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Supplementary Materials

Zn(II)-to-Cu(II) Transmetalation in an Amide Functionalized Complex and Catalytic Applications in Styrene Oxidation and Nitroaldol Coupling

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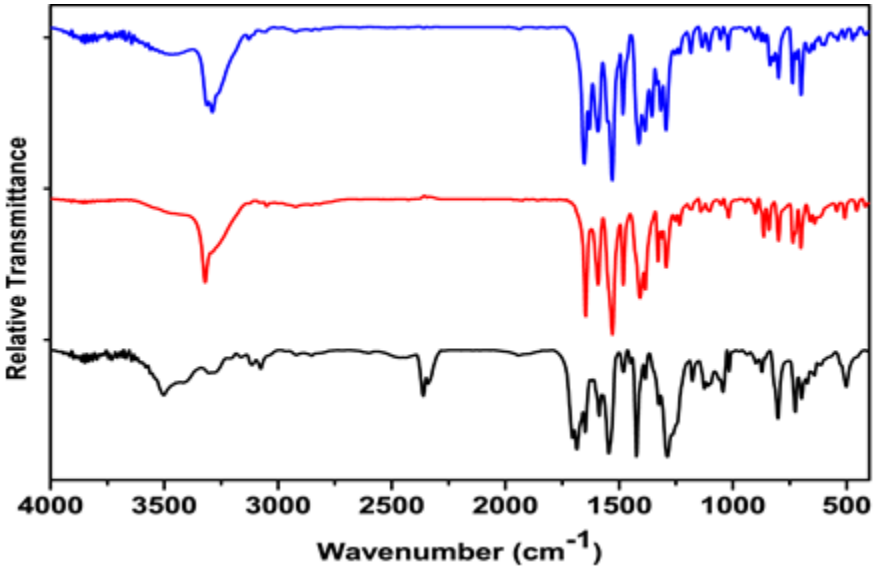

Figure S1. IR spectra of **HL** (black), **1** (red) and **2** (blue).

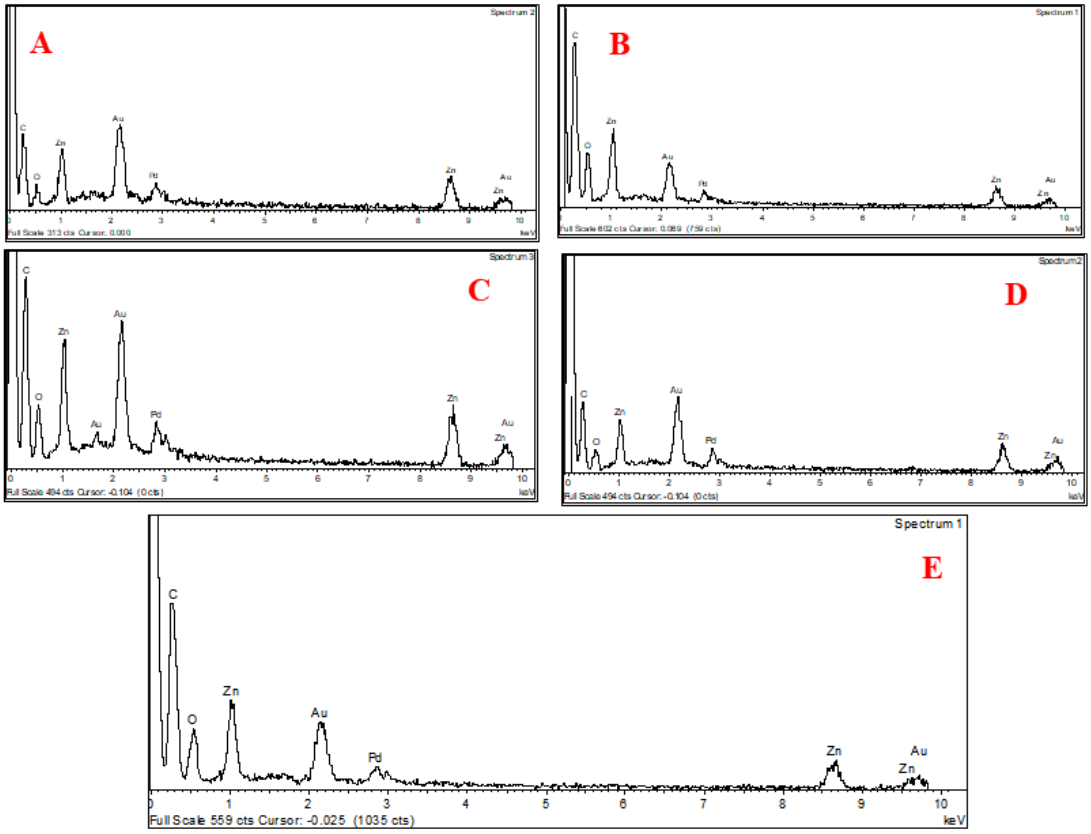

Figure S2. EDS of the samples to identify any eventual replacement of Zn(II) in **1** by another metal ion, using Pb(II) (A) Co(II) (B), Cd(II) (C), Mn(II) (D) or Ni(II) (E) salts.

Table S1. Hydrogen bond geometry (Å, °) in compounds 1 and 2.

Compound	D-H···A	D···H (Å)	H···A (Å)	D···A (Å)	<D–H···A(°)
1	N1-H1N···O3	0.78(3)	2.240(3)	3.006(2)	168(3)
	O4-H4B···N2	0.878(16)	1.857(17)	2.721(2)	168(2)
	O4-H4A···O2	0.855(17)	1.876(18)	2.714(2)	166(2)
2	N1-H1N···O3	0.88(2)	2.17(3)	3.013(6)	158(6)
	O4-H4A···O2	0.78(7)	1.90(8)	2.667(6)	168(7)
	O4-H4B···N2	0.95(7)	1.86(7)	2.729(6)	151(6)

Table S2. Cartesian atomic coordinates (in Å) of the calculated equilibrium structures (nuclear charges are given in the first column).

$[Zn(H_2O)_6]^{2+}$			
30	−0.000987	−0.000453	0.000563
8	1.373575	0.193074	−1.534027
8	−1.375843	−0.195658	1.534704
8	−1.537983	0.312787	−1.349393
8	1.537129	−0.312705	1.349421
8	0.082826	2.030045	0.403932
8	−0.086330	−2.030555	−0.403645
1	1.170556	0.408141	−2.458538
1	2.340630	0.174385	−1.451950
1	−2.342851	−0.175432	1.452429
1	−1.173400	−0.409973	2.459516
1	−1.994582	−0.372578	−1.863266
1	−1.952535	1.161027	−1.574630
1	1.952549	−1.160557	1.574537
1	1.991640	0.372742	1.865033
1	−0.435262	2.484859	1.087320
1	0.602006	2.708032	−0.057363
1	−0.603606	−2.708843	0.059324
1	0.431578	−2.485232	−1.087256
$[Cu(H_2O)_6]^{2+}$			
29	−0.015578	0.006754	0.007245
8	0.680907	1.927917	0.342005
8	−0.600413	−1.941678	−0.371350
8	−1.975058	0.721490	0.542832
8	1.982761	−0.686501	−0.507286
8	0.431531	−0.533421	1.823275
8	−0.452098	0.541907	−1.810898
1	0.132464	2.669867	0.645065
1	1.602307	2.234004	0.341672
1	−1.485812	−2.340164	−0.393270
1	0.028583	−2.620763	−0.664808
1	−2.595379	1.028481	−0.137760
1	−2.488309	0.669479	1.364729
1	2.507618	−0.649608	−1.322604
1	2.592956	−0.985692	0.185599
1	0.097414	−1.364731	2.201340
1	0.581268	0.092178	2.552033
1	−0.609066	−0.085589	−2.536394
1	−0.109499	1.368471	−2.191611
1			
30	0.000000	0.000000	0.100930
8	1.602261	0.072160	1.365498

8	−0.117239	2.240313	1.651051
8	−0.074746	1.783560	−0.540223
8	−0.798632	8.531380	−2.007689
7	−0.024570	9.110681	0.064662
7	0.565098	12.539986	1.138478
6	−0.126740	2.600482	0.452539
6	−0.202350	4.047832	0.113054
6	0.000000	10.509477	−0.028588
6	−0.343491	12.624386	−1.073234
1	−0.664010	13.229759	−1.918477
6	−0.427505	11.240011	−1.138613
1	−0.804561	10.726304	−2.015784
6	0.154835	13.231037	0.073103
1	0.229517	14.316876	0.142365
6	0.483928	11.219393	1.076700
1	0.822809	10.667400	1.960573
6	−0.339544	6.771382	−0.483117
6	−0.183482	4.476358	−1.215611
1	−0.110582	3.734180	−2.006843
6	−0.257707	5.828202	−1.509705
1	−0.257574	6.184659	−2.537286
6	−0.420443	8.208047	−0.894515
6	−0.305768	4.985326	1.140500
1	−0.339491	4.633198	2.168592
6	−0.375083	6.338448	0.845467
1	−0.500575	7.049617	1.661726
1	0.384867	8.732298	0.910058
1	1.435808	−0.732636	1.896175
1	1.366585	0.851682	1.905988
8	−1.602261	−0.072160	1.365498
8	0.117239	−2.240313	1.651051
8	0.074746	−1.783560	−0.540223
8	0.798632	−8.531380	−2.007689
7	0.024570	−9.110681	0.064662
7	−0.565098	−12.539986	1.138478
6	0.126740	−2.600482	0.452539
6	0.202350	−4.047832	0.113054
6	0.000000	−10.509477	−0.028588
6	0.343491	−12.624386	−1.073234
1	0.664010	−13.229759	−1.918477
6	0.427505	−11.240011	−1.138613
1	0.804561	−10.726304	−2.015784
6	−0.154835	−13.231037	0.073103
1	−0.229517	−14.316876	0.142365
6	−0.483928	−11.219393	1.076700
1	−0.822809	−10.667400	1.960573
6	0.339544	−6.771382	−0.483117
6	0.183482	−4.476358	−1.215611
1	0.110582	−3.734180	−2.006843
6	0.257707	−5.828202	−1.509705
1	0.257574	−6.184659	−2.537286
6	0.420443	−8.208047	−0.894515
6	0.305768	−4.985326	1.140500
1	0.339491	−4.633198	2.168592
6	0.375083	−6.338448	0.845467
1	0.500575	−7.049617	1.661726

1	−0.384867	−8.732298	0.910058
1	−1.435808	0.732636	1.896175
1	−1.366585	−0.851682	1.905988
trans−**2**			
29	−0.018271	−1.436395	−0.283459
8	−0.249396	−2.311967	1.446945
8	−1.868966	−1.198066	−0.407453
8	−8.923826	0.065012	−1.662938
8	−2.086819	−0.877328	−2.626091
7	−8.509974	0.930709	0.413979
7	−11.042977	2.479145	2.522776
6	−9.790498	1.347445	0.803474
6	−3.985148	−0.607144	−1.248222
6	−6.685444	−0.001816	−0.873989
6	−2.540449	−0.913325	−1.469736
6	−12.153760	2.258904	1.817139
1	−13.083242	2.635963	2.245562
6	−9.902274	2.031126	2.020106
1	−9.000061	2.221328	2.612148
6	−5.854291	−0.226228	0.226895
1	−6.255371	−0.207401	1.240214
6	−6.159359	−0.108592	−2.163172
1	−6.828191	0.041041	−3.007657
6	−4.817189	−0.395817	−2.349200
1	−4.389096	−0.465953	−3.346514
6	−12.153261	1.589881	0.599152
1	−13.085079	1.434093	0.059589
6	−10.957499	1.120587	0.072195
1	−10.912242	0.599101	−0.877157
6	−8.142083	0.319100	−0.762592
6	−4.513558	−0.530771	0.040043
1	−3.862325	−0.716515	0.890229
1	−7.761423	1.216927	1.033154
1	−0.921569	−3.004219	1.494361
1	0.666101	−2.679622	1.633754
8	0.310570	−1.619351	−2.187337
8	1.772544	−0.964441	0.002489
8	8.735506	−0.090671	1.986238
8	2.289185	−2.633140	1.418847
7	8.537427	0.936490	−0.048539
7	11.245822	2.714276	−1.712286
6	9.814645	1.491808	−0.207937
6	3.992641	−1.128558	0.781396
6	6.633397	−0.224461	0.890980
6	2.587365	−1.632555	0.747124
6	12.201707	2.680978	−0.781775
1	13.144959	3.164301	−1.039002
6	10.091327	2.133248	−1.421327
1	9.316757	2.171774	−2.195372
6	5.682051	0.466661	0.135771
1	5.945407	1.389481	−0.381138
6	6.246202	−1.357422	1.609587
1	6.993534	−1.866292	2.214409
6	4.938797	−1.810113	1.549055
1	4.623250	−2.694253	2.097832
6	12.029839	2.071299	0.454845

1	12.839008	2.069621	1.182026
6	10.819990	1.462160	0.759772
1	10.646336	0.972494	1.711359
6	8.060365	0.205469	1.015471
6	4.370518	0.016964	0.081610
1	3.621814	0.559124	−0.490438
1	7.934962	1.009276	−0.859197
1	1.061061	−1.105545	−2.516404
1	−0.550639	−1.310658	−2.619166
cis−**2**			
29	−0.113003	−4.622158	0.100915
8	−1.269456	−5.945552	0.931580
8	1.241054	−3.319397	0.041691
8	6.500552	1.488393	−1.470273
8	2.789603	−4.385796	−1.196107
7	5.418823	2.296867	0.375461
7	6.273373	5.427938	2.025877
6	6.080555	3.516786	0.572040
6	3.182398	−2.142667	−0.570376
6	4.748058	0.168591	−0.562442
6	2.356876	−3.386263	−0.589066
6	7.187747	5.930478	1.194022
1	7.613444	6.896323	1.468609
6	5.743097	4.255314	1.712331
1	4.994263	3.857151	2.406231
6	3.471194	0.179672	0.006211
1	3.053680	1.098993	0.416944
6	5.224728	−1.002692	−1.154805
1	6.209798	−0.984655	−1.615651
6	4.451119	−2.151479	−1.152921
1	4.811976	−3.073057	−1.603306
6	7.593221	5.278883	0.035687
1	8.343036	5.728184	−0.612018
6	7.037874	4.049452	−0.293246
1	7.329030	3.503051	−1.184033
6	5.639945	1.367549	−0.615059
6	2.693214	−0.968947	0.002136
1	1.694056	−0.968036	0.430253
1	4.775093	2.035093	1.112170
1	−0.879585	−6.473370	1.641329
1	−2.039210	−5.382792	1.298513
8	1.043540	−6.063540	−0.498424
8	−1.463534	−3.323234	−0.029853
8	−7.022844	1.369178	0.204375
8	−2.935445	−4.130383	1.469717
7	−5.170359	2.630922	−0.254809
7	−5.235797	6.244367	−0.705989
6	−5.732900	3.907139	−0.395964
6	−3.366917	−2.035559	0.468955
6	−4.924864	0.257839	0.149178
6	−2.540618	−3.262726	0.666227
6	−6.546892	6.493150	−0.702842
1	−6.842140	7.535894	−0.825353
6	−4.853763	4.984911	−0.556450
1	−3.774049	4.798385	−0.561276
6	−3.695841	0.143500	−0.506714

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6	−5.378927	−0.796249	0.944870
1	−6.350212	−0.699791	1.425066
6	−4.600901	−1.929515	1.112659
1	−4.931815	−2.752426	1.741801
6	−7.503092	5.496292	−0.553078
1	−8.561651	5.747490	−0.557027
6	−7.102402	4.176171	−0.396529
1	−7.816244	3.370389	−0.269812
6	−5.818554	1.451154	0.033403
6	−2.922616	−0.997971	−0.350281
1	−1.968371	−1.102761	−0.861197
1	−4.158045	2.609557	−0.242286
1	1.848057	−5.571538	−0.895116
1	0.675797	−6.672154	−1.153089