

Metal-ligand bond lengths and strengths: are they correlated? A detailed CSD analysis

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Table of contents

Table S.1 Stability constants and related values of ΔG^0	1
Figure S.1. Searches for number of compounds with different oxidation states for Cu alcohol compounds	1
Table S.2 Comparison of bond lengths for t5 and t6 Cu alcohols and Cu alkoxides, Figure 2 shows the combined data for both coordination numbers for alkoxide and alcohol.	2
Table S.3 Some representative copper and zinc complexes.	2
Figure S.2 Bond length comparison carboxylate and keto Cu(t4) coordinated complexes.....	3
Figure S.3 Bond length comparison carboxylate and keto Cu(t5) coordinated complexes.....	3
Figure S.4 Bond length comparison carboxylate and keto Cu(t6) coordinated complexes.....	3
Table S.4 Cu-O and C=O bond lengths for keto coordination Cu(II) neutral carboxylic acid complexes.	4
Table S.5 Zn-N distances for four-coordinated zinc imidazole and imidazolates	5
Table S.6 Cu triazole compounds bond length distribution (\AA)	6
Table S.7 Zn-N and Zn-O distances for four-coordinate Zn-imidazole, Zn-pyridine and Zn-carboxylate compounds from the CSD	6
Table S.8 Triazole systems with different numbers of Zn coordination. bond length distribution	7
Figure S.6 Bond lengths in Zn triazoles. See table S.8 for data.	8
Figure S.7 Bond lengths in Zn triazoles.	8
Table S.9 Calculation of force constants and vibrational energy assuming a regular harmonic oscillator extended 0,05 \AA	9
Table S.10 Constants and values used in the calculations in table S.9	9
Table S.11 Calculation of ion-dipole coulombic interaction bond extension 0,05 \AA ,	9
Table S.12 Calculation of ion-ion coulombic interaction, bond extension 0,05 \AA	9
Table S.13 Constants and values used in calculations in tables S.11 and S.12	9
Table S.14 Reference codes and bond lengths for Cu-carboxylic acid compounds	9

Table S.1 Stability constants and related values of ΔG^0 .

Data acquired from "SILLÉN, L. G. & MARTELL, A. E. 1971. Stability constants of metal-ion complexes. Supplement, London, Chemical Society". Mean log K calculated from list of values in the table.

Equation $ML_{n-1} + L \rightleftharpoons ML_n$	Cu	medium	Zn	Equation $ML_{n-1} + L \rightleftharpoons ML_n$	Cu	medium	Zn
Ligand -Cu ²⁺ bond log k _{st}		T=298K	log k _{st}	Ligand -Cu ²⁺ bond cont. log k _{st}		T=298K	log k _{st}
Imidazoles				Carboxylic acids			
imidazole	4.33	K ₂ SO ₄	2.13	acetic acid	7.9	NaClO ₄	2.32
4-aminomethylimidazole	9.05		not found	propanoic acid	2.3	NaClO ₄	2.41
4(5)aminomethyl-2-methylimidazole	9.09		not found	2-methylpropanoic acid	2.44	NaClO ₄	not found
2-(2-pyridyl)imidazole	7.94		4.39	benzoic acid	3.3	NaClO ₄	2.32
4-(2-pyridyl)imidazole	8.76		5.419	4-methylbenzoic acid	3.44	NaClO ₄	2.43
2-(2-hydroxyethyl)benzimidazole	11.8		4	mean log k	3.876		2.37
mean log k	8.495		3.985	$\Delta G^0 = -RT \ln K$ (low log K=2.3)	-13.12	kJ/mol	
$\Delta G^0 = -RT \ln K$ (low log K=4.33)	-24.70 kJ/mol			$\Delta G^0 = -RT \ln K$ (high log K=7.9)	-45.07	kJ/mol	
$\Delta G^0 = -RT \ln K$ (high log K=11.8)	-67.32 kJ/mol			Ethanol	0.26		Not found
Pyridines				$\Delta G^0 = -RT \ln K$ (log K=0.26)	- 1.48	kJ/mol	
pyridine	2.65	NaClO ₄	2.08	Propanone	0.57		Not found
2-methylpyridine	1.3		<1	$\Delta G^0 = -RT \ln K$ (log K=0.57)	-3.25	kJ/mol	
3-methylpyridine	2.77		< 1				
2-aminomethylpyridine	9.5		5.2				
2-amino-3-methylpyridine	1.91	KNO ₃	not found				
2-hydroxymethylpyridine	3.41	KNO ₃	1.9				
3-hydroxymethylpyridine	2.43	KNO ₃	1.9				
2,5-dimethylpyridine	1.78	KNO ₃	not found				
2-(2-aminoethyl)pyridine	7.3	KNO ₃	7.8				
2-phenylpyridine	1.3	NaClO ₄	<1				
mean log k	3.435		3.776				
$\Delta G^0 = -RT \ln K$ (low log K=1.3)	-7.42 kJ/mol						
$\Delta G^0 = -RT \ln K$ (high log K=7.3)	-41.65 kJ/mol						

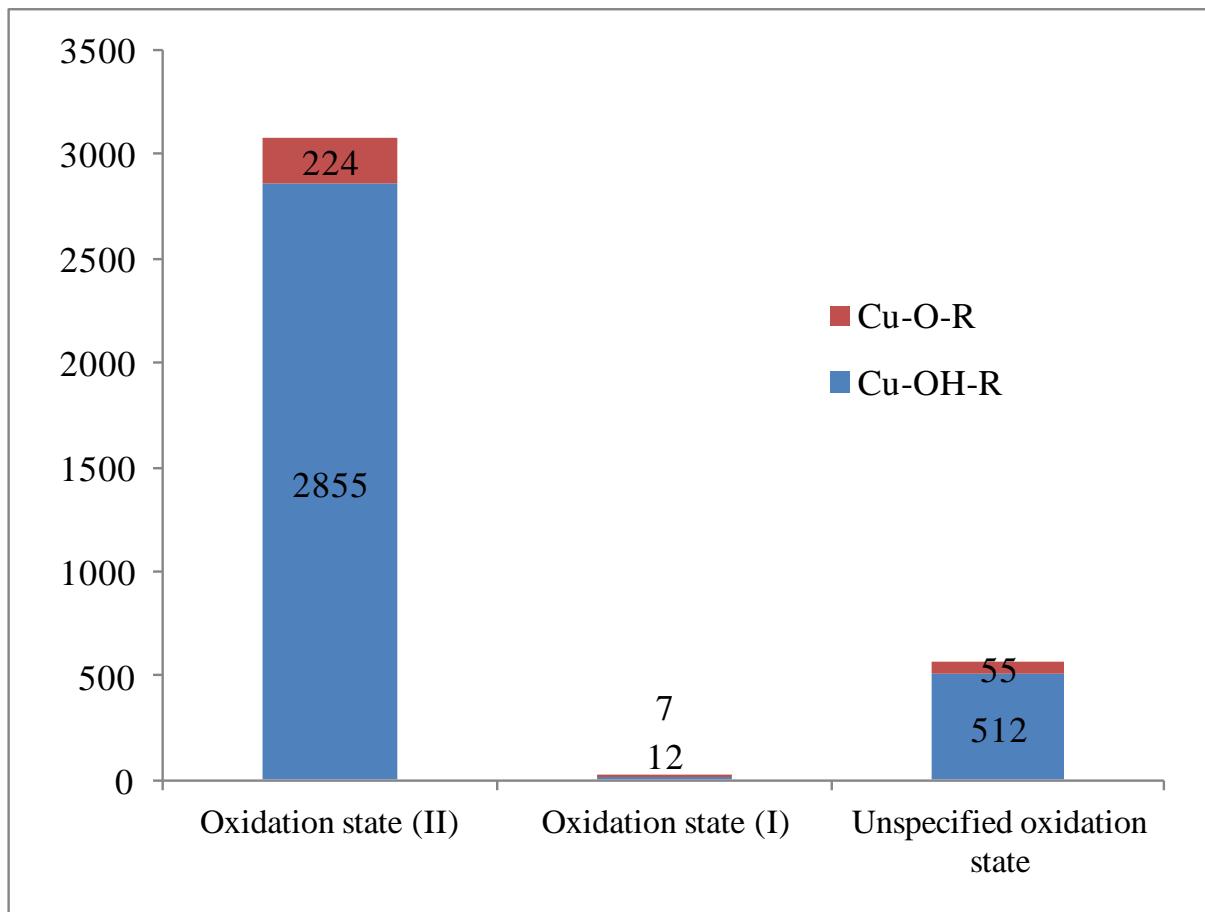


Figure S.1. Searches for number of compounds with different oxidation states for Cu alcohol and alcooxide compounds

Table S.2 Comparison of bond lengths for t5 and t6 Cu alcohols and Cu alkoxides. Fig. 2 shows the combined data for both coordination numbers for alkoxide and alcohol.

BL (Å) box	alcohols		alkoxides		BL (Å) box	alcohols continued		alkoxides continued	
	Cu t6 -OH-R	Cu t5 -OH-R	Cu t5 -O-R	Cu t6 -O-R		Cu t6 -OH-R	Cu t5 -OH-R	Cu t5 -O-R	Cu t6 -O-R
1.830	0	0	0	0	2.280	24	10	1	0
1.840	0	0	0	0	2.290	13	9	0	0
1.850	0	0	0	0	2.300	7	14	0	0
1.860	0	0	1	0	2.310	14	11	1	0
1.870	0	0	0	0	2.320	21	9	1	0
1.880	0	0	2	0	2.330	20	10	0	0
1.890	0	0	4	0	2.340	16	10	1	0
1.900	0	0	5	0	2.350	11	14	0	0
1.910	0	0	9	0	2.360	16	15	2	0
1.920	1	0	6	1	2.370	13	15	0	0

1.930	2	2	8	4	2.380	4	8	0	1
1.940	4	4	10	6	2.390	12	12	1	1
1.950	11	3	12	3	2.400	10	13	0	0
1.960	5	9	7	2	2.410	4	10	0	0
1.970	14	8	1	4	2.420	10	14	1	0
1.980	14	9	6	3	2.430	8	3	0	0
1.990	17	8	2	3	2.440	3	9	0	0
2.000	22	11	4	2	2.450	4	11	0	1
2.010	19	12	1	1	2.460	1	14	0	0
2.020	12	7	2	0	2.470	4	9	0	1
2.030	9	5	4	1	2.480	2	16	1	0
2.040	8	7	1	0	2.490	1	9	0	0
2.050	8	3	0	1	2.500	3	8	0	0
2.060	5	2	0	0	2.530		8	0	1
2.070	7	3	0	0	2.540	0	6	0	0
2.080	4	2	0	0	2.550	1	6	0	0
2.090	2	2	0	0	2.560	0	3	0	0
2.100	7	1	0	1	2.570	1	6	0	1
2.110	3	1	1	0	2.580	2	4	0	0
2.120	1	4	0	0	2.590	1	1	0	0
2.130	3	4	2	0	2.600	0	4	0	0
2.140	6	8	0	0	2.610	0	1	0	0
2.150	4	6	0	1	2.620	3	1	0	0
2.160	9	12	0	2	2.630	0	2	0	0
2.170	4	6	0	0	2.640	0	3	0	0
2.180	6	3	0	0	2.650	0	2	0	0
2.190	5	5	0	0	2.660	1	3	0	0
2.200	9	7	0	0	2.670	0	2	0	0
2.210	10	2	1	0	2.680	1	1	0	0
2.220	17	1	1	0	2.690	0	0	0	0
2.230	9	3	0	0	2.700	0	1	0	0
2.240	11	5	0	1	2.710	0	0	0	0
2.250	18	4	0	0	2.720	0	1	0	0

2.260	19	2	0	0	2.730	0	0	0	0
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Table S.3 Some representative copper and zinc complexes. Only the longest BL is reported for CUHMAM01.

Group	Refcode	BL1 (Å)	BL2 (Å)	BL3 (Å)	BL4 (Å)	BL5 (Å)	BL6 (Å)
Cu alcohols	ETDOCU01	1.964	1.998	2.33	2	2.312	1.956
Cu alcohols	RELCUG01	2.223	1.968	2.022	1.968	2.223	2.022
Cu alcohols	RELCUG04	2.162	1.972	2.076	1.972	2.162	2.076
Zn alcohols	CIRJIW	2.086	2.086	2.086	2.086		
Cu alkoxide	BESHUD	1.864	1.864				
Cu alkoxide t4	LIVFAY	1.911	1.912	1.969	1.943		
Cu alkoxide t4	JIWVIU	1.968	1.968	1.916	1.916		
Cu carboxylate	MAZSAI	1.93					
Cu carboxylate	CUHMAM01	2.683					
Cu triazole	HOXLUB	1.947	2.008				

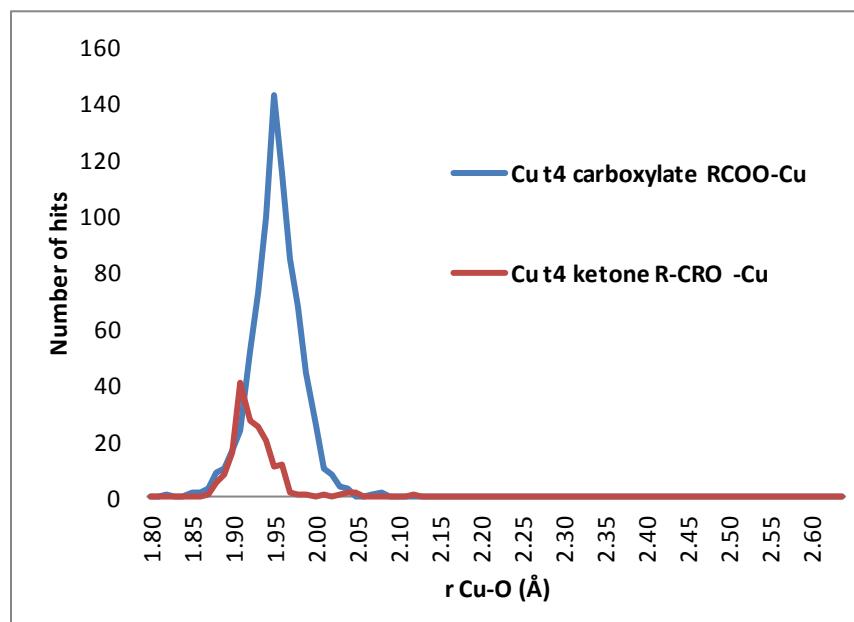


Fig. S.2 Bond length comparison carboxylate and keto Cu(t4) coordinated complexes. Number of hits: Carboxylates =802(peak 1.950Å), Ketones=177 (peak 1.910Å)

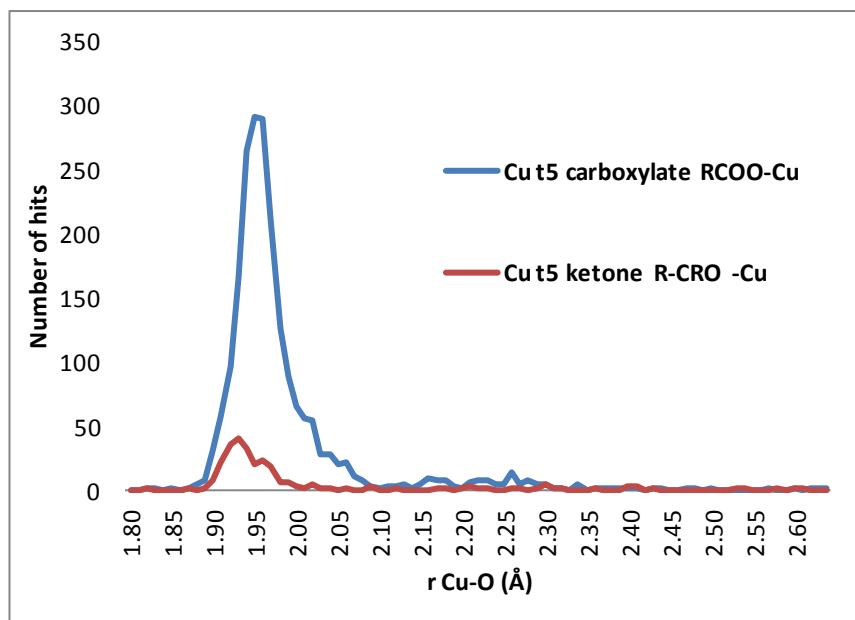


Fig. S.3 Bond length comparison carboxylate and keto Cu(t5) coordinated complexes.

Number of hits: Carboxylates =2074 (peak 1.950 Å), Ketones=264 (peak 1.930 Å)

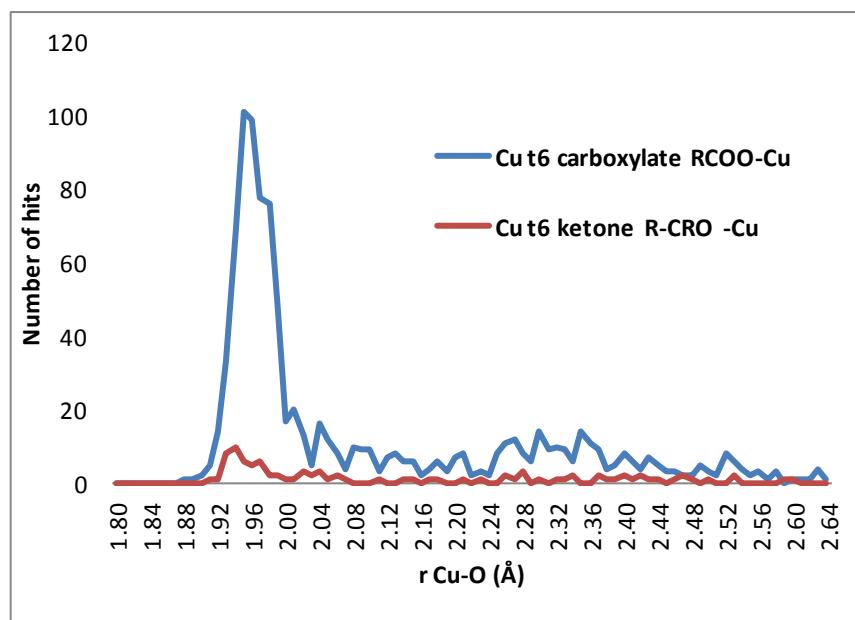


Fig. S.4 Bond length comparison carboxylate and keto Cu(t6) coordinated complexes.
Number of hits: Carboxylates =947 (peak 1.950 Å), Ketones=95 (peak 1.940 Å)

Table S.4 Cu-O and C=O bond lengths for keto coordination Cu(II) neutral carboxylic acid complexes.

Refcode	bond length (Å)	bond length (Å)	Refcode	bond length (Å)	bond length (Å)	Refcode	bond length (Å)	bond length (Å)
	O-Cu	C=O		O-Cu	C=O		O-Cu	C=O
ABUWOK	2.559	1.206	HEDTAC01	2.466	1.217	IFUPOO	2.421	1.201
ACACCV10	2.197	1.211	HIPZIP	2.278	1.221	IFUPOO	2.451	1.204
APIXUT	1.968	1.277	HIXDUN	1.96	1.279	IIATAO	2.424	1.204
AROSOP	2.541	1.203	HIXDUN	1.938	1.271	IYAREF	2.450	1.212
AROSOP	2.723	1.212	HOVLIN	1.953	1.338	KALDUX	2.475	1.217
AXONAC	2.306	1.216	HPYRCU	2.322	1.236	KALQET	2.193	1.202
BAGSOR	1.964	1.265	HPYRCU	2.452	1.211	KIJKUJ	2.183	1.215
BASNAL	2.481	1.214	HPYRCU	2.375	1.209	LALXUT	2.176	1.186
BEHBIZ	1.987	1.238	HPYRCU	2.326	1.235	LALXUT	2.179	1.215
BETGUD	1.99	1.252	TEBYUU01	2.401	1.200	LOBYEH	2.372	1.225
BODRIW	2.324	1.217	TONSOE	1.962	1.244	MEYXIX	2.459	1.209
CANYIA	2.354	1.209	TONSOE	2.454	1.22	MODCOY	2.176	1.223
CIDWES	2.521	1.212	ULONUE	1.948	1.242	MOLDAT	2.451	1.226
CIDWIW	2.485	1.212	ULONUE	1.944	1.268	MUGNCU	2.559	1.220
CIDWIW	2.032	1.230	UNOPIX	2.394	1.221	MUGNCU10	2.558	1.220
COQWAH	2.582	1.213	VELNOQ	2.542	1.208	NANPAU	2.381	1.218
DESQAT	2.317	1.206	XATMUA	1.942	1.252	NEDREU	1.962	1.269
DICWER	2.461	1.210	YAFXAF	2.287	1.214	NEHLAO	2.480	1.205
DOKPOI01	2.435	1.204	YEHJUR	1.985	1.256	NEQXOX	2.316	1.200
DUKBAN	2.220	1.249	YEHJUR	2.330	1.226	NUHYIZ	2.410	1.216
DUQXOD	2.457	1.222	ZUDXOL	2.386	1.215	NUHYIZ	2.355	1.213
EBOGOS01	2.349	1.219	AXEZUZ	2.540	1.206	PUMSAS	2.418	1.203
ECEPOR	2.463	1.215	EYUFAG	1.984	1.249	QAGTEZ	1.935	1.282
EKAWUJ	2.523	1.210	GANPUI	2.446	1.216	QAGTEZ	1.950	1.258
EMAWOE	2.511	1.212	YEXSAV01	2.298	1.223	QIDSAY	2.350	1.214
ESIPUR	2.208	1.210	YEXSAV02	2.296	1.223	QIDSAY	2.338	1.219
ESIPUR02	2.212	1.214	ZOGWOH	2.267	1.213	QIXGOU	2.162	1.225
ETOYOC	2.240	1.232	HPYRCU01	2.314	1.271	QQQFMV01	2.321	1.212
ETPACU01	2.518	1.217	HPYRCU01	2.300	1.231	QQQFMV02	2.328	1.206

FAKRUE	2.207	1.213	IBUHIX	2.394	1.222	RAKWAB	1.972	1.252
FIVCAO	2.496	1.213	IBUHIX01	2.312	1.218	RAKWAB01	1.967	1.249
FIWFIA	2.008	1.240	IBUJAR	2.296	1.212	RAZGOP	2.525	1.210
GABDIX	1.967	1.256	IBUJOF	2.329	1.218	RAZNAH01	2.427	1.216
GABDOD	2.264	1.213	IBUJOF	2.264	1.225	SAPBER	2.511	1.205
GOMPEE	1.943	1.269	IBUJUL	2.320	1.209	SUGRAN	2.295	1.208
GUGROP	2.186	1.202	IBUJUL	2.263	1.215	SUGRAN01	2.296	1.203
HAMLIR	1.974	1.254	PAQRUW	2.341	1.229	TAHQIE	2.308	1.214
LATXEL	2.215	1.22	QQQFMV03	2.313	1.208	TEBYUU	2.405	1.197
HEDTAC	2.467	1.211						

Table S.5 Zn-N distances for four-coordinated zinc imidazole and imidazolates

BL box (Å)	BL frequency Zn t4 -Him		BL frequency Zn t4 -im-Zn t4		BL frequency Zn t4 -im-Zn t4		BL frequency Zn t4 -Rim	
	1	0	0	0	1	0	0	0
1.830	1	0	0	0	0	0	0	0
1.840	0	1	0	0	0	0	0	0
1.850	0	0	0	0	0	0	0	0
1.860	0	0	0	0	0	0	0	0
1.870	0	0	0	1	0	0	0	0
1.880	0	0	0	0	0	0	0	0
1.890	0	0	0	0	0	0	0	0
1.900	0	0	0	0	0	0	0	0
1.910	1	1	1	1	0	0	0	0
1.920	1	1	1	1	1	1	1	1
1.930	2	0	1	1	0	0	0	0
1.940	0	4	0	0	1	1	1	1
1.950	3	2	1	1	1	1	1	1
1.960	4	1	1	1	2	2	2	2
1.970	9	6	4	4	6	6	6	6
1.980	26	8	6	6	24	24	24	24
1.990	36	13	15	15	50	50	50	50
2.000	48	9	11	11	98	98	98	98
2.010	51	6	8	8	126	126	126	126
2.020	37	3	1	1	96	96	96	96

2.030	27	0	3	94
2.040	25	1	3	59
2.050	13	1	0	28
2.060	7	1	1	20
2.070	5	0	0	7
2.080	4	1	2	12
2.090	2	0	0	3
2.100	3	1	0	5
2.110	0	0	0	0
2.120	1	0	0	1
2.130	0	0	0	1
2.140	0	0	0	0
2.150	0	0	0	0
2.160	0	0	0	0
2.170	0	0	0	0
2.180	0	0	0	0
2.190	0	0	0	0
2.200	0	0	0	0
2.210	0	0	0	0
2.220	0	0	0	0
2.230	0	0	0	0
2.240	0	0	0	0
2.250	0	0	0	0
2.260	0	0	0	0
2.270	0	0	0	0
2.280	0	0	0	0
2.290	0	0	0	0
2.300	0	0	0	0

Table S.6 Cu triazole compounds bond length distribution (Å)

BL Å) Box	1.2.4 tri Cu- triazolate	1.2 Cu- triazole	4-Cu- triazole	BL Å) Box Cont.	1.2.4 tri Cu- triazolate	1.2 Cu- triazole	4-Cu- triazole
1.850	2	1	2	2.030	3	11	26
1.860	10	0	12	2.040	2	8	26
1.870	30	0	27	2.050	2	4	8
1.880	22	2	20	2.060	3	5	9
1.890	16	1	7	2.070	1	4	3
1.900	23	5	16	2.080	2	2	3
1.910	17	3	11	2.090	0	1	1
1.920	11	2	10	2.100	0	1	3
1.930	8	2	6	2.110	0	0	1
1.940	15	1	14	2.120	2	0	1
1.950	31	1	16	2.130	1	1	1
1.960	29	5	14	2.140	0	1	0
1.970	52	5	39	2.150	1	0	1
1.980	21	7	37	2.160	0	0	2
1.990	13	17	39	2.170	0	2	2
2.000	16	10	38	2.180	0	2	1
2.010	12	19	60	2.190	0	1	0
2.020	6	16	45	2.200	0	0	0

Table S.7 Zn-N and Zn-O distances for four-coordinate Zn-imidazole, Zn-pyridine and Zn-carboxylate compounds from the CSD. Total number of hits 752(pyridines), 1549(carboxylates) and 318(imidazoles). BL with most hits is colour marked

BL Box (Å)	Zn t4 pyri- dine	Zn t4 carbox- ylate	Zn t4 imid- azole	BL Box (Å) cont.	Zn t4 pyridine	Zn t4 carboxylate	Zn t4 imidazole
1.740	0	0	0	2.020	48	28	36
1.750	0	0	0	2.030	74	12	28
1.760	0	0	0	2.040	101	12	25
1.770	0	0	0	2.050	127	3	13
1.780	0	0	1	2.060	122	1	7
1.790	0	0	0	2.070	105	6	5
1.800	0	0	0	2.080	44	4	4

1.810	0	0	0	2.090	16	1	2
1.820	0	1	0	2.100	18	2	2
1.830	0	0	0	2.110	6	4	0
1.840	0	0	0	2.120	12	4	1
1.850	0	2	0	2.130	12	2	0
1.860	0	1	0	2.140	6	2	0
1.870	0	0	0	2.150	3	1	0
1.880	0	1	0	2.160	8	0	0
1.890	0	4	0	2.170	0	0	0
1.900	0	7	0	2.180	1	0	0
1.910	0	22	1	2.190	0	0	0
1.920	0	60	1	2.200	2	0	0
1.930	0	118	2	2.210	3	0	0
1.940	0	159	1	2.220	4	0	0
1.950	0	235	4	2.230	0	0	0
1.960	0	260	5	2.240	2	0	0
1.970	1	220	10	2.250	0	0	0
1.980	1	146	28	2.260	0	0	0
1.990	1	121	38	2.270	1	1	0
2.000	6	55	52	2.280	0	0	0
2.010	28	54	52	2.290	0	0	0

Table S.8 Bond length distribution for triazole systems coordinating different numbers of Zn .

BL (Å) Box	tri-Zn trz charged	di-Zn trz -R uncharged	di-Zn trz -H	Zn-4N trz	Zn-1N trz
1.800	0	0	0	0	0
1.810	0	0	0	0	0
1.820	0	0	0	0	0
1.830	0	0	0	0	0
1.840	0	0	0	0	0
1.850	0	0	0	0	0
1.860	0	0	0	0	0
1.870	0	0	0	0	0
1.880	0	0	0	0	0
1.890	0	0	0	0	0
1.900	0	0	0	0	0
1.910	0	0	0	0	0
1.920	0	0	0	0	0
1.930	0	0	0	0	0
1.940	0	0	0	0	0
1.950	1	0	0	0	0
1.960	2	0	0	0	0
1.970	1	0	0	0	1
1.980	5	0	0	0	0
1.990	27	0	1	0	1
2.000	28	0	0	1	5
2.010	50	0	0	5	11
2.020	29	0	0	8	11
2.030	23	0	0	9	10
2.040	17	1	0	9	8
2.050	18	0	0	7	9
2.060	7	0	0	1	11
2.070	4	3	0	4	11
2.080	9	1	0	0	8
2.090	4	0	0	0	4

2.100	7	1	0	0	7
2.110	1	0	0	2	3
2.120	5	3	0	0	5
2.130	11	2	0	2	5
2.140	6	3	0	1	5
2.150	2	3	1	1	2
2.160	3	4	0	3	3
2.170	1	2	0	1	3
2.180	3	2	0	3	1
2.190	0	3	0	0	2
2.200	2	0	0	2	0
2.210	3	1	0	1	0
2.220	1	0	0	2	1
2.230	1	1	0	0	2
2.240	0	0	1	0	0
2.250	1	0	1	0	0
2.260	0	0	0	0	0
2.270	1	0	0	0	0
2.280	0	0	0	0	0
2.290	0	0	0	0	0
2.300	0	0	0	0	0
2.310	0	0	0	0	0
2.320	0	0	0	0	0
2.330	0	0	0	0	0
2.340	0	0	0	0	0
2.350	0	0	0	0	1

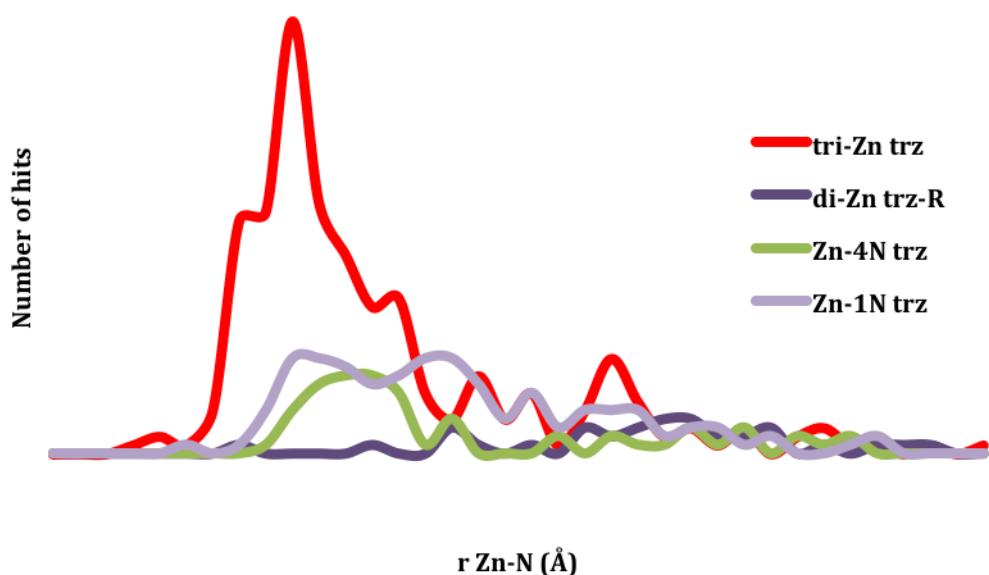


Fig. S.6 Bond lengths in Zn triazoles. See table S.8 for data.

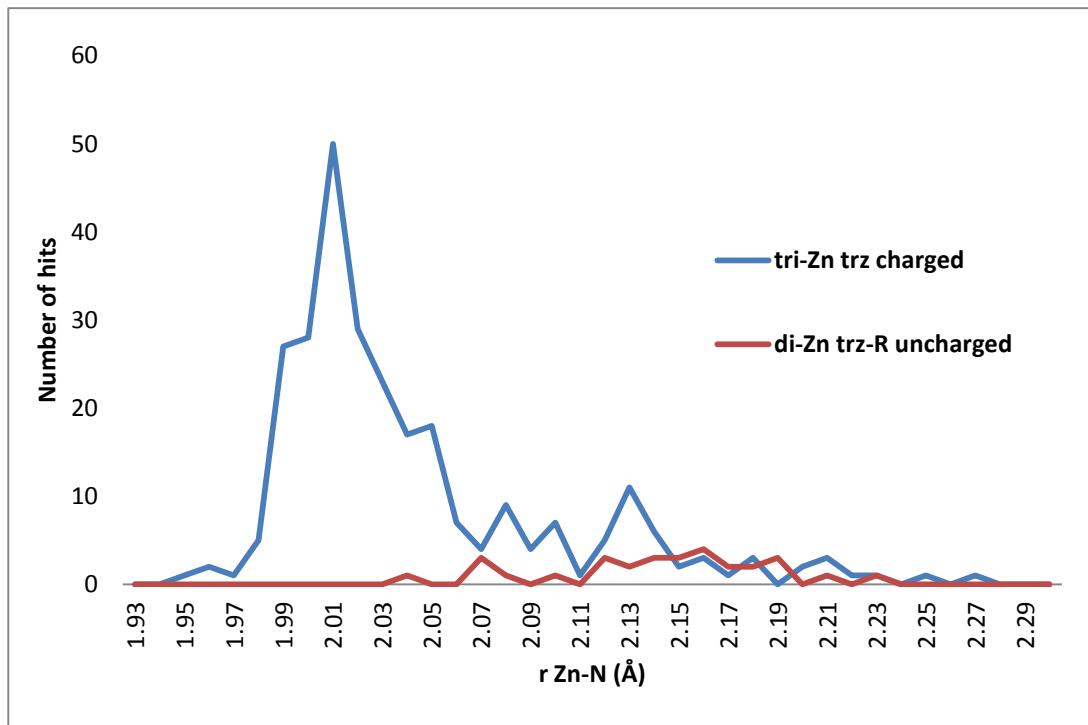


Fig. S.7 Bond lengths in Zn triazoles. Total number of hits tri-ZN = 273 for di-Zn hits = 30

Table S.9 Calculation of force constants and vibrational energy assuming a regular harmonic oscillator extended 0.05 Å

Compound	μ reduced mass (g)	v wave number (cm^{-1})	f (hz)	k force constant (N/m) $k=4\pi^2 f^2 \mu$	vibrational ground state per atom $E_{\text{eq}}=hf(v+0.5)$	E_{eq} (kJ/mol)	$E_{\text{ext}} = 0.5Kx^2$ (at 0.05 Å)	$E_{\text{ext}} = 0.5Kx^2$ (at 0.05 Å) (kJ/mol)
zn(Py) ₂ Cl ₂	8.17E-26	204.000	6.116E+12	120.688	2.0262E-21	1.2202	1.5086E-21	0.9085
Zn (imH) ₂ Cl ₂	7.35E-26	239.000	7.165E+12	148.952	2.3738E-21	1.4295	1.8619E-21	1.1212
Cu(Py) ₂ Cl ₂	8.00E-26	270.000	8.094E+12	206.893	2.6817E-21	1.6149	2.5862E-21	1.5574
Cu (imH) ₂ Cl ₂	7.21E-26	306.500	9.189E+12	240.251	3.0442E-21	1.8332	3.0031E-21	1.8085

Table S.10 Constants and values used in the calculations in table S.9

Complex	complex mass (u)	atomic mass (u)
zn(Py) ₂ Cl ₂	199.0812	65.39
Zn (imH) ₂ Cl ₂	136.9692	65.39
Cu(Py) ₂ Cl ₂	199.0812	63.546
Cu (imH) ₂ Cl ₂	136.9692	63.546
constants		
u	1.66E-27	
Pi	3.1415927	
h	6.63E-34	
N _A	6.022E+23	
x BL ext	0.05 Å	
Compound	BL (Å)	
Zn-ImH	2.01E-10	
Zn-Pyr	2.05E-10	
Zn-carb	1.96E-10	

Table S.11 Calculation of ion-dipole coulombic interaction bond extension 0.05 Å, r equals peak bond length for class.

$E = (k^* \text{dipole moment})/\text{BL}^2$ Q assumed to be 1					Energy of bond extension 0.05 Å		
				BL_{eq}	$\text{BL}_{\text{ext}} 0.05 \text{ Å}$		
formula	dipole moment (D)	BL (Å)	E_c (J)	E (kJ/mol)	E_{ext} (kJ/mol)	ΔE_{ext} (kJ/mol)	
imidazole (in dioxan)	3.95	2.01	4.6961E-19	282.80	269.2373	-13.56	
Pyridine (in CCl ₄)	2.41	2.05	2.7545E-19	165.88	158.0705	-7.80	

benzoic acid	1.72	1.96	2.1505E-19	129.51	123.1427	-6.36
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Table S.12 Calculation of ion-ion coulombic interaction, bond extension 0.05 Å

E = (k*Q ₁ Q ₂)/BL Q assumed to be 1		BL _{eq}	BL _{ext} 0.05 Å	Energy of bond extension 0.05 Å	
Compound	BL (Å)	E _c (J)	E _{eq} (kJ/mol)	E _{ext} (kJ/mol)	ΔE _{ext} (kJ/mol)
imidazole (in dioxan)	2.01	1.1478E-18	691.21	674.43	-16.78
Pyridine (in CCl ₄)	2.05	1.1254E-18	677.72	661.58	-16.14
benzoic acid	1.96	1.1771E-18	708.84	691.21	-17.63

Table S.13 Constants and values used in calculations in tables S.11 and S.12

Constants	
1 D	3.33564E-30 C*m
k (e*3.33564E-30(4Πε ₀) ⁻¹) dipole-ion interaction	4.80321E-39
k (e ² (4Πε ₀) ⁻¹) ion-ion interaction	2.3071E-28
N _A	6.0220E+23

Table S.14 Reference codes and bond lengths for Cu-carboxylic acid compounds

Ref-code	MAZSAI	MAZSAI	YAQJAD	MAZSAI	MAZSAI	MAZSAI	MAZSAI	BAGSOR	KUBYIQ	UJITOX	TEZKAL	HAJRIU01	AWOTIQ
BL (Å)	1.93	1.94	1.95	1.95	1.98	1.98	1.99	2.01	2.46	2.51	2.54	2.58	2.75