Electronic Supplementary Information

Supramolecular features in the engineering of 3d metal complexes with phenyl-substituted imidazoles as ligands: the case of copper(II)

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Table S1. Hydrogen-Bonding Geometry (Å, º) in compounds **1**–**7***

D–H· · ·A	D–H	H· · ·A	D· · ·A	<(DHA)	Symmetry operation of A
1					
C2–H2···Cl	0.93	2.87	3.596(3)	136	1–x, –y, 1–z
C6–H6A···Cl	0.96	2.97	3.797(2)	145	1–x, –y, 1–z
C9–H9···Cl	0.93	2.82	3.697(2)	158	1+x, y, z
C10–H10···C_g^{i}	0.93	2.79	3.581(2)	143	1+x, 1+y, z
C18–H18···C_g^{ii}	0.93	2.70	3.537(2)	151	–1+x, y, z
2					
C2–H2···Br	0.93	3.05	3.790(7)	138	–1–x, 1–y, 1–z
C6–H6A···Br	0.96	3.13	3.891(6)	138	–1–x, 1–y, 1–z
C9–H9···Br	0.93	2.89	3.780(7)	160	1+x, y, z
C10–H10···C_g^{i}	0.93	2.83	3.611(8)	143	1+x, 1+y, z
C18–H18···C_g^{ii}	0.93	2.76	3.599(7)	151	–1+x, y, z
3·0.6MeOH					
C12A–H12A···O2	0.93	2.69	3.570(4)	160	1+x, –1+y, z
C17A–H17A···O1	0.93	2.74	3.443(9)	133	1+x, –1+y, z
C6B–H6B1···O6	0.96	2.63	3.586(4)	172	1–x, y, 3/2–z
C9B–H9B···O5	0.93	2.39	3.145(17)	138	5/2–x, 1/2–y, 2–z
C10B–H10B···O3	0.93	2.88	3.571(6)	132	5/2–x, 1/2–y, 2–z
C11B–H11B···O1	0.93	2.38	3.231(7)	152	3/2+x, –1/2+y, z
C9A–H9A···C_g^{iii}	0.93	2.89	3.665(5)	141	–1/2+x, 1/2–y, –1/2+z
C16A–H16A···C_g^{iv}	0.93	3.03	3.808(5)	143	–1/2+x, –1/2+y, z
4·H_2O					
C2A–H2A···O6	0.93	2.67	3.511(5)	152	1+x, y, z
C6A–H6A1···O7	0.96	2.55	3.416(5)	150	1+x, y, z
C16A–H16A···O4	0.93	2.61	3.525(5)	167	2–x, 1–y, 2–z
C18B–H18B···O4	0.93	2.68	3.529(5)	152	2–x, –y, 2–z
C11C–H11C···O4	0.93	2.35	3.061(4)	133	2–x, –y, 2–z
C17C–H17C···O3	0.93	2.45	3.351(4)	162	1–x, –y, 2–z
C10D–H10D···O5	0.93	2.76	3.571(6)	146	1–x, 1–y, 1–z
C17D–H17D···O3	0.93	2.74	3.625(5)	160	1–x, 1–y, 2–z
C6A–H6A2··· C_g^{v}	0.96	2.65	3.413(6)	137	1+x, y, z
C10A–H10A···C_g^{vi}	0.93	2.90	3.739(6)	150	1–x, 1–y, 2–z
C6C–H6C1···C_g^{vii}	0.96	3.02	3.828(5)	143	–1+x, y, z
5·MeCN·H_2O					
C18A–H18A···O3	0.93	2.67	3.524(2)	153	–x, 1–y, 1–z
C11B–H11B···O3	0.93	2.37	3.095(2)	135	–x, 1–y, 1–z
C17B–H17B···O2	0.93	2.46	3.366(2)	165	1–x, 1–y, 1–z
C10C–H10C···O7	0.93	2.51	3.402(3)	161	1–x, –y, 2–z
C17C–H17C···O2	0.93	2.62	3.482(3)	155	1–x, –y, 1–z
C2D–H2D···O8	0.93	2.66	3.487(4)	149	–1+x, y, z
C6D–H6D3···O5	0.96	2.50	3.400(3)	157	–1+x, y, z
C16D–H16D···O3	0.93	2.64	3.538(3)	163	–x, –y, 1–z
C20–H20A···O7	0.96	2.44	3.218(3)	138	x, y, –1+z
C16B–H16B···C_g^{viii}	0.93	3.19	3.877(4)	133	x, 1+y, z

C6D–H6D2···C_g^{ix}	0.96	2.75	3.479(3)	133	–1+x, y, z
C10D–H10D···C_g^{x}	0.93	3.00	3.809(3)	146	1–x, –y, 1–z
6·Me_2CO·1.6H_2O					
C2A–H2A···O10	0.93	2.44	3.173(3)	136	1/2–x, 1/2+y, –1/2+z
C15A–H15A···O8A	0.93	2.92	3.625(4)	134	1/2–x, –1/2+y, –1/2+z
C17A–H17A···O9	0.93	2.60	3.451(6)	153	–x, 1–y, –1/2+z
C2B–H2B···O11	0.93	2.44	3.323(5)	159	1/2–x, –1/2+y, –1/2+z
C6B–H6B1···O3	0.96	2.60	3.341(3)	134	1/2–x, –1/2+y, –1/2+z
C6C–H6C3···O4	0.96	2.76	3.554(3)	141	x, y, –1+z
C17C–H17C···O7A	0.93	2.53	3.344(4)	146	1–x, 1–y, –1/2+z
C15C–H15C···O9	0.93	2.72	3.488(6)	141	1/2–x, 1/2+y, –1/2+z
C2D–H2D···O2	0.93	2.87	3.698(3)	149	1/2–x, 1/2+y, –1/2+z
C6D–H6D3···O4	0.96	2.87	3.647(3)	139	1/2–x, 1/2+y, –1/2+z
C8D–H8D···O11	0.93	2.41	3.165(5)	138	1/2–x, –1/2+y, –1/2+z
C16D–H16D···O3	0.93	2.73	3.609(3)	158	1–x, 1–y, –1/2+z
C20–H20C···O2	0.93	2.60	3.439(3)	146	1/2–x, 1/2+y, –1/2+z
C6D–H6D2···C_g^{xi}	0.96	2.97	3.724(4)	136	1/2–x, 1/2+y, 1/2+z
7					
O2–H2···O3	0.85(4)	2.15(4)	2.975(5)	165(4)	x, y, –1+z
C2A–H2A···O3	0.93	2.43	3.285(5)	153	1–x, 1–y, 1–z
C2B–H2B···O3	0.93	2.58	3.315(5)	136	x, y, –1+z
C6A–H6A2···O4	0.96	2.58	3.403(6)	144	x, y, z
C11B–H11B···O5	0.93	2.64	3.453(5)	146	x, y, z
C15B–H15B···O6	0.93	2.68	3.355(6)	130	1/2+x, 1/2–y, –1/2+z
C17A–H17A···O6	0.93	2.90	3.611(6)	134	x, y, z
C17B–H17B···O3	0.93	2.71	3.590(5)	158	–1/2+x, 1/2–y, –1/2+z
C20–H20C···O4	0.96	2.74	3.575(6)	146	x, y, –1+z
C16A–H16A···C_g^{xii}	0.93	2.90	3.684(5)	143	–1/2+x, 1/2–y, 1/2+z
C16B–H16B···C_g^{xiii}	0.93	2.78	3.541(5)	139	1/2–x, –1/2+y, 1/2–z

* Ring centroids: (i) C13 to C18; (ii) C7 to C12; (iii) C7B to C12B; (iv) C13B to C18B; (v) C13D to C18D; (vi) C13A to C18A; (vii) C13B to C18B; (viii) C13C to C18C; (ix) C13C to C18C; (x) C13D to C18D; (xi) C13A to C18A; (xii) C13B to C18B; (xiii) N1A to C5A.

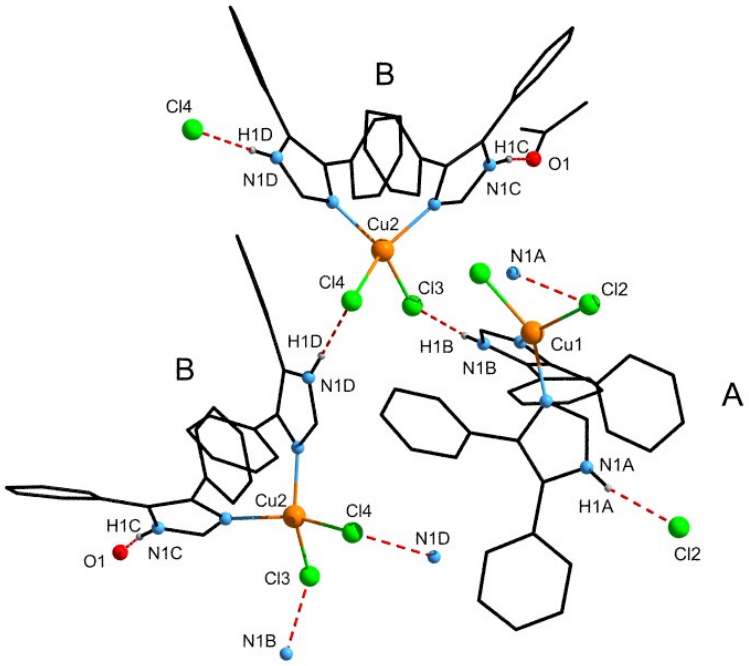


Figure S1. Part of the supramolecular structure of compound **8**. Strong N–H···Cl bonding between the NH groups and the coordinated chloride ions of the two independent (A and B) $[CuCl_2(HL')_2]$ units of the structure guide effectively its 3D self-assembly.

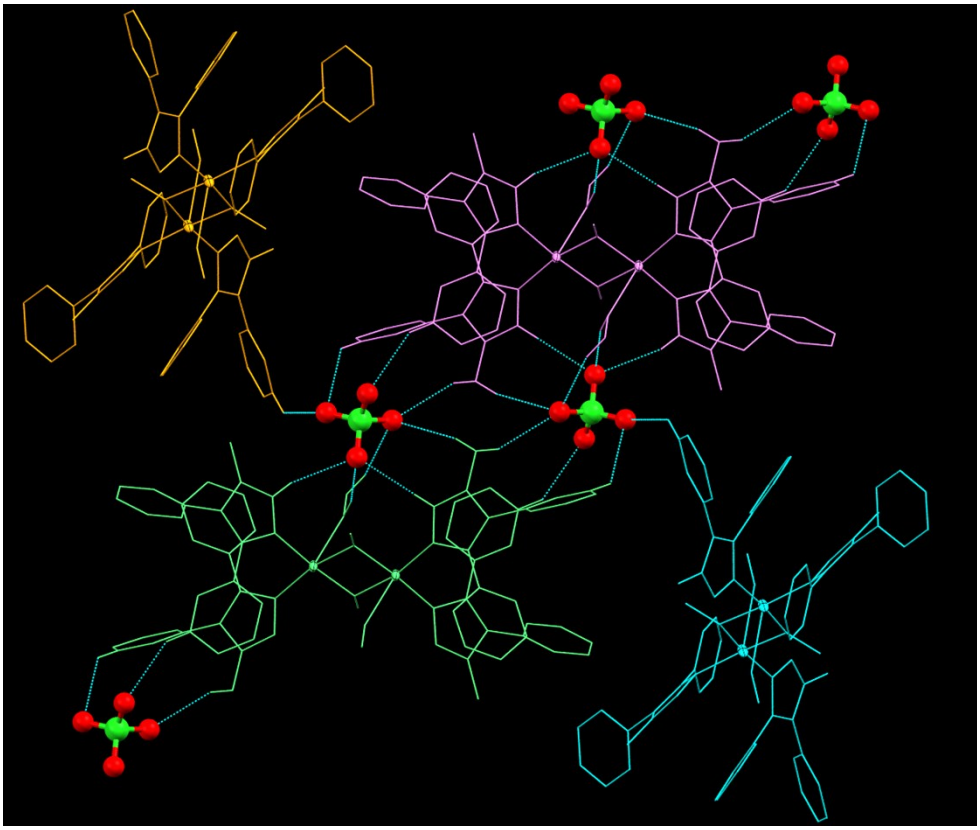


Figure S2. The network of weak C–H···O interactions in the crystal packing of compound **7** organized by the perchlorate counterions and the surrounding ligands of the complexes. Only contact H-atoms are drawn.

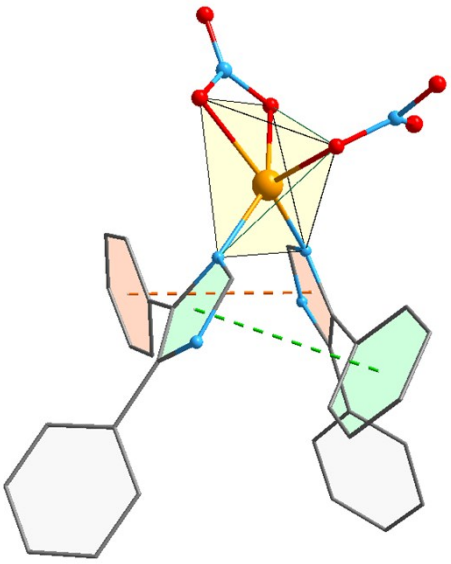


Figure S3. The molecular structure of complex **11**. The two intramolecular π···π patterns together with the distorted square-pyramidal N_2O_3 environment of the copper centre are also shown. Hydrogen atoms have been omitted.

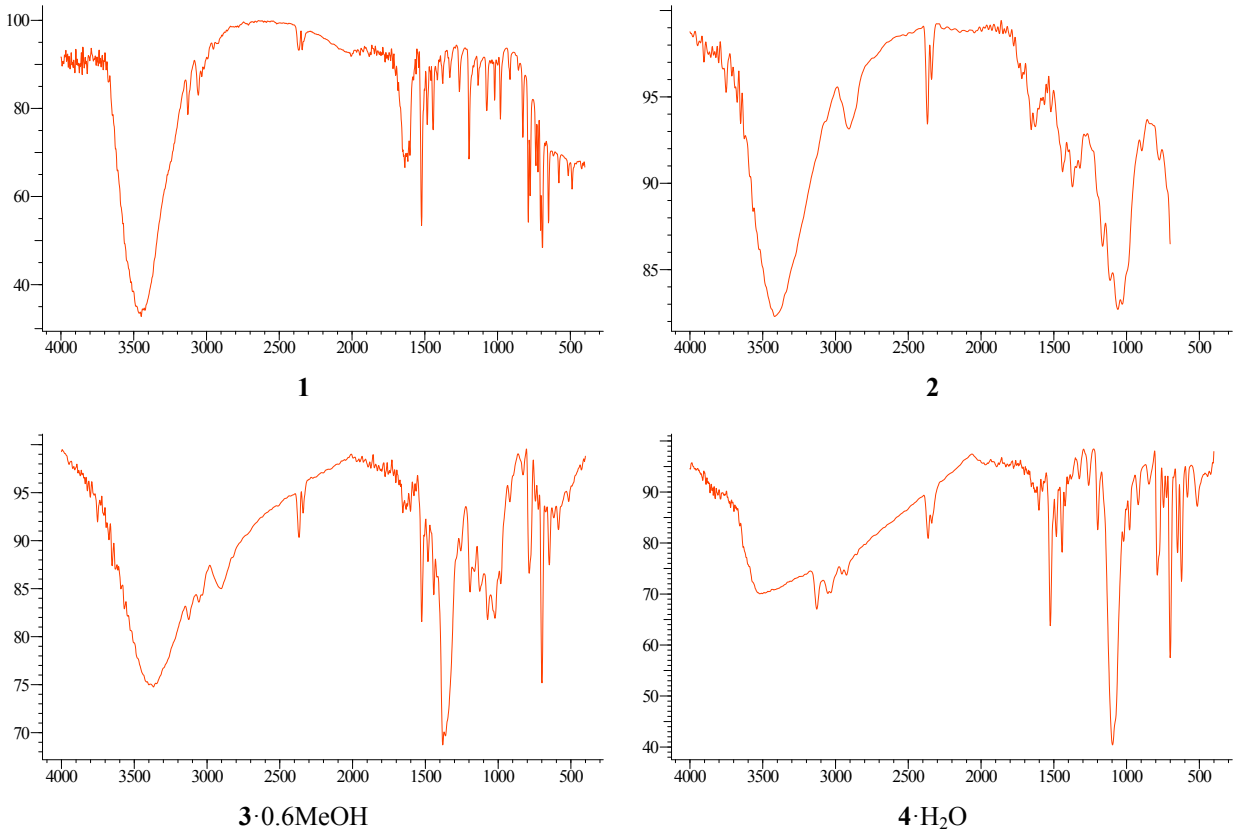
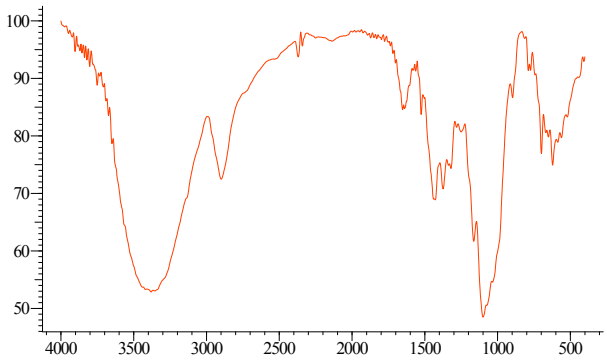
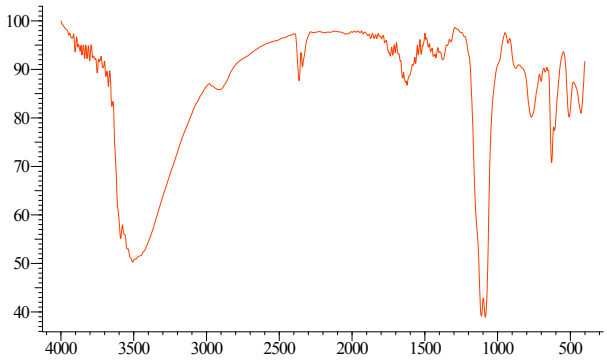


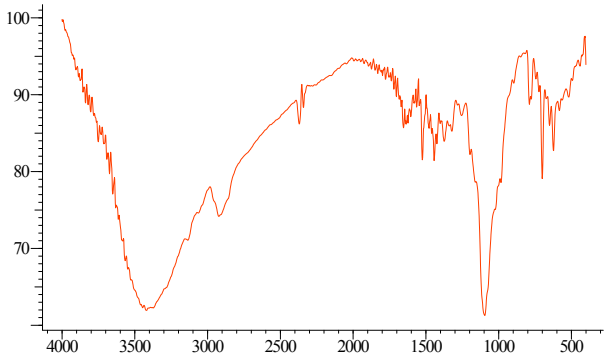
Figure S4. IR spectra for compounds **1–11** (*continued on next page*)



5·MeCN·H_2O



6·Me_2CO·1.6H_2O



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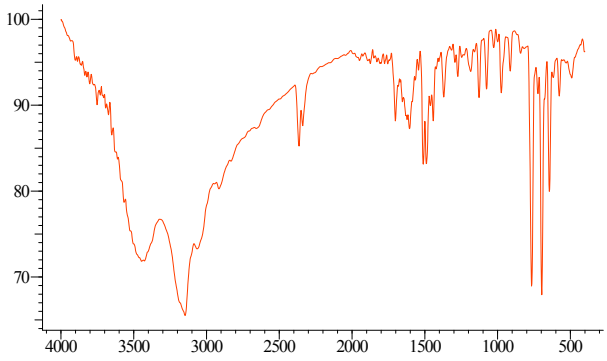
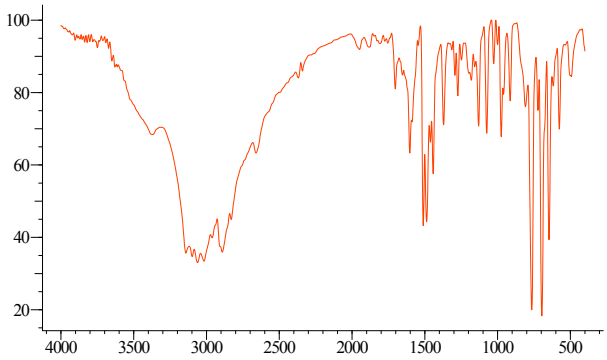
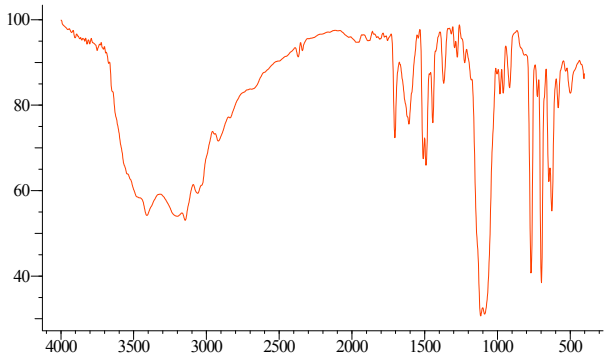


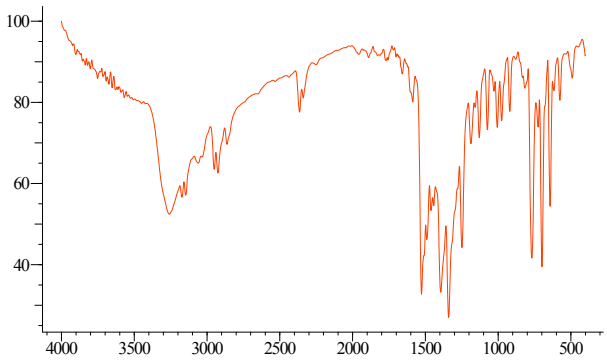
8·Me_2CO·0.25H_2O



9·0.62H_2O



10·EtOH·CH_2Cl_2·H_2O



11·MeCN

Figure S4. IR spectra for compounds **1–11.**