246	-1.138412
20	6	0	-2.441679	-1.609941	0.471160
21	6	0	-3.868286	-1.666016	0.244266
22	1	0	-1.972954	-2.463714	0.965193
23	6	0	-4.512020	-0.775175	-0.643149
24	6	0	-4.625035	-2.649592	0.914311
25	6	0	-5.996381	-2.742888	0.701814
26	6	0	-6.623231	-1.856440	-0.180095
27	6	0	-5.879903	-0.874022	-0.851567
28	1	0	6.464923	1.280675	1.989952
29	1	0	8.879137	1.542690	1.504554
30	1	0	9.867372	0.445122	-0.495599
31	1	0	6.031711	-1.203903	-1.515708
32	1	0	8.448816	-0.924273	-2.002121
33	1	0	-3.939245	-0.128698	-1.308999
34	1	0	-4.132656	-3.332984	1.600917
35	1	0	-6.575211	-3.505406	1.212458
36	1	0	-7.691156	-1.937332	-0.358848
37	1	0	-6.370209	-0.222399	-1.568066
38	1	0	-0.130882	-2.906292	-0.372191
39	1	0	-0.147933	1.438554	0.151638
40	6	0	-4.070567	3.842308	0.029937
41	8	0	-3.309652	2.958119	-0.148323
42	8	0	-4.796206	4.710769	0.191876

Cu Structure 2 CO2 Bound to OH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.676391	-0.476518	0.011570
2	6	0	2.898639	-1.632314	-0.034578
3	6	0	1.495914	-1.547516	-0.079182
4	6	0	0.825709	-0.308531	-0.054631
5	6	0	1.612708	0.849078	0.014334
6	6	0	3.001761	0.751235	0.044243
7	6	0	-0.648213	-0.230872	-0.114934
8	6	0	-1.460137	-1.082006	0.646353
9	6	0	-2.851345	-1.013759	0.534207
10	6	0	-1.292295	0.689190	-0.955730
11	6	0	-2.690848	0.742076	-1.058614
12	6	0	-3.518058	-0.107953	-0.312515
13	1	0	0.921871	-2.466303	-0.150619
14	1	0	3.360053	-2.613204	-0.043913
15	1	0	1.169780	1.837199	0.064973
16	1	0	-0.701652	1.346503	-1.585603
17	1	0	-3.134606	1.430654	-1.771422
18	1	0	-1.016606	-1.793516	1.338569
19	8	0	-3.671646	-1.849208	1.288189
20	7	0	-4.892744	-0.104148	-0.281709
21	7	0	5.046329	-0.394510	-0.014140
22	6	0	5.817138	-1.408203	-0.327147
23	6	0	7.294647	-1.348451	-0.276285
24	1	0	5.396413	-2.360327	-0.668508
25	6	0	7.952998	-0.152642	0.026104
26	6	0	8.029016	-2.506758	-0.547715
27	6	0	9.424527	-2.465571	-0.513627
28	6	0	10.081971	-1.270860	-0.217345
29	6	0	9.347953	-0.115441	0.051068
30	6	0	-5.507790	1.018605	-0.406022
31	6	0	-6.984989	1.020965	-0.403674
32	1	0	-4.973182	1.967344	-0.475604
33	6	0	-7.742816	-0.118913	-0.712255
34	6	0	-7.655659	2.203458	-0.069286
35	6	0	-9.051965	2.240127	-0.023889
36	6	0	-9.791955	1.095452	-0.309827
37	6	0	-9.138198	-0.083034	-0.658343
38	1	0	7.519933	-3.436884	-0.785143
39	1	0	9.995036	-3.364704	-0.722543
40	1	0	11.167499	-1.241596	-0.199627
41	1	0	7.377109	0.742538	0.226849
42	1	0	9.858369	0.815279	0.276624
43	1	0	-7.260791	-1.005407	-1.127671
44	1	0	-7.087870	3.101636	0.160131
45	1	0	-9.555973	3.165224	0.237112
46	1	0	-10.876787	1.127465	-0.280972
47	1	0	-9.708424	-0.966248	-0.929105
48	8	0	3.688873	1.882329	0.112747
49	1	0	4.654383	1.688173	0.154391
50	29	0	-5.728523	-1.706629	0.631257
51	1	0	-3.157771	-2.502745	1.790564
52	6	0	6.463777	4.042072	0.524807
53	8	0	6.591323	5.189378	0.653987
54	8	0	6.337953	2.879283	0.394259

Cu Structure 2 CO2 Bound to Metal

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.950170	-0.198432	0.155600
2	6	0	-4.209544	0.901392	-0.274227
3	6	0	-2.807656	0.830534	-0.354906
4	6	0	-2.100383	-0.330860	0.013592
5	6	0	-2.849318	-1.425625	0.466108
6	6	0	-4.238502	-1.346583	0.528221
7	6	0	-0.628198	-0.398504	-0.087439
8	6	0	0.186593	0.657349	0.342095
9	6	0	1.573895	0.581516	0.192631
10	6	0	0.010306	-1.519825	-0.638116
11	6	0	1.404840	-1.578090	-0.783749
12	6	0	2.234349	-0.527651	-0.369033
13	1	0	-2.264143	1.693630	-0.726849
14	1	0	-4.699368	1.825254	-0.560055
15	1	0	-2.374958	-2.343955	0.793134
16	1	0	-0.583687	-2.347604	-1.011770
17	1	0	1.839467	-2.445122	-1.272181
18	1	0	-0.250106	1.536887	0.808641
19	8	0	2.388375	1.608883	0.633293
20	7	0	3.611073	-0.490254	-0.373455
21	7	0	-6.317547	-0.310055	0.215799
22	6	0	-7.129139	0.550086	-0.351727
23	6	0	-8.601175	0.483920	-0.217854
24	1	0	-6.748215	1.365010	-0.976100
25	6	0	-9.211526	-0.574065	0.462562
26	6	0	-9.379598	1.492293	-0.793952
27	6	0	-10.770928	1.440078	-0.685411
28	6	0	-11.380640	0.381296	-0.011182
29	6	0	-10.602770	-0.625250	0.561184
30	6	0	4.251719	-1.595797	-0.207153
31	6	0	5.727335	-1.572607	-0.271520
32	1	0	3.741487	-2.536510	0.005156
33	6	0	6.438474	-0.568110	-0.945403
34	6	0	6.445267	-2.585930	0.374735
35	6	0	7.842760	-2.583674	0.365423
36	6	0	8.536807	-1.568021	-0.287549
37	6	0	7.835346	-0.562529	-0.946813
38	1	0	-8.907405	2.314198	-1.325090
39	1	0	-11.375513	2.223399	-1.130860
40	1	0	-12.463204	0.339998	0.064533
41	1	0	-8.601312	-1.354715	0.902285
42	1	0	-11.076381	-1.451223	1.081880
43	1	0	5.911601	0.145754	-1.575925
44	1	0	5.913961	-3.382040	0.890196
45	1	0	8.384074	-3.377920	0.869495
46	1	0	9.622484	-1.573101	-0.301115
47	1	0	8.369972	0.199421	-1.506329
48	8	0	-4.906215	-2.407616	0.964920
49	1	0	-5.863487	-2.174976	0.960004
50	29	0	4.478207	1.288817	0.059113
51	1	0	1.875500	2.376973	0.932829
52	6	0	7.146918	2.587261	0.557839
53	8	0	5.963525	2.587974	0.514128
54	8	0	8.301340	2.601771	0.600622

Mn Structure 1 CO2 Bound to OH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.502764	-0.168174	0.036806
2	6	0	-0.804768	-1.401590	-0.159360
3	6	0	0.571962	-1.452352	-0.198055
4	6	0	-0.757297	1.050490	0.146741
5	6	0	0.611687	1.023013	0.127314
6	6	0	1.303381	-0.221746	-0.021513
7	1	0	-1.300949	1.983151	0.248471
8	1	0	-1.387443	-2.308928	-0.291457
9	25	0	4.061764	-1.849162	-0.411562
10	7	0	2.690444	-0.368539	-0.046857
11	7	0	-2.842444	-0.063595	0.077793
12	6	0	-3.675212	-0.916235	0.601712
13	6	0	-5.096292	-0.930631	0.336038
14	1	0	-3.303997	-1.643086	1.334725
15	6	0	-5.681764	-0.043084	-0.593664
16	6	0	-5.904853	-1.866846	1.012790
17	6	0	-7.271718	-1.920046	0.761816
18	6	0	-7.841319	-1.038796	-0.163323
19	6	0	-7.045976	-0.101442	-0.839025
20	6	0	3.475832	0.439093	0.621920
21	6	0	4.895946	0.518834	0.362794
22	1	0	3.058971	1.110590	1.376202
23	6	0	5.486751	-0.147668	-0.733558
24	6	0	5.700484	1.298441	1.219649
25	6	0	7.066825	1.411758	0.985665
26	6	0	7.641018	0.748670	-0.103877
27	6	0	6.849927	-0.029927	-0.962076
28	1	0	-5.459076	-2.548236	1.732695
29	1	0	-7.893074	-2.637970	1.286770
30	1	0	-8.910148	-1.073952	-0.353128
31	1	0	-5.065933	0.692959	-1.096390
32	1	0	-7.498152	0.588126	-1.544215
33	1	0	4.865356	-0.407678	-1.618530
34	1	0	5.249768	1.803406	2.069516
35	1	0	7.680906	2.026075	1.636238
36	1	0	8.703902	0.848987	-0.300535
37	1	0	7.295659	-0.488179	-1.839561
38	1	0	1.178130	1.946848	0.191879
39	1	0	1.101675	-2.388247	-0.342804
40	6	0	-3.954486	3.381673	-0.319896
41	8	0	-2.895385	3.594891	0.132613
42	8	0	-5.004599	3.148797	-0.773959

Mn Structure 1 CO2 Bound to Metal

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.599106	-0.652841	-0.088953
2	6	0	1.862090	0.573343	-0.105228
3	6	0	0.483943	0.585854	-0.113849
4	6	0	1.891355	-1.897890	-0.132085
5	6	0	0.522031	-1.910835	-0.124743
6	6	0	-0.208062	-0.679589	-0.092700
7	1	0	2.465542	-2.817371	-0.166728
8	1	0	2.417285	1.506883	-0.121544
9	25	0	-2.972120	0.939787	-0.146754
10	7	0	-1.598412	-0.571208	-0.071324
11	7	0	3.940419	-0.712046	-0.087500
12	6	0	4.760423	0.080000	0.535492
13	6	0	6.174696	0.174327	0.250572
14	1	0	4.386963	0.682471	1.373214
15	6	0	6.766030	-0.561527	-0.800002
16	6	0	6.969897	1.035903	1.033903
17	6	0	8.329182	1.165001	0.769678
18	6	0	8.904564	0.434272	-0.275262
19	6	0	8.122630	-0.428164	-1.057928
20	6	0	-2.346820	-1.488465	0.491743
21	6	0	-3.769061	-1.576762	0.247945
22	1	0	-1.896657	-2.239900	1.144837
23	6	0	-4.401421	-0.787796	-0.738648
24	6	0	-4.533038	-2.489352	1.004903
25	6	0	-5.900128	-2.612749	0.780600
26	6	0	-6.515544	-1.827524	-0.199778
27	6	0	-5.765072	-0.916392	-0.958123
28	1	0	6.519226	1.600345	1.846096
29	1	0	8.940603	1.824938	1.376111
30	1	0	9.967609	0.528242	-0.476855
31	1	0	6.154057	-1.239604	-1.386242
32	1	0	8.581269	-0.998584	-1.859030
33	1	0	-3.805433	-0.343734	-1.559160
34	1	0	-4.049982	-3.091021	1.769791
35	1	0	-6.482560	-3.327710	1.352633
36	1	0	-7.578640	-1.935517	-0.391465
37	1	0	-6.241648	-0.355747	-1.756214
38	1	0	-0.017531	-2.851452	-0.175753
39	1	0	-0.076485	1.514796	-0.118826
40	6	0	-4.782104	3.632767	0.061889
41	8	0	-5.422386	4.588144	0.138267
42	8	0	-4.122971	2.652052	-0.014117

Mn Structure 2 CO2 Bound to OH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.598624	-0.495587	-0.014340
2	6	0	-2.829553	-1.657337	0.027594
3	6	0	-1.426257	-1.583216	0.073087
4	6	0	-0.746789	-0.349129	0.053637
5	6	0	-1.525067	0.814531	-0.011162
6	6	0	-2.914807	0.727205	-0.041990
7	6	0	0.727638	-0.283021	0.115093
8	6	0	1.533512	-1.137097	-0.649232
9	6	0	2.925220	-1.079368	-0.536798
10	6	0	1.378224	0.629132	0.959532
11	6	0	2.777045	0.671025	1.063243
12	6	0	3.598417	-0.181861	0.313705
13	1	0	-0.859249	-2.506622	0.141323
14	1	0	-3.298283	-2.634786	0.033080
15	1	0	-1.074860	1.799553	-0.057993
16	1	0	0.792232	1.288791	1.591222
17	1	0	3.226662	1.353314	1.778404
18	1	0	1.084733	-1.844409	-1.342602
19	8	0	3.787504	-1.906389	-1.271937
20	7	0	4.971559	-0.198790	0.289752
21	7	0	-4.968045	-0.403542	0.010802
22	6	0	-5.746419	-1.412531	0.319797
23	6	0	-7.223426	-1.341518	0.268593
24	1	0	-5.332973	-2.369066	0.657752
25	6	0	-7.872672	-0.139651	-0.029431
26	6	0	-7.966561	-2.495339	0.535228
27	6	0	-9.361708	-2.443581	0.500698
28	6	0	-10.010063	-1.242840	0.208795
29	6	0	-9.267300	-0.091913	-0.054814
30	6	0	5.596128	0.929064	0.413555
31	6	0	7.073493	0.920324	0.411003
32	1	0	5.066750	1.880141	0.465774
33	6	0	7.822631	-0.226162	0.715987
34	6	0	7.753121	2.098990	0.080938
35	6	0	9.149705	2.125588	0.037064
36	6	0	9.880969	0.974271	0.318723
37	6	0	9.218255	-0.200669	0.662249
38	1	0	-7.464536	-3.430146	0.769292
39	1	0	-9.939029	-3.339219	0.705891
40	1	0	-11.095332	-1.205384	0.190751
41	1	0	-7.289996	0.751962	-0.226422
42	1	0	-9.770629	0.843483	-0.276944
43	1	0	7.333072	-1.102462	1.154790
44	1	0	7.191243	3.000230	-0.149721
45	1	0	9.660823	3.048556	-0.217919
46	1	0	10.965868	0.996781	0.288137
47	1	0	9.781277	-1.089492	0.929708
48	8	0	-3.593619	1.863752	-0.106526
49	1	0	-4.560397	1.676470	-0.149250
50	25	0	5.866942	-1.603813	-0.753147
51	1	0	3.306588	-2.561426	-1.805345
52	6	0	-6.346867	4.047438	-0.508308
53	8	0	-6.459718	5.197010	-0.631103
54	8	0	-6.235616	2.882487	-0.384160

Mn Structure 2 CO2 Bound to Metal

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.823297	-0.185413	0.164238
2	6	0	-4.082799	0.839496	-0.422371
3	6	0	-2.682599	0.747940	-0.511053
4	6	0	-1.976551	-0.357054	0.004208
5	6	0	-2.724994	-1.373708	0.612716
6	6	0	-4.112719	-1.276696	0.681708
7	6	0	-0.506355	-0.448636	-0.106275
8	6	0	0.320175	0.650103	0.163224
9	6	0	1.704984	0.544285	0.008011
10	6	0	0.118207	-1.639706	-0.505831
11	6	0	1.510135	-1.727525	-0.660679
12	6	0	2.351356	-0.636475	-0.404569
13	1	0	-2.139714	1.547738	-1.005353
14	1	0	-4.571692	1.718681	-0.826356
15	1	0	-2.251117	-2.241668	1.056972
16	1	0	-0.485926	-2.506709	-0.752813
17	1	0	1.936200	-2.654359	-1.033015
18	1	0	-0.105464	1.589036	0.509060
19	8	0	2.595207	1.586674	0.284680
20	7	0	3.718845	-0.611432	-0.477374
21	7	0	-6.190593	-0.276910	0.257864
22	6	0	-7.005066	0.502353	-0.412227
23	6	0	-8.475417	0.465995	-0.251113
24	1	0	-6.628627	1.220624	-1.148113
25	6	0	-9.081878	-0.483989	0.576264
26	6	0	-9.256369	1.391373	-0.949999
27	6	0	-10.646292	1.364800	-0.816908
28	6	0	-11.252208	0.413159	0.004431
29	6	0	-10.471852	-0.510930	0.699358
30	6	0	4.364582	-1.687365	-0.125273
31	6	0	5.839436	-1.683158	-0.210759
32	1	0	3.854957	-2.554952	0.291949
33	6	0	6.546544	-0.786782	-1.026486
34	6	0	6.560916	-2.603455	0.559222
35	6	0	7.958117	-2.613267	0.530636
36	6	0	8.648423	-1.701943	-0.264737
37	6	0	7.943218	-0.791315	-1.046361
38	1	0	-8.787150	2.128928	-1.595352
39	1	0	-11.252860	2.083898	-1.357773
40	1	0	-12.333802	0.390597	0.099384
41	1	0	-8.469669	-1.201282	1.110910
42	1	0	-10.942595	-1.254089	1.334814
43	1	0	6.015054	-0.181080	-1.767299
44	1	0	6.031206	-3.312530	1.189815
45	1	0	8.501688	-3.336240	1.130696
46	1	0	9.733694	-1.713411	-0.289479
47	1	0	8.471795	-0.111089	-1.707263
48	8	0	-4.780569	-2.262519	1.269723
49	1	0	-5.736168	-2.024737	1.245500
50	25	0	4.686134	1.011594	-0.075666
51	1	0	2.141369	2.413339	0.519487
52	6	0	6.557642	3.541753	0.740744
53	8	0	5.748119	2.726765	0.466052
54	8	0	7.339203	4.349684	1.009760

Zn Structure 1 CO2 Bound to OH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.611137	-0.031994	0.049789
2	6	0	0.911090	1.187500	0.381183
3	6	0	-0.454623	1.219160	0.378915
4	6	0	0.838536	-1.185987	-0.338314
5	6	0	-0.527235	-1.146281	-0.332700
6	6	0	-1.212135	0.043058	0.078439
7	1	0	1.375173	-2.086682	-0.614872
8	1	0	1.482296	2.086338	0.589290
9	30	0	-3.963093	2.014600	-0.197965
10	7	0	-2.565423	0.103135	0.142462
11	7	0	2.939731	-0.122140	-0.017301
12	6	0	3.813398	0.578470	0.673345
13	6	0	5.166207	0.760292	0.277808
14	1	0	3.511387	1.009869	1.635550
15	6	0	5.659582	0.256611	-0.960276
16	6	0	6.031806	1.492668	1.137701
17	6	0	7.347185	1.714503	0.769893
18	6	0	7.816620	1.213828	-0.456860
19	6	0	6.972541	0.488945	-1.319856
20	6	0	-3.371767	-0.881672	0.474302
21	6	0	-4.780362	-0.856912	0.198379
22	1	0	-2.977649	-1.686483	1.097870
23	6	0	-5.316133	-0.168819	-0.941120
24	6	0	-5.669146	-1.484566	1.101538
25	6	0	-7.040711	-1.373183	0.917156
26	6	0	-7.559068	-0.668178	-0.185100
27	6	0	-6.703994	-0.085661	-1.119227
28	1	0	5.655205	1.872330	2.083760
29	1	0	8.015083	2.266031	1.423021
30	1	0	8.851625	1.381871	-0.740436
31	1	0	4.997859	-0.316691	-1.599355
32	1	0	7.360334	0.104662	-2.257396
33	1	0	-4.662764	0.053532	-1.783663
34	1	0	-5.275026	-2.020666	1.960190
35	1	0	-7.718569	-1.835341	1.627821
36	1	0	-8.633799	-0.611046	-0.327853
37	1	0	-7.105441	0.392811	-2.006781
38	1	0	-1.105860	-2.014244	-0.633667
39	1	0	-0.988315	2.136949	0.612760
40	6	0	4.198953	-3.072361	-0.032385
41	8	0	3.142477	-3.542232	-0.217841
42	8	0	5.244998	-2.587108	0.152957

Zn Structure 1 CO2 Bound to Metal

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.473422	-0.783426	-0.076650
2	6	0	1.765424	0.459371	-0.042732
3	6	0	0.387908	0.504227	-0.036929
4	6	0	1.736155	-2.009442	-0.155872
5	6	0	0.367035	-1.990752	-0.135285
6	6	0	-0.333222	-0.744741	-0.053565
7	1	0	2.287426	-2.939780	-0.234191
8	1	0	2.345319	1.377254	-0.044702
9	30	0	-3.055586	0.932736	-0.290126
10	7	0	-1.705154	-0.596483	0.032040
11	7	0	3.821851	-0.851131	-0.125857
12	6	0	4.657053	-0.123383	0.551376
13	6	0	6.070496	-0.052023	0.255841
14	1	0	4.303215	0.457777	1.414126
15	6	0	6.634652	-0.764135	-0.825597
16	6	0	6.892946	0.762819	1.060736
17	6	0	8.252416	0.869477	0.787597
18	6	0	8.800798	0.162660	-0.287864
19	6	0	7.991598	-0.653390	-1.092253
20	6	0	-2.485371	-1.523776	0.523823
21	6	0	-3.911411	-1.570829	0.291069
22	1	0	-2.042924	-2.341466	1.091605
23	6	0	-4.534127	-0.732732	-0.660304
24	6	0	-4.689770	-2.490573	1.024134
25	6	0	-6.061337	-2.574471	0.809029
26	6	0	-6.667028	-1.741276	-0.137211
27	6	0	-5.902229	-0.821896	-0.870918
28	1	0	6.461744	1.307338	1.897143
29	1	0	8.885241	1.495288	1.408456
30	1	0	9.863449	0.240864	-0.497885
31	1	0	5.997381	-1.400801	-1.430616
32	1	0	8.429239	-1.202983	-1.919535
33	1	0	-3.989648	-0.594257	-1.609179
34	1	0	-4.211193	-3.128877	1.761031
35	1	0	-6.654452	-3.299531	1.357688
36	1	0	-7.729993	-1.830091	-0.337928
37	1	0	-6.370568	-0.253938	-1.668764
38	1	0	-0.193950	-2.917241	-0.211415
39	1	0	-0.150382	1.448209	-0.007791
40	6	0	-3.146910	4.134092	0.129593
41	8	0	-3.439962	5.237009	0.258023
42	8	0	-2.831310	2.992822	-0.002483

Zn Structure 2 CO2 Bound to OH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.725681	-0.478768	0.005094
2	6	0	2.947442	-1.633520	-0.054604
3	6	0	1.544968	-1.547910	-0.102855
4	6	0	0.875095	-0.309082	-0.068322
5	6	0	1.662253	0.847616	0.014735
6	6	0	3.051206	0.749044	0.048047
7	6	0	-0.598753	-0.230345	-0.132733
8	6	0	-1.413158	-1.087708	0.620295
9	6	0	-2.806055	-1.017887	0.501007
10	6	0	-1.239756	0.698325	-0.966036
11	6	0	-2.637708	0.753212	-1.072140
12	6	0	-3.467920	-0.104307	-0.341205
13	1	0	0.971683	-2.466926	-0.181874
14	1	0	3.408751	-2.614595	-0.072686
15	1	0	1.222169	1.836982	0.072048
16	1	0	-0.646310	1.366318	-1.581270
17	1	0	-3.077700	1.449379	-1.780376
18	1	0	-0.970424	-1.795105	1.316026
19	8	0	-3.654276	-1.848885	1.242960
20	7	0	-4.833714	-0.098723	-0.299909
21	7	0	5.102443	-0.402020	-0.005571
22	6	0	5.866872	-1.407591	-0.335460
23	6	0	7.344369	-1.348906	-0.279705
24	1	0	5.446896	-2.356940	-0.687691
25	6	0	8.002146	-0.156425	0.036700
26	6	0	8.079216	-2.504741	-0.560279
27	6	0	9.474624	-2.464417	-0.521226
28	6	0	10.131516	-1.272921	-0.211107
29	6	0	9.397025	-0.119940	0.066359
30	6	0	-5.454731	1.022046	-0.425810
31	6	0	-6.934033	1.026792	-0.427307
32	1	0	-4.920389	1.971542	-0.455887
33	6	0	-7.691220	-0.109797	-0.751168
34	6	0	-7.605382	2.206000	-0.084691
35	6	0	-9.001803	2.242896	-0.043823
36	6	0	-9.741248	1.101264	-0.343076
37	6	0	-9.086776	-0.073983	-0.700981
38	1	0	7.569578	-3.431836	-0.808722
39	1	0	10.046075	-3.361552	-0.736720
40	1	0	11.216969	-1.244431	-0.189205
41	1	0	7.425004	0.736179	0.245463
42	1	0	9.906943	0.808357	0.303362
43	1	0	-7.226614	-0.941516	-1.281601
44	1	0	-7.038205	3.100378	0.159119
45	1	0	-9.505624	3.166816	0.221733
46	1	0	-10.826199	1.135142	-0.328124
47	1	0	-9.656535	-0.949170	-0.996747
48	8	0	3.748386	1.884041	0.126449
49	1	0	4.707118	1.668648	0.168953
50	30	0	-5.813379	-1.685213	0.693679
51	1	0	-3.167875	-2.553299	1.706290
52	6	0	6.378703	4.076591	0.548734
53	8	0	6.411117	2.908401	0.420292
54	8	0	6.347212	5.231944	0.675956

Zn Structure 2 CO2 Bound to Metal

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.839967	-0.305924	0.118359
2	6	0	-4.073350	0.852359	0.002806
3	6	0	-2.670362	0.778050	-0.049111
4	6	0	-1.988257	-0.451538	0.037275
5	6	0	-2.763657	-1.610802	0.176298
6	6	0	-4.153324	-1.524087	0.212638
7	6	0	-0.514047	-0.519024	-0.031477
8	6	0	0.295661	0.378974	0.677994
9	6	0	1.688566	0.317162	0.554457
10	6	0	0.131864	-1.477973	-0.825783
11	6	0	1.529744	-1.524228	-0.936846
12	6	0	2.355148	-0.626914	-0.249536
13	1	0	-2.106288	1.698331	-0.172273
14	1	0	-4.544918	1.827163	-0.056116
15	1	0	-2.313972	-2.592922	0.274852
16	1	0	-0.459333	-2.176195	-1.408444
17	1	0	1.973517	-2.247424	-1.615317
18	1	0	-0.154620	1.113817	1.339933
19	8	0	2.541244	1.209030	1.240772
20	7	0	3.723942	-0.616040	-0.214111
21	7	0	-6.223077	-0.393610	0.123027
22	6	0	-6.991788	0.586228	-0.251929
23	6	0	-8.468348	0.516014	-0.185648
24	1	0	-6.580878	1.524083	-0.644169
25	6	0	-9.112870	-0.667298	0.187392
26	6	0	-9.215830	1.651043	-0.513756
27	6	0	-10.610568	1.599205	-0.465425
28	6	0	-11.254245	0.416603	-0.098713
29	6	0	-10.507162	-0.715718	0.226164
30	6	0	4.352423	-1.736928	-0.294295
31	6	0	5.831676	-1.727628	-0.303541
32	1	0	3.822027	-2.687970	-0.296019
33	6	0	6.576111	-0.599536	-0.682061
34	6	0	6.516200	-2.883828	0.087935
35	6	0	7.913100	-2.905535	0.122896
36	6	0	8.639867	-1.771471	-0.231171
37	6	0	7.972182	-0.619751	-0.637834
38	1	0	-8.714981	2.570200	-0.806326
39	1	0	-11.192326	2.480206	-0.717608
40	1	0	-12.339153	0.378267	-0.069001
41	1	0	-8.523261	-1.542103	0.437438
42	1	0	-11.007623	-1.636666	0.508527
43	1	0	6.098681	0.203042	-1.247911
44	1	0	5.958612	-3.771814	0.373408
45	1	0	8.427597	-3.812275	0.424700
46	1	0	9.725119	-1.794194	-0.219915
47	1	0	8.534721	0.243457	-0.979841
48	8	0	-4.853354	-2.660104	0.343573
49	1	0	-5.801214	-2.403510	0.372213
50	30	0	4.620750	1.008622	0.653638
51	1	0	2.044865	1.899356	1.713549
52	6	0	5.675553	3.946248	-0.399992
53	8	0	5.010920	2.990594	-0.157939
54	8	0	6.318556	4.872207	-0.634634

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