The antimicrobial properties of some copper(II) and platinum(II) 1,10-phenathroline complexes

Supplementary data

Neville S. Ng[a], Peter Leverett[a], David E. Hibbs[b], Qianfan Yang[c], Jerikho C. Bulanadi[a], Ming Jie Wu[a], and Janice R. Aldrich-Wright[a*]

a) School of Science and Health
University of Western Sydney
Locked Bag 1797, Penrith South DC, 2751, NSW Australia

b) Faculty of Pharmacy,
The University of Sydney,
NSW 2006, Australia

c) Beijing National Laboratory for Molecular Sciences (BNLMS),
Center for Molecular Sciences, State Key Laboratory for Structural Chemistry for Unstable and Stable Species, Institute of Chemistry, Chinese Academy of Sciences (ICCAS). Zhongguancun North First Street 2,100190 Beijing, PR China

* Please address editorial correspondence to Prof. Janice R. Aldrich-Wright via e-mail: j.aldrich-wright@uws.edu.au or via facsimile: +61 2 4620 3025.

Synthesis of copper(II) complexes

Compound abbreviations are defined in Table S1. Stock solutions of perchlorate isolates for spectral analysis prepared in 50% acetonitrile (v/v) with concentrations 5-25 mM. For UV spectra, stock solutions were diluted to final concentrations of 5-15 μM for visualisation of 200-400 nm spectra, and 2.3-5.8 mM for visualisation of 400-800 nm bands. Samples were read in square-base quartz cuvettes with a path length of 10 mm. UV spectra were obtained in double beam mode at 600 nm/min, with a data interval of 1 nm, and average time of 0.1 sec at ~23 °C. UV spectra of $\mathbf{1}_{\mathbf{Cu}}$-$\mathbf{21}_{\mathbf{Cu}}$ are provided in Figure S2 and Figure S2.

Table S1. List of compounds referred to in this document.

No	Copper(II) complex	No	Platinum(II) complex
1$_{Cu}$	[Cu(phen)(*SS*-dach)]$(ClO_4)_2$	**1**$_{Pt}$	[Pt(phen)(*SS*-dach)]Cl_2
2$_{Cu}$	[Cu(phen)(*RR*-dach)]$(ClO_4)_2$	**2**$_{Pt}$	[Pt(phen)(*RR*-dach)]Cl_2
3$_{Cu}$	[Cu(4mephen)(*SS*-dach)]$(ClO_4)_2$	**3**$_{Pt}$	[Pt(4mephen)(*SS*-dach)]Cl_2
4$_{Cu}$	[Cu(4mephen)(*RR*-dach)]$(ClO_4)_2$	**4**$_{Pt}$	[Pt(4mephen)(*RR*-dach)]Cl_2
5$_{Cu}$	[Cu(5mephen)(*SS*-dach)]$(ClO_4)_2$	**5**$_{Pt}$	[Pt(5mephen)(*SS*-dach)]Cl_2
6$_{Cu}$	[Cu(5mephen)(*RR*-dach)]$(ClO_4)_2$	**6**$_{Pt}$	[Pt(5mephen)(*RR*-dach)]Cl_2
7$_{Cu}$	[Cu(47me$_2$phen)(*SS*-dach)]$(ClO_4)_2$	**7**$_{Pt}$	[Pt(47me$_2$phen)(*SS*-dach)]Cl_2
8$_{Cu}$	[Cu(47me$_2$phen)(*RR*-dach)]$(ClO_4)_2$	**8**$_{Pt}$	[Pt(47me$_2$phen)(*RR*-dach)]Cl_2
9$_{Cu}$	[Cu(56me$_2$phen)(*SS*-dach)]$(ClO_4)_2$	**9**$_{Pt}$	[Pt(56me$_2$phen)(*SS*-dach)]Cl_2
10$_{Cu}$	[Cu(56me$_2$phen)(*RR*-dach)]$(ClO_4)_2$	**10**$_{Pt}$	[Pt(56me$_2$phen)(*RR*-dach)]Cl_2
11$_{Cu}$	[Cu(3478me$_4$phen)(*SS*-dach)]$(ClO_4)_2$	**11**$_{Pt}$	[Pt(3478me$_4$phen)(*SS*-dach)]Cl_2
12$_{Cu}$	[Cu(3478me$_4$phen)(*RR*-dach)]$(ClO_4)_2$	**12**$_{Pt}$	[Pt(3478me$_4$phen)(*RR*-dach)]Cl_2
13$_{Cu}$	[Cu(5Clphen)(*SS*-dach)]$(ClO_4)_2$	**13**$_{Pt}$	[Pt(5Clphen)(*SS*-dach)]Cl_2
14$_{Cu}$	[Cu(5Clphen)(*RR*-dach)]$(ClO_4)_2$	**14**$_{Pt}$	[Pt(5Clphen)(*RR*-dach)]Cl_2
15$_{Cu}$	[Cu(38Br$_2$phen)(*SS*-dach)]Cl.ClO4	**15**$_{Pt}$	[Pt(phen)(en)]Cl_2
16$_{Cu}$	[Cu(38Br$_2$phen)(*RR*-dach)]Cl.ClO4	**16**$_{Pt}$	[Pt(56me$_2$phen)(en)]Cl_2
17$_{Cu}$	[Cu(5NO$_2$phen)(*SS*-dach)]$(ClO_4)_2$		
18$_{Cu}$	[Cu(5NO$_2$phen)(*RR*-dach)]$(ClO_4)_2$		
19$_{Cu}$	[Cu(DIP)(*SS*-dach)]$(ClO_4)_2$		
20$_{Cu}$	[Cu(DIP)(*RR*-dach)]$(ClO_4)_2$		
21$_{Cu}$	[Cu(56me$_2$phen)$_3$]$(ClO_4)_2$.56me$_2$phen		

No	Intercalator
1$_{IL}$	1,10-phenanthroline (phen)
2$_{IL}$	4-methyl-1,10-phenanthroline (4mephen)
3$_{IL}$	5-methyl-1,10-phenanthroline (5mephen)
4$_{IL}$	4,7-dimethyl-1,10-phenanthroline (47me$_2$phen)
5$_{IL}$	5,6-dimethyl-1,10-phenanthroline (56me$_2$phen)
6$_{IL}$	3,4,7,8-tetramethyl-1,10-phenanthroline (3478me$_4$phen)
7$_{IL}$	5-chloro-1,10-phenanthroline (5Clphen)
8$_{IL}$	3,8-dibromo-1,10-phenanthroline (38Br$_2$phen)
9$_{IL}$	5-nitro-1,10-phenanthroline (5NO$_2$phen)
10$_{IL}$	4,7-diphenyl-1,10-phenanthroline (DIP)

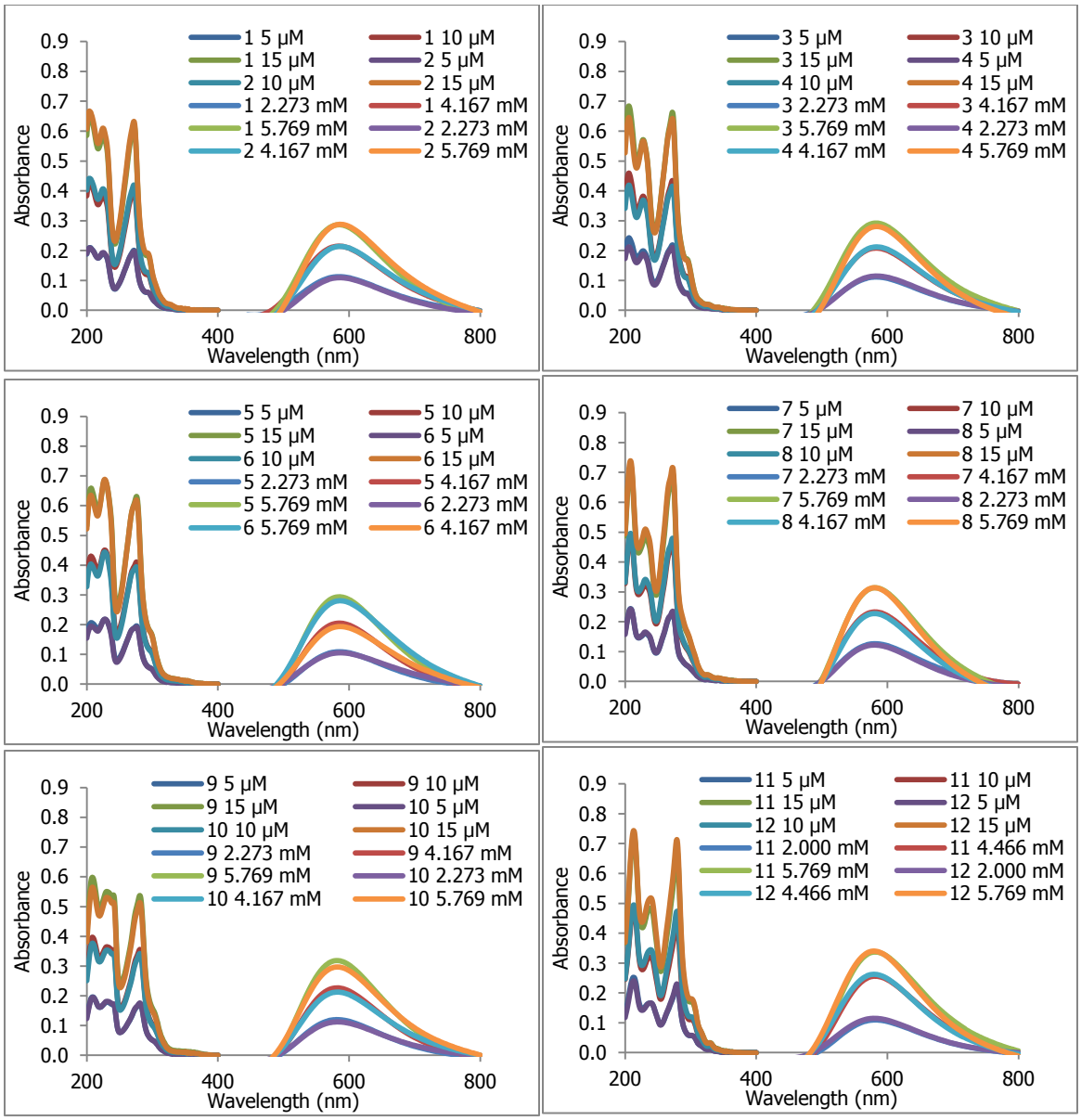


Figure S1.UV spectra of copper(II) complexes $\mathbf{1_{Cu}}$-$\mathbf{12_{Cu}}$.

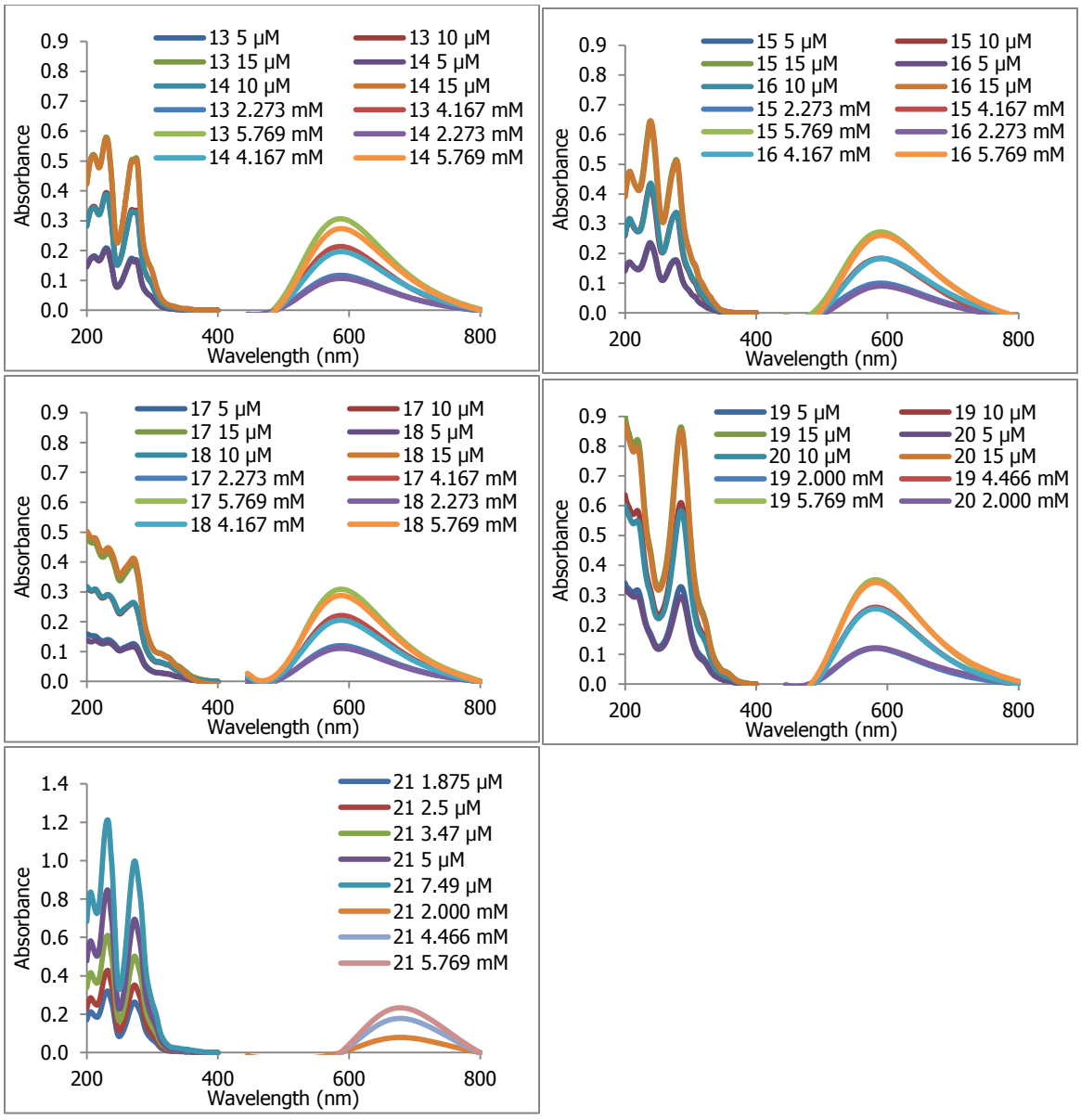


Figure S2.UV spectra of copper(II) complexes **13_{Cu}-21_{Cu}**.

For CD spectra, stock solutions were diluted to 15 µM for 200-400 nm spectra and 5.8 mM for 400-800 nm. Samples were read in the same cuvettes described for UV. Instrument parameters were configured to a scan rate of 200 nm/min, bandwidth of 2 nm, data pitch of 0.5 nm, and response time of 1 s with ≥ 5 accumulations. Spectra was corrected by that of the solvent, 50% acetonitrile (v/v). For all readings, the temperature of the instrument was 23°C. Spectra are provided in Figure S3 and Figure S4.

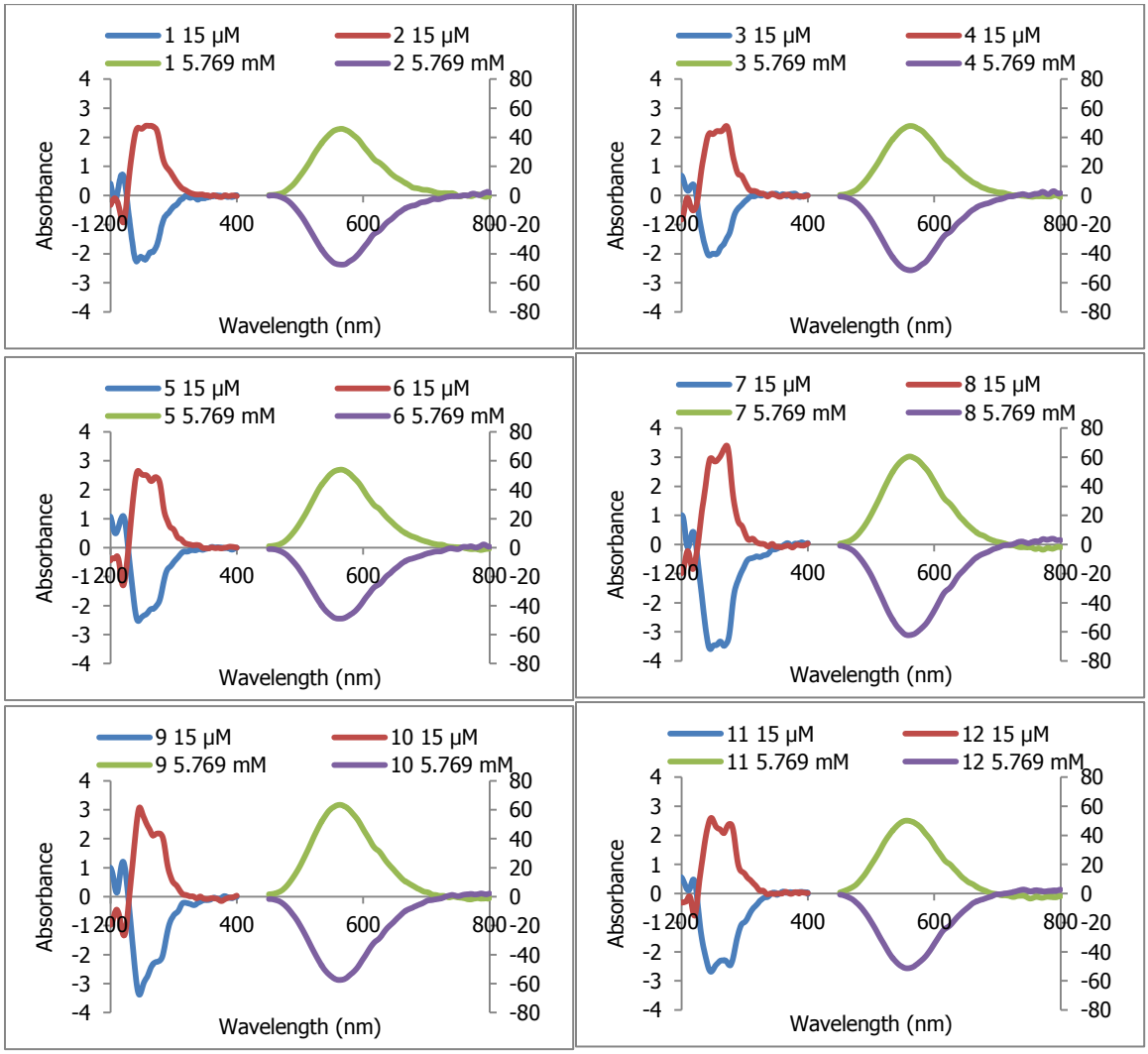


Figure S3. CD spectra of copper(II) complexes $\mathbf{1}_{Cu}$-$\mathbf{12}_{Cu}$.

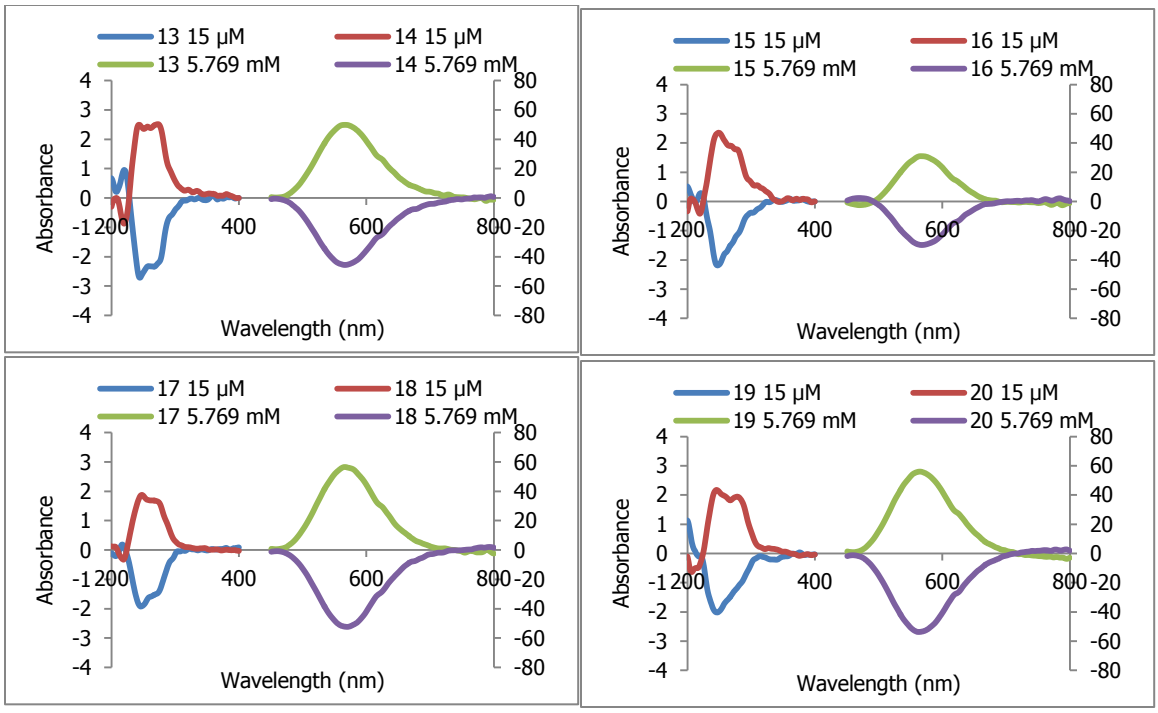


Figure S4. CD spectra of copper(II) complexes $\mathbf{13}_{Cu}$-$\mathbf{20}_{Cu}$.

ESI-MS was carried out in positive ionisation mode scanned in the range m/z = 50-1000 at a capillary voltage of 3.5 kV, cone voltage of 63.5 kV, extractor voltage of 8.4 kV and source temperature of 300°C. Each acetonitrile-dissolved sample at a final concentration of 20 μM was injected via a Waters Aquity AutoSampler with a run time of 2 minutes and a flow rate of 10 μL/min with a binary solvent system of water and acetonitrile. Idle samples were maintained at a temperature of 10°C. Peaks of **20$_{Cu}$** assigned as $[Cu(I_L)(A_L)]ClO_4^+$ (608) and $[Cu(I_L)_2]^{2+}$ (727) are portrayed in Figure S5. All other complexes showed a similar pattern of fragmentation indicating presence of $[Cu(I_L)(A_L)]^{2+}$, and to a lesser extent $[Cu(I_L)_2]^{2+}$ in freshly dissolved samples.

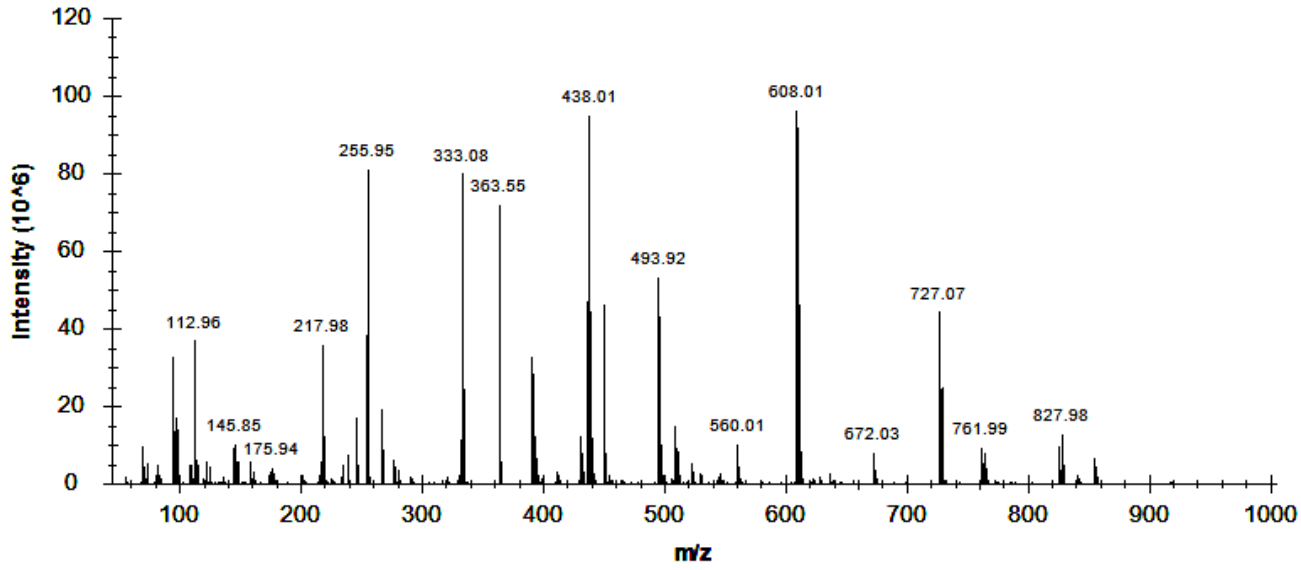


Figure S5. ESI-MS spectra of **20$_{Cu}$**.

Synthesis of platinum(II) complexes

Compound abbreviations are defined in Table S1. $\mathbf{1_{Pt}}$-$\mathbf{16_{Pt}}$ were synthesised by means of an established method.[1] Potassium tetrachloroplatinate (0.415 g, 1 mmol) was dissolved in water (50 mL) and stirred with A_L (*SS*-dach or *RR*-dach, 0. 114 g, 1 mmol.) in water (30 mL) for 1 h. The solution was left in the fridge overnight and the orange-yellow precipitate collected via vacuum filtrated and washed with water and ethanol before drying with diethyl ether. The $[Pt(A_L)Cl_2]$ intermediate was dissolved in water (100 mL), and intercalating ligand ($\mathbf{1_{IL}}$-$\mathbf{10_{IL}}$, 1 mmol.) was added. The mixture was refluxed for 24 h or until clear, and the yellow solution was cooled to room temperature and filtered to remove insoluble impurities. The solution was reduced (~40 mL) and filtered through a Waters Porakpak RP Rxn® column (activated with MeOH, 10 mL before washed with water, 2 × 10 mL). A saturated solution of potassium hexafluorophosphate (5 mL) was added to the filtrate to produce a yellow precipitate. The precipitate was dried with vacuum filtration, washed with water, ethanol and diethyl ether (5 mL each). The water insoluble hexafluorophospate salt was then dissolved in acetone, and tetrabutylammonium chloride was added to precipitate a chloride salt. The yellow product was washed with acetone to remove any excess tetrabutylammonium chloride before drying with diethyl ether (yields 38-96%). Characterisation the previously synthesised platinum(II) complexes $\mathbf{1_{Pt}}$-$\mathbf{16_{Pt}}$ as chloride salts were consistent with literature and are described below (Table S2).

1 Table S2. Structural characterisation of previously published Pt(II) complexes.

#	Yield	ESI-MS (m:z)	CD λ_{max}/nm (mdeg.L.mol-1)× 10^4	^{1}H NMR δ (400 MHz, D_2O)	[^{1}H-^{195}Pt]-HMQC NMR δ (85 MHz, D_2O)	Ref.
1$_{Pt}$	96%	488 [M - 2H$^+$]$^+$	203 (-8), 311 (20), 247 (-8), 261 (20), 227 (-8), 334 (20)	8.84 (d, 2H, *J* = 4.38 Hz); 8.78 (d, 2H, *J* = 8.28 Hz); 7.96 (s, 2H); 7.93 (dd, 2H, *J* = 4.4, 8.3 Hz) 2.72 (bd, 2H); 2.21 (bd, 2H); 1.65 (bd, 2H); 1.48 (bd, 2H); 1.24 (bd, 2H)	-2823	2
2$_{Pt}$	83%	489 [M - H$^+$]$^+$	205 (8), 307 (20), 248.5 (8), 260 (20), 227 (8), 335 (20)	8.84 (d, 2H, *J* = 4.38 Hz); 8.78 (d, 2H, *J* = 8.28 Hz); 7.96 (s, 2H); 7.93 (d, 2H, *J* = 4.4, 8.3 Hz) 2.72 (bd, 2H); 2.21 (bd, 2H); 1.65 (bd, 2H); 1.48 (bd, 2H); 1.24 (bd, 2H)	-2823	2
3$_{Pt}$	62%	502 [M - 2H$^+$]$^+$	206 (-8), 306.5 (20), 247.5 (-8), 262 (20), 228 (-8), 332.5 (20)	8.76 (d, 1H, *J* = 5.33 Hz); 8.69 (d, 1H, *J* = 5.33 Hz); 8.56 (d, 1H, *J* = 5.33 Hz) 7.87 (s, 1H); 7.83 (s, 1H); 7.81 – 7.89 (dd, 1H, *J* = 5.22, 11.56 Hz); 7.69 (d, 1H, *J* = 5.33 Hz); 2.88 (s, 3H); 2.71 (bd, 2H); 2.22 (bd, 2H); 1.66 (bd, 2H); 1.49 (bd, 2H); 1.24 (bt, 2H)	-2826	3
4$_{Pt}$	72%	502 [M - 2H$^+$]$^+$	205.5 (6), 302.5 (20), 248 (6), 259.5 (20), 229 (6), 333 (20)	8.76 (d, 1H, *J* = 5.33 Hz); 8.69 (d, 1H, *J* = 5.33 Hz); 8.56 (d, 1H, *J* = 5.33 Hz) 7.87 (s, 1H); 7.83 (s, 1H); 7.81 – 7.89 (dd, 1H, *J* = 5.22, 11.56 Hz); 7.69 (d, 1H, *J* = 5.33 Hz); 2.88 (s, 3H); 2.71 (bd, 2H); 2.22 (bd, 2H); 1.66 (bd, 2H); 1.49 (bd, 2H); 1.24 (bt, 2H)	-2826	3
5$_{Pt}$	84%	502 [M - 2H$^+$]$^+$	204 (-8), 292 (20), 246.5 (-8), 262 (20), 226.5 (-8), 336.5 (20)	9.28 (d, 1H, *J* = 5.38 Hz); 9.20 (d, 1H, *J* = 5.35 Hz); 9.15 (d, 1H, *J* = 8.47 Hz) 8.99 (d, 1H, *J* = 8.35 Hz) 8.26 (dd, 1H, *J* = 5.39, 8.52 Hz); 8.19 (dd, 1H *J* = 5.41, 8.32 Hz); 8.12 (s, 1H); 2.86 (s, 3H); 2.80 (bd, 2H); 2.31 (bd, 2H); 1.73 (bd, 2H); 1.58 (bd, 2H); 1.32 (bt, 2H)	-2806	3
6$_{Pt}$	83%	503 [M - H$^+$]$^+$	204 (9), 289.5 (20), 248 (9), 262 (20), 228 (9), 336.5 (20)	9.28 (d, 1H, *J* = 5.38 Hz); 9.20 (d, 1H, *J* = 5.35 Hz); 9.15 (d, 1H, *J* = 8.47 Hz) 8.99 (d, 1H, *J* = 8.35 Hz) 8.26 (dd, 1H, *J* = 5.39, 8.52 Hz); 8.19 (dd, 1H *J* = 5.41, 8.32 Hz); 8.12 (s, 1H); 2.86 (s, 3H); 2.80 (bd, 2H); 2.31 (bd, 2H); 1.73 (bd, 2H); 1.58 (bd, 2H); 1.32 (bt, 2H)	-2806	3
7$_{Pt}$	78%	516 [M - 2H$^+$]$^+$	207.5 (-8), 304 (20), 247.5 (-8), 261 (20), 229.5 (-8), 331.5 (20)	9.09 (d, 2H, *J* = 5.23 Hz); 8.40 (s, 2H) 8.08 (d, 2H, *J* = 5.41 Hz); 2.92 (s, 6H) 2.69 (bd, 2H), 2.21 (bd, 2H); 1.65 (bd, 2H); 1.47 (bd, 2H); 1.23 (bt, 2H)	-2833	3
8$_{Pt}$	73%	517 [M - H$^+$]$^+$	205.5 (9), 304.5 (20), 248 (9), 260 (20), 230 (9), 329.5 (20)	9.09 (d, 2H, *J* = 5.23 Hz); 8.40 (s, 2H) 8.08 (d, 2H, *J* = 5.41 Hz); 2.92 (s, 6H) 2.69 (bd, 2H), 2.21 (bd, 2H); 1.65 (bd, 2H); 1.47 (bd, 2H); 1.23 (bt, 2H)	-2833	3
9$_{Pt}$	68%	516 [M - 2H$^+$]$^+$	207 (-7), 287.5 (20), 245 (-7), 265.5 (20), 226 (-7), 340 (20)	9.25 (d, 2H, *J* = 5.23 Hz); 9.17 (d, 2H, *J* =8.65 Hz); 8.22 (dd, 2H, *J* = 5.20, 8.64 Hz); 3.06 (s, 6H); 2.78 (bd, 2H); 2.29 (bd, 2H); 1.73 (bd, 2H); 1.55 (bd, 2H); 1.31 (bt, 2H)	-2838	3
10$_{Pt}$	81%	516 [M - 2H$^+$]$^+$	205.5 (7), 289.5 (20), 244.5 (7), 263 (20), 226.5 (7), 339.5 (20)	9.25 (d, 2H, *J* = 5.23 Hz); 9.17 (d, 2H, *J* =8.65 Hz); 8.22 (dd, 2H, *J* = 5.20, 8.64 Hz); 3.06 (s, 6H); 2.78 (bd, 2H); 2.29 (bd, 2H); 1.73 (bd, 2H); 1.55 (bd, 2H); 1.31 (bt, 2H)	-2838	3
11$_{Pt}$	71%	544 [M - 2H$^+$]$^+$	213 (-8), 303 (20), 249 (-8), 265.5 (20), 233.5 (-8), 331.5 (20)	9.14 (s, 2H); 8.30 (s, 2H); 2.77 (s, 6H); 2.71 (bd, 2H); 2.58 (s, 6H); 2.24 (bd, 2H); 1.67 (bd, 2H); 1.51 (bd, 2H); 1.25 (bt, 3H)	-2823	3
12$_{Pt}$	58%	545 [M - H$^+$]$^+$	213 (10), 301 (20), 250 (10), 264 (20), 233 (10), 334 (20)	9.14 (s, 2H); 8.30 (s, 2H); 2.77 (s, 6H); 2.71 (bd, 2H); 2.58 (s, 6H); 2.24 (bd, 2H); 1.67 (bd, 2H); 1.51 (bd, 2H); 1.25 (bt, 3H)	-2823	3
13$_{Pt}$	69%	522 [M - 2H$^+$]$^+$	207 (-10), 296 (20), 248.5 (-10), 264.5 (20), 228 (-10), 338.5 (20)	9.54 (d, 1H, *J* = 5.20 Hz); 9.46 (d, 1H, *J* = 4.40 Hz); 9.17 (d, 1H, *J* = 8.40 Hz); 9.07 (d, 1H, *J* = 8.40 Hz); 8.63 (s, 1H); 8.34 (dd, 1H, *J* = 5.2 Hz, *J* = 8.4 Hz); 8.26 (dd, 1H, *J* = 5.2 Hz, *J* = 8.4 Hz); 2.73 (bd, 2H); 2.22 (bd, 2H); 1.65 (bd, 2H); 1.49 (bd, 2H); 1.24 (bd, 2H)	-2828	3
14$_{Pt}$	73%	522 [M - 2H$^+$]$^+$	205 (9), 297 (20), 249 (9), 263 (20), 228.5 (9), 339 (20)	9.54 (d, 1H, *J* = 5.20 Hz); 9.46 (d, 1H, *J* = 4.40 Hz); 9.17 (d, 1H, *J* = 8.40 Hz); 9.07 (d, 1H, *J* = 8.40 Hz); 8.63 (s, 1H); 8.34 (dd, 1H, *J* = 5.2 Hz, *J* = 8.4 Hz); 8.26 (dd, 1H, *J* = 5.2 Hz, *J* = 8.4 Hz); 2.73 (bd, 2H); 2.22 (bd, 2H); 1.65 (bd, 2H); 1.49 (bd, 2H); 1.24 (bd, 2H)	-2828	3
15$_{Pt}$	66%	434 [M - 2H$^+$]$^+$	No spectrum	9.20 (m, 2H); 9.15 (d, 2H, *J* = 8.00 Hz); 8.37 (s, 2H); 8.28 (dd, 2H, *J* = 8.00 Hz) 2.92 (s, 4H)	-2849	4
16$_{Pt}$	75%	462 [M - 2H$^+$]$^+$	No spectrum	9.25 (d, 2H, *J* = 5.23 Hz); 9.17 (d, 2H, *J* =8.65 Hz); 8.22 (dd, 2H, *J* = 5.20, 8.64 Hz); 3.06 (s, 4H); 2.8 (s, 6H)	-2869	4

CD experiments for platinum(II) complexes were conducted as described previously. Chloride complexes were dissolved in H_2O to produce stock solutions of 5 mM. For characterisation of the 200-400 nm CD region, stock solutions of 5 mM were diluted to 20 µM in 3 mL circular quartz cuvettes provided by Starna UK with a path length of 5 mm. Enantiomeric pairs of platinum complexes $\mathbf{1_{Pt}}$-$\mathbf{1\backslash 4_{Pt}}$ produced CD spectra with peaks of equal magnitude and opposite signs, confirming relative chiral purity (Figure S6). As expected, no CD spectra was observed for achiral complexes $\mathbf{15_{Pt}}$ and $\mathbf{16_{Pt}}$ (data not shown).

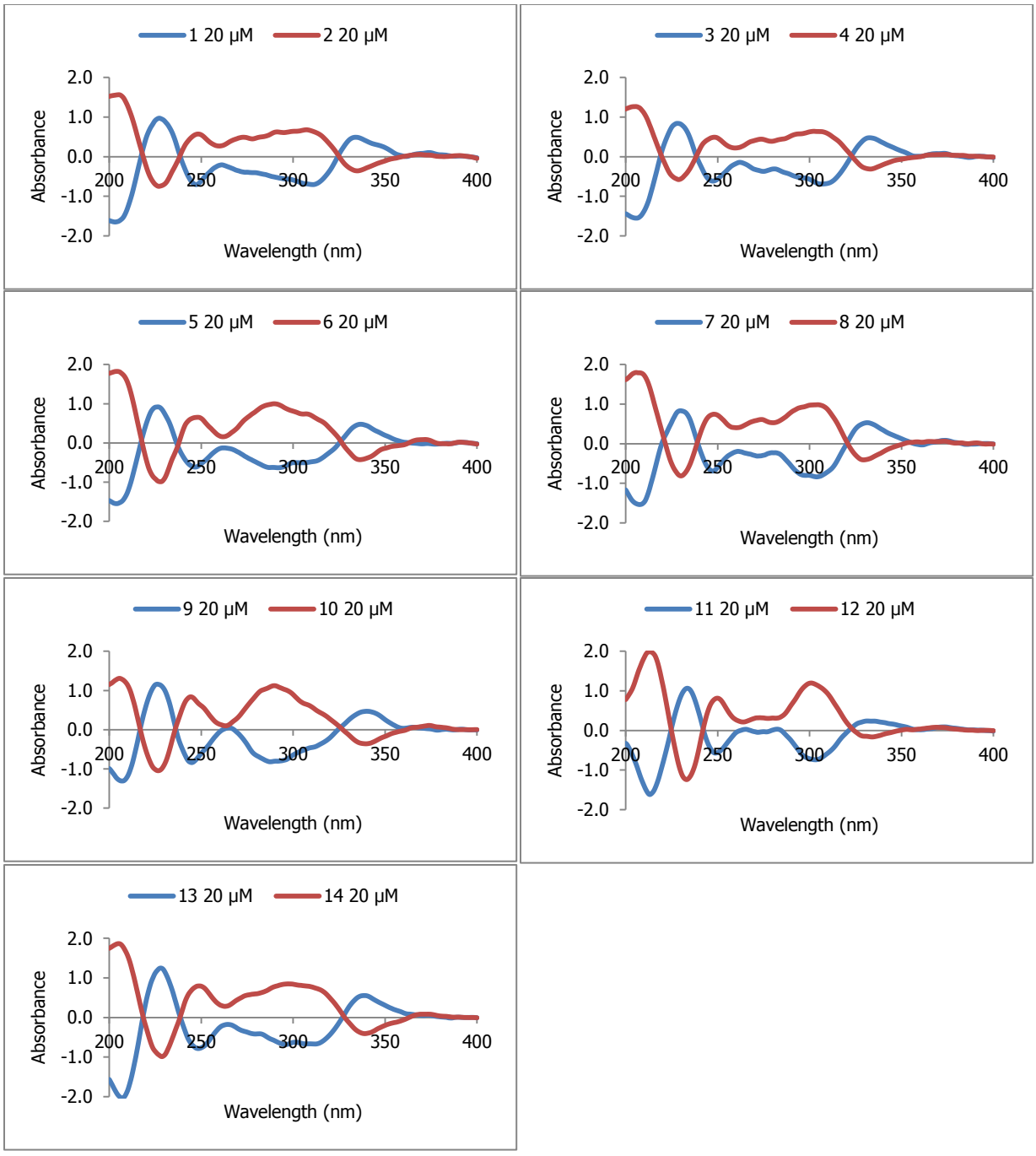


Figure S6. CD spectra of previously published compounds $\mathbf{1_{Pt}}$-$\mathbf{14_{Pt}}$.

NMR samples were prepared with ~2 mg of product dissolved in D_2O at 25 ˚C. For one-dimensional ^1H spectra, a spectral width of 20 ppm was used with 65536 data points and a relaxation delay of 3.7 s. For two-dimensional HMQC spectra 8 transients were recorded and averaged, using a 12 ppm spectral width with 256 increments in the t_1 dimension and 1024 data points in the t_2 dimension. The following abbreviations apply to spin multiplicity: s (singlet), d (doublet), bd (broad doublet), dd (doublet of doublets)

Platinum complexes $\mathbf{1_{Pt}}$-$\mathbf{16_{Pt}}$ exhibit several resonances in the aromatic region of the intercalating ligand between 9 and 7 ppm and aliphatic resonances between 5 and 1 ppm. Each spectrum was assigned and each was consistent with previous documented instances (Table S2). ^1H NMR spectra of $\mathbf{1_{Pt}}$-$\mathbf{16_{Pt}}$ were assigned to the proton labelling system outlined in Figure S7.

In the one-dimensional ^1H NMR spectrum of [Pt(phen)(*SS*-dach)]Cl_2 ($\mathbf{1_{Pt}}$), two overlapping doublets, a singlet and one doublet of doublet are observed in the aromatic region, all with an integrating for the expected eight aromatic protons of the symmetrical phenanthroline ligand. As the protons H5/6 are not coupled to adjacent protons, so the singlet at 8.19 ppm can be assigned to the H5/6. To differentiate between the two doublets, the coupling constants were compared, as it has been shown that a proton located on a carbon alpha to a nitrogen of a pyridyl ring has a smaller coupling constant than a proton located further away from the nitrogen.[5] Therefore, the doublet at 8.96 ppm with J = 5.3 Hz, is assigned as the H2/9 resonance and the doublet at 8.94 ppm, with J = 8.6 Hz, assigned to the H4/7 resonance. The doublet of doublet protons at 8.04 ppm can be attributed to the resonance for H3/8.

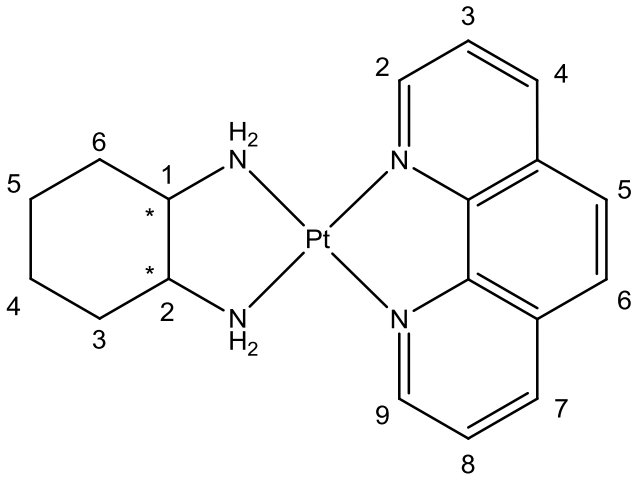


Figure S7. Numbering scheme for complexes **1_{Pt}-16_{Pt}.** * indicates a chiral centre for **1_{Pt}-14_{Pt}**. 3', 4' = H and 5', 6' are absent for **15_{Pt}-16_{Pt}.**

In the aliphatic region of the [Pt(phen)(*SS*-dach)]Cl_2 (**1_{Pt}**) spectrum, five signals are observed; four broad doublets and a broad triplet, each integrating to 2 protons, indicating symmetry within the ancillary ligand. Resonances corresponding to the amine protons were not observed due to the proton exchange with D_2O. The broad resonance at 2.75 ppm was assigned to protons H1'/ H2' due to the deshielding effects of the neighbouring nitrogen. In the DQCOSY spectrum cross peak is observed from the H1/H2 broad singlet resonance to the two doublets at 2.26 ppm and 1.52 ppm, which can then be assigned as the H3/6 proton resonances. The doublet at 1.52 ppm, displays two cross peaks; one with the doublet at 1.63 ppm and the other to the broad triplet at 1.29 ppm, which are then assigned as the H4/H5 proton resonances. [^{1}H-^{195}Pt]-HMQC spectra were recorded as an efficient means of observing ^{195}Pt resonances. A ^{195}Pt resonance of -2823 ppm indicates that phen and dach are coordinated to a central platinum metal as this shift is synonymous with the values determined from other platinum complexes of the formula $[Pt(I_L)(A_L)]^{2+}$.

ESI-MS was carried out with similar conditions above however with final samples in H_2O. The presence of a charged ion generally corresponding to $[M - H^+]^+$ or $[M - 2H^+]^+$ in all cases was confirmed by ESI-MS, with an example of $\mathbf{9_{Pt}}$ 516 $[M - 2H^+]^+$ provided in Figure S8.

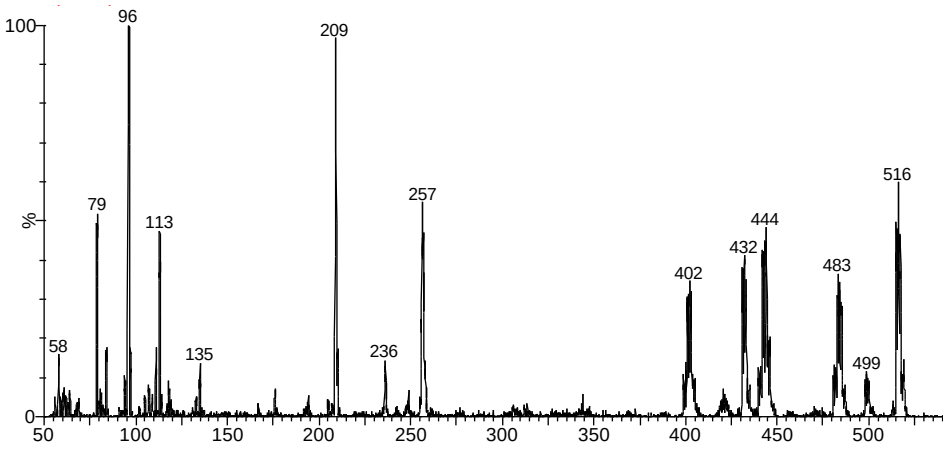


Figure S8. ESI-MS spectra of $\mathbf{9_{Pt}}$.

X-ray crystallography

Table S3. Crystallographic data for [Cu(*RR*-dach)(4mephen)]$(ClO_4)_2$ (**4_{Cu}**) [Cu(*RR*-dach)(56me$_2$phen)(H_2O)]$(ClO_4)_2$.1.5H_2O (**21_{Cu}**) and [Cu(56me$_2$phen)$_3$]$(ClO_4)_2$.56me$_2$phen.2H_2O (**10_{Cu}**)

	4_{Cu}	**10_{Cu}**	**21_{Cu}**
Empirical formula	$C_{19}H_{24}Cl_2CuN_4O_8$	$C_{20}H_{31}Cl_2CuN_4O_{10\cdot50}$	$C_{56}H_{52}Cl_2CuN_8O_{10}$
Formula weight	570.87	629.93	1131.512
Crystal system	Triclinic	Triclinic	Triclinic
Space group	P1	P1	P-1
Temperature (K)	150(2) K	293(2)	293(2) K
a (Å)	9.7307(8)	7.3727(9)	12.128(4)
b (Å)	10.6054(9)	13.5040(17)	13.222(4)
c (Å)	12.7338(11)	13.6633(17)	18.328(6)
α (°)	109.9840(10)	96.441(2)	104.820(4)
β (°)	109.5500(10)	94.312(2)	105.834(4)
γ (°)	94.7620(10)	98.423(2)	99.840(4)
V (Å^3)	1134.51(17)3	1331.3	2640.4(14)
Z	2	2	2
D_c (mg/m^3)	1.671	1.524	1.398
Absorption coefficient (mm^{-1})	1.253	1.082	0.58
θ range for data collection (°)	1.85 to 28.31	1.51 to 26.96	1.22 to 28.34
Reflections	9005	10201	20774
Independent reflections	7622 [$R_{(int)}$ = 0.0138]	8662 [$R_{(int)}$ = 0.0243]	11558 [$R_{(int)}$ = 0.1511]
GooF on F2	1.039	0.982	1.003
Final R [I>2*σ*(I)] R1	0.0458	0.0635	0.1441
Final R [I>2*σ*(I)] wR_2	0.1191	0.1673	0.3552
R indices (all data) R1	0.0565	0.0956	0.3537
R indices (all data) wR_2	0.1262	0.1967	0.4596
Crystal size (mm)	0.25 x 0.15 x 0.15	0.05 x 0.05 x 0.08	0.06x 0.04 x 0.04
F(000)	586	646	1150
Completeness to θ = 28.30°	87.90%	95.50%	87.50%
Refinement method	Full-matrix least-squares on F2	Full-matrix least-squares on F2	Full-matrix least-squares on F2
Data	7622	8662	11558
Restraints	21	9	0
Parameters	615	437	332
Index ranges	$-12 \le h \le 12$ $-13 \le k \le 13$ $-16 \le l \le 15$	$-9 \le h \le 6$ $-17 \le k \le 17$ $-17 \le l \le 17$	$-15 \le h \le 14$ $-17 \le k \le 17$ $-22 \le l \le 24$
Min., max. Δρ/e-3	1.153 and -0.709	1.408, -0.458	2.496, -0.597

Table S4. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for [Cu(*RR*-dach)(4mephen)](ClO_4)$_2$ (**4$_{Cu}$**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
Cu(1)	2953(1)	8266(1)	4313(1)	34(1)	C(23)	5138(10)	3515(10)	10022(9)	52(2)
N(11)	1251(7)	9070(7)	3637(6)	41(2)	C(24)	3689(9)	2853(8)	8993(8)	40(2)
N(12)	3837(7)	10262(6)	5452(5)	35(1)	C(25)	3179(10)	1377(9)	8265(8)	50(2)
C(11)	-44(8)	8436(9)	2704(7)	46(2)	C(26)	1858(11)	835(9)	7357(9)	48(2)
C(12)	-1053(9)	9191(11)	2271(8)	50(2)	C(27)	875(9)	1708(8)	7045(8)	39(2)
C(13)	-747(9)	10588(10)	2787(8)	50(2)	C(28)	-540(10)	1183(8)	6098(7)	44(2)
C(14)	582(9)	11295(10)	3791(8)	51(2)	C(29)	-1389(9)	2107(8)	5852(7)	42(2)
C(15)	1028(10)	12723(9)	4440(8)	50(2)	C(210)	-853(8)	3495(8)	6549(7)	41(2)
C(16)	2334(11)	13348(10)	5429(9)	53(2)	C(211)	1335(8)	3101(8)	7707(6)	32(2)
C(17)	3355(10)	12569(8)	5781(8)	44(2)	C(212)	2764(8)	3729(9)	8713(7)	38(2)
C(18)	4775(11)	13140(9)	6777(8)	52(2)	C(213)	6185(10)	2647(11)	10391(11)	74(3)
C(19)	5674(10)	12274(8)	7046(7)	47(2)	N(23)	-311(7)	6717(6)	8010(5)	34(1)
C(110)	5164(9)	10830(8)	6381(7)	39(2)	N(24)	2342(6)	7912(6)	9886(5)	32(1)
C(111)	2970(9)	11089(8)	5161(7)	40(2)	C(214)	-194(6)	8087(5)	8895(5)	29(1)
C(112)	1576(9)	10477(8)	4173(7)	37(2)	C(215)	-1192(7)	8930(7)	8373(6)	34(2)
C(113)	-1837(10)	11404(11)	2348(9)	64(3)	C(216)	-1017(7)	10317(7)	9355(7)	45(2)
N(13)	4700(7)	7603(6)	5152(5)	34(1)	C(217)	609(7)	11094(6)	10045(6)	49(2)
N(14)	2311(6)	6314(7)	3025(5)	32(1)	C(218)	1615(7)	10213(7)	10495(7)	40(2)
C(114)	4426(6)	6115(5)	4598(5)	30(1)	C(219)	1429(6)	8849(6)	9495(5)	34(1)
C(115)	5838(8)	5574(7)	4898(6)	38(2)	Cl(2)	-763(2)	4819(2)	9933(2)	33(1)
C(116)	5552(8)	4035(7)	4189(6)	48(2)	O(21)	692(5)	5697(6)	10282(4)	42(1)
C(117)	4733(8)	3633(6)	2837(6)	45(1)	O(22)	-976(6)	4936(7)	11015(5)	63(2)
C(118)	3317(7)	4184(7)	2534(6)	40(2)	O(23)	-1900(6)	5263(7)	9193(6)	61(2)
C(119)	3636(6)	5698(6)	3221(5)	30(1)	O(24)	-770(8)	3446(6)	9291(6)	59(2)
Cl(1)	5157(2)	9393(2)	3045(2)	35(1)	Cl(3)	4708(2)	7655(3)	8188(2)	55(1)
O(11)	3722(5)	8602(6)	2700(4)	44(1)	O(31)	3165(6)	6917(7)	7711(5)	64(2)
O(12)	5528(6)	9086(7)	2003(5)	61(2)	O(32)	4852(7)	8673(6)	7688(5)	58(2)
O(13)	6220(6)	9059(6)	3966(5)	53(1)	O(33)	5286(8)	8231(8)	9409(5)	94(3)
O(14)	5149(7)	10821(6)	3560(6)	62(2)	O(34)	5466(9)	6594(6)	7701(8)	91(2)
Cu(2)	1443(1)	5974(1)	8684(1)	31(1)	Cl(4)	9939(2)	6613(2)	4905(2)	46(1)
N(21)	3123(6)	5112(6)	9311(6)	30(1)	O(41)	11506(7)	7299(8)	5321(6)	74(2)
N(22)	476(7)	4010(6)	7454(6)	34(1)	O(42)	9745(8)	5789(7)	5512(6)	72(2)
C(21)	4439(8)	5678(9)	10225(7)	42(2)	O(43)	9470(9)	5732(10)	3692(7)	121(3)
C(22)	5468(8)	4907(9)	10584(8)	47(2)	O(44)	9094(11)	7589(11)	5067(12)	137(4)

Table S5. Bond lengths [Å] and angles [°] for [Cu(*RR*-dach)(4mephen)]$(ClO_4)_2$ (**4$_{Cu}$**).

Bond	Length [Å]	Bond	Length [Å]	Bond	Length [Å]	Bond	Length [Å]
Cu(1)-N(11)	1.998(6)	C(113)-H(11C)	0.98	Cu(2)-O(31)	2.702(5)	N(24)-H(24A)	0.92
Cu(1)-N(13)	2.005(6)	N(13)-C(114)	1.450(8)	N(21)-C(21)	1.324(10)	N(24)-H(24B)	0.92
Cu(1)-N(12)	2.022(6)	N(13)-H(13A)	0.92	N(21)-C(212)	1.351(10)	C(214)-C(219)	1.514(7)
Cu(1)-N(14)	2.036(6)	N(13)-H(13B)	0.92	N(22)-C(210)	1.324(9)	C(214)-C(215)	1.518(8)
Cu(1)-O(11)	2.528(5)	N(14)-C(119)	1.479(8)	N(22)-C(211)	1.377(9)	C(214)-H(214)	1
Cu(1)-O(41)#1	2.560(6)	N(14)-H(14A)	0.92	C(21)-C(22)	1.402(10)	C(215)-C(216)	1.521(9)
N(11)-C(11)	1.328(10)	N(14)-H(14B)	0.92	C(21)-H(21)	0.95	C(215)-H(21D)	0.99
N(11)-C(112)	1.369(10)	C(114)-C(115)	1.514(9)	C(22)-C(23)	1.357(12)	C(215)-H(21E)	0.99
N(12)-C(111)	1.324(10)	C(114)-C(119)	1.540(7)	C(22)-H(22)	0.95	C(216)-C(217)	1.521(9)
N(12)-C(110)	1.338(10)	C(114)-H(114)	1	C(23)-C(24)	1.472(13)	C(216)-H(21F)	0.99
C(11)-C(12)	1.406(11)	C(115)-C(116)	1.518(10)	C(23)-C(213)	1.496(11)	C(216)-H(21G)	0.99
C(11)-H(11)	0.95	C(115)-H(11D)	0.99	C(24)-C(212)	1.397(10)	C(217)-C(218)	1.517(9)
C(12)-C(13)	1.359(13)	C(115)-H(11E)	0.99	C(24)-C(25)	1.458(12)	C(217)-H(21H)	0.99
C(12)-H(12)	0.95	C(116)-C(117)	1.518(8)	C(25)-C(26)	1.322(12)	C(217)-H(21I)	0.99
C(13)-C(14)	1.395(13)	C(116)-H(11F)	0.99	C(25)-H(25)	0.95	C(218)-C(219)	1.514(9)
C(13)-C(113)	1.507(11)	C(116)-H(11G)	0.99	C(26)-C(27)	1.440(11)	C(218)-H(21J)	0.99
C(14)-C(15)	1.400(13)	C(117)-C(118)	1.524(9)	C(26)-H(26)	0.95	C(218)-H(21K)	0.99
C(14)-C(112)	1.427(11)	C(117)-H(11H)	0.99	C(27)-C(211)	1.371(11)	C(219)-H(219)	1
C(15)-C(16)	1.363(13)	C(117)-H(11I)	0.99	C(27)-C(28)	1.401(12)	Cl(2)-O(24)	1.403(6)
C(15)-H(15)	0.95	C(118)-C(119)	1.488(9)	C(28)-C(29)	1.383(12)	Cl(2)-O(23)	1.423(5)
C(16)-C(17)	1.401(12)	C(118)-H(11J)	0.99	C(28)-H(28)	0.95	Cl(2)-O(22)	1.426(6)
C(16)-H(16)	0.95	C(118)-H(11K)	0.99	C(29)-C(210)	1.377(11)	Cl(2)-O(21)	1.465(5)
C(17)-C(18)	1.431(12)	C(119)-H(119)	1	C(29)-H(29)	0.95	Cl(3)-O(33)	1.347(6)
C(17)-C(111)	1.444(12)	Cl(1)-O(11)	1.410(5)	C(210)-H(210)	0.95	Cl(3)-O(32)	1.447(5)
C(18)-C(19)	1.369(12)	Cl(1)-O(12)	1.429(6)	C(211)-C(212)	1.446(10)	Cl(3)-O(31)	1.450(6)
C(18)-H(18)	0.95	Cl(1)-O(14)	1.431(6)	C(213)-H(21A)	0.98	Cl(3)-O(34)	1.470(7)
C(19)-C(110)	1.419(11)	Cl(1)-O(13)	1.450(5)	C(213)-H(21B)	0.98	Cl(4)-O(44)	1.378(9)
C(19)-H(19)	0.95	Cu(2)-N(23)	1.994(6)	C(213)-H(21C)	0.98	Cl(4)-O(42)	1.389(5)
C(110)-H(110)	0.95	Cu(2)-N(24)	1.996(6)	N(23)-C(214)	1.471(8)	Cl(4)-O(43)	1.392(8)
C(111)-C(112)	1.414(11)	Cu(2)-N(21)	2.005(6)	N(23)-H(23A)	0.92	Cl(4)-O(41)	1.465(7)
C(113)-H(11A)	0.98	Cu(2)-N(22)	2.034(7)	N(23)-H(23B)	0.92		
C(113)-H(11B)	0.98	Cu(2)-O(21)	2.476(4)	N(24)-C(219)	1.488(8)		

Bond	Angle [°]	Bond	Angle [°]	Bond	Angle [°]
N(11)-Cu(1)-N(13)	174.3(3)	C(116)-C(115)-H(11D)	109.2	N(22)-C(210)-C(29)	122.8(7)
N(11)-Cu(1)-N(12)	81.3(3)	C(114)-C(115)-H(11E)	109.2	N(22)-C(210)-H(210)	118.6
N(13)-Cu(1)-N(12)	94.0(2)	C(116)-C(115)-H(11E)	109.2	C(29)-C(210)-H(210)	118.6
N(11)-Cu(1)-N(14)	101.0(3)	H(11D)-C(115)-H(11E)	107.9	C(27)-C(211)-N(22)	122.5(7)
N(13)-Cu(1)-N(14)	84.2(2)	C(117)-C(116)-C(115)	111.9(5)	C(27)-C(211)-C(212)	122.6(7)
N(12)-Cu(1)-N(14)	169.9(2)	C(117)-C(116)-H(11F)	109.2	N(22)-C(211)-C(212)	114.9(7)
N(11)-Cu(1)-O(11)	83.1(2)	C(115)-C(116)-H(11F)	109.2	N(21)-C(212)-C(24)	124.5(8)
N(13)-Cu(1)-O(11)	100.3(2)	C(117)-C(116)-H(11G)	109.2	N(21)-C(212)-C(211)	118.4(6)
N(12)-Cu(1)-O(11)	92.3(2)	C(115)-C(116)-H(11G)	109.2	C(24)-C(212)-C(211)	117.1(8)
N(14)-Cu(1)-O(11)	78.4(2)	H(11F)-C(116)-H(11G)	107.9	C(23)-C(213)-H(21A)	109.5
N(11)-Cu(1)-O(41)#1	90.6(2)	C(116)-C(117)-C(118)	112.8(6)	C(23)-C(213)-H(21B)	109.5
N(13)-Cu(1)-O(41)#1	87.6(2)	C(116)-C(117)-H(11H)	109	H(21A)-C(213)-H(21B)	109.5
N(12)-Cu(1)-O(41)#1	104.6(2)	C(118)-C(117)-H(11H)	109	C(23)-C(213)-H(21C)	109.5
N(14)-Cu(1)-O(41)#1	85.2(2)	C(116)-C(117)-H(11I)	109	H(21A)-C(213)-H(21C)	109.5
O(11)-Cu(1)-O(41)#1	160.9(2)	C(118)-C(117)-H(11I)	109	H(21B)-C(213)-H(21C)	109.5
C(11)-N(11)-C(112)	118.3(7)	H(11H)-C(117)-H(11I)	107.8	C(214)-N(23)-Cu(2)	109.5(4)
C(11)-N(11)-Cu(1)	128.8(6)	C(119)-C(118)-C(117)	111.3(5)	C(214)-N(23)-H(23A)	109.8
C(112)-N(11)-Cu(1)	112.7(5)	C(119)-C(118)-H(11J)	109.4	Cu(2)-N(23)-H(23A)	109.8
C(111)-N(12)-C(110)	118.1(7)	C(117)-C(118)-H(11J)	109.4	C(214)-N(23)-H(23B)	109.8
C(111)-N(12)-Cu(1)	112.6(5)	C(119)-C(118)-H(11K)	109.4	Cu(2)-N(23)-H(23B)	109.8
C(110)-N(12)-Cu(1)	129.2(5)	C(117)-C(118)-H(11K)	109.4	H(23A)-N(23)-H(23B)	108.2
N(11)-C(11)-C(12)	120.9(9)	H(11J)-C(118)-H(11K)	108	C(219)-N(24)-Cu(2)	109.9(4)
N(11)-C(11)-H(11)	119.5	N(14)-C(119)-C(118)	115.0(5)	C(219)-N(24)-H(24A)	109.7
C(12)-C(11)-H(11)	119.5	N(14)-C(119)-C(114)	107.1(5)	Cu(2)-N(24)-H(24A)	109.7
C(13)-C(12)-C(11)	121.6(9)	C(118)-C(119)-C(114)	112.2(4)	C(219)-N(24)-H(24B)	109.7
C(13)-C(12)-H(12)	119.2	N(14)-C(119)-H(119)	107.4	Cu(2)-N(24)-H(24B)	109.7
C(11)-C(12)-H(12)	119.2	C(118)-C(119)-H(119)	107.4	H(24A)-N(24)-H(24B)	108.2
C(12)-C(13)-C(14)	119.4(8)	C(114)-C(119)-H(119)	107.4	N(23)-C(214)-C(219)	108.4(5)
C(12)-C(13)-C(113)	122.0(9)	O(11)-Cl(1)-O(12)	109.0(3)	N(23)-C(214)-C(215)	114.5(5)
C(14)-C(13)-C(113)	118.5(9)	O(11)-Cl(1)-O(14)	108.9(4)	C(219)-C(214)-C(215)	110.9(4)
C(13)-C(14)-C(15)	125.9(8)	O(12)-Cl(1)-O(14)	111.0(4)	N(23)-C(214)-H(214)	107.6

Table S5. Cont.

C(13)-C(14)-C(112)	116.4(9)	O(11)-Cl(1)-O(13)	108.5(3)	C(219)-C(214)-H(214)	107.6
C(15)-C(14)-C(112)	117.7(8)	O(12)-Cl(1)-O(13)	110.9(4)	C(215)-C(214)-H(214)	107.6
C(16)-C(15)-C(14)	123.0(8)	O(14)-Cl(1)-O(13)	108.5(4)	C(214)-C(215)-C(216)	110.8(5)
C(16)-C(15)-H(15)	118.5	Cl(1)-O(11)-Cu(1)	119.1(3)	C(214)-C(215)-H(21D)	109.5
C(14)-C(15)-H(15)	118.5	N(23)-Cu(2)-N(24)	84.8(2)	C(216)-C(215)-H(21D)	109.5
C(15)-C(16)-C(17)	120.1(9)	N(23)-Cu(2)-N(21)	176.5(3)	C(214)-C(215)-H(21E)	109.5
C(15)-C(16)-H(16)	120	N(24)-Cu(2)-N(21)	98.5(2)	C(216)-C(215)-H(21E)	109.5
C(17)-C(16)-H(16)	120	N(23)-Cu(2)-N(22)	93.9(2)	H(21D)-C(215)-H(21E)	108.1
C(16)-C(17)-C(18)	124.1(8)	N(24)-Cu(2)-N(22)	178.6(3)	C(217)-C(216)-C(215)	112.1(5)
C(16)-C(17)-C(111)	120.0(9)	N(21)-Cu(2)-N(22)	82.8(2)	C(217)-C(216)-H(21F)	109.2
C(18)-C(17)-C(111)	115.9(8)	N(23)-Cu(2)-O(21)	94.7(2)	C(215)-C(216)-H(21F)	109.2
C(19)-C(18)-C(17)	118.9(8)	N(24)-Cu(2)-O(21)	84.0(2)	C(217)-C(216)-H(21G)	109.2
C(19)-C(18)-H(18)	120.5	N(21)-Cu(2)-O(21)	84.4(2)	C(215)-C(216)-H(21G)	109.2
C(17)-C(18)-H(18)	120.5	N(22)-Cu(2)-O(21)	95.53(19)	H(21F)-C(216)-H(21G)	107.9
C(18)-C(19)-C(110)	120.1(8)	N(23)-Cu(2)-O(31)	96.2(2)	C(218)-C(217)-C(216)	112.0(5)
C(18)-C(19)-H(19)	120	N(24)-Cu(2)-O(31)	78.0(2)	C(218)-C(217)-H(21H)	109.2
C(110)-C(19)-H(19)	120	N(21)-Cu(2)-O(31)	85.8(2)	C(216)-C(217)-H(21H)	109.2
N(12)-C(110)-C(19)	122.5(8)	N(22)-Cu(2)-O(31)	102.7(2)	C(218)-C(217)-H(21I)	109.2
N(12)-C(110)-H(110)	118.8	O(21)-Cu(2)-O(31)	157.98(17)	C(216)-C(217)-H(21I)	109.2
C(19)-C(110)-H(110)	118.8	C(21)-N(21)-C(212)	117.9(6)	H(21H)-C(217)-H(21I)	107.9
N(12)-C(111)-C(112)	117.5(7)	C(21)-N(21)-Cu(2)	130.2(5)	C(219)-C(218)-C(217)	112.5(5)
N(12)-C(111)-C(17)	124.5(8)	C(212)-N(21)-Cu(2)	111.8(5)	C(219)-C(218)-H(21J)	109.1
C(112)-C(111)-C(17)	118.0(7)	C(210)-N(22)-C(211)	117.8(7)	C(217)-C(218)-H(21J)	109.1
N(11)-C(112)-C(111)	115.6(7)	C(210)-N(22)-Cu(2)	130.2(5)	C(219)-C(218)-H(21K)	109.1
N(11)-C(112)-C(14)	123.3(8)	C(211)-N(22)-Cu(2)	111.8(5)	C(217)-C(218)-H(21K)	109.1
C(111)-C(112)-C(14)	121.1(8)	N(21)-C(21)-C(22)	122.8(8)	H(21J)-C(218)-H(21K)	107.8
C(13)-C(113)-H(11A)	109.5	N(21)-C(21)-H(21)	118.6	N(24)-C(219)-C(214)	107.7(4)
C(13)-C(113)-H(11B)	109.5	C(22)-C(21)-H(21)	118.6	N(24)-C(219)-C(218)	115.2(5)
H(11A)-C(113)-H(11B)	109.5	C(23)-C(22)-C(21)	121.0(8)	C(214)-C(219)-C(218)	109.8(5)
C(13)-C(113)-H(11C)	109.5	C(23)-C(22)-H(22)	119.5	N(24)-C(219)-H(219)	108
H(11A)-C(113)-H(11C)	109.5	C(21)-C(22)-H(22)	119.5	C(214)-C(219)-H(219)	108
H(11B)-C(113)-H(11C)	109.5	C(22)-C(23)-C(24)	117.5(7)	C(218)-C(219)-H(219)	108
C(114)-N(13)-Cu(1)	110.4(4)	C(22)-C(23)-C(213)	122.9(9)	O(24)-Cl(2)-O(23)	110.0(4)
C(114)-N(13)-H(13A)	109.6	C(24)-C(23)-C(213)	119.5(9)	O(24)-Cl(2)-O(22)	109.4(4)
Cu(1)-N(13)-H(13A)	109.6	C(212)-C(24)-C(25)	119.1(8)	O(23)-Cl(2)-O(22)	111.0(4)
C(114)-N(13)-H(13B)	109.6	C(212)-C(24)-C(23)	116.2(8)	O(24)-Cl(2)-O(21)	109.5(4)
Cu(1)-N(13)-H(13B)	109.6	C(25)-C(24)-C(23)	124.7(7)	O(23)-Cl(2)-O(21)	108.9(3)
H(13A)-N(13)-H(13B)	108.1	C(26)-C(25)-C(24)	122.2(7)	O(22)-Cl(2)-O(21)	107.9(3)
C(119)-N(14)-Cu(1)	107.3(4)	C(26)-C(25)-H(25)	118.9	Cl(2)-O(21)-Cu(2)	119.2(3)
C(119)-N(14)-H(14A)	110.3	C(24)-C(25)-H(25)	118.9	O(33)-Cl(3)-O(32)	111.1(4)
Cu(1)-N(14)-H(14A)	110.3	C(25)-C(26)-C(27)	120.1(8)	O(33)-Cl(3)-O(31)	111.5(4)
C(119)-N(14)-H(14B)	110.3	C(25)-C(26)-H(26)	119.9	O(32)-Cl(3)-O(31)	111.3(4)
Cu(1)-N(14)-H(14B)	110.3	C(27)-C(26)-H(26)	119.9	O(33)-Cl(3)-O(34)	112.6(6)
H(14A)-N(14)-H(14B)	108.5	C(211)-C(27)-C(28)	118.8(7)	O(32)-Cl(3)-O(34)	106.4(4)
N(13)-C(114)-C(115)	113.2(5)	C(211)-C(27)-C(26)	118.8(8)	O(31)-Cl(3)-O(34)	103.7(5)
N(13)-C(114)-C(119)	106.6(4)	C(28)-C(27)-C(26)	122.3(8)	Cl(3)-O(31)-Cu(2)	133.9(3)
C(115)-C(114)-C(119)	111.1(5)	C(29)-C(28)-C(27)	118.1(7)	O(44)-Cl(4)-O(42)	108.9(5)
N(13)-C(114)-H(114)	108.6	C(29)-C(28)-H(28)	121	O(44)-Cl(4)-O(43)	111.9(7)
C(115)-C(114)-H(114)	108.6	C(27)-C(28)-H(28)	121	O(42)-Cl(4)-O(43)	106.0(5)
C(119)-C(114)-H(114)	108.6	C(210)-C(29)-C(28)	120.0(7)	O(44)-Cl(4)-O(41)	109.4(5)
C(114)-C(115)-C(116)	112.2(5)	C(210)-C(29)-H(29)	120	O(42)-Cl(4)-O(41)	112.8(4)
C(114)-C(115)-H(11D)	109.2	C(28)-C(29)-H(29)	120	O(43)-Cl(4)-O(41)	107.8(4)

1 Symmetry transformations used to generate equivalent atoms: #1 x-1,y,z

2

3

4

5

Table S6. Anisotropic displacement parameters ($Å^2 \times 10^3$) for [Cu(*RR*-dach)(4mephen)]$(ClO_4)_2$ (**4**$_{Cu}$). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}	Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	38(1)	33(1)	33(1)	13(1)	14(1)	16(1)	C(23)	60(5)	68(6)	77(6)	50(5)	56(5)	42(5)
N(11)	46(4)	55(5)	39(4)	25(4)	28(3)	24(3)	C(24)	51(4)	41(4)	59(5)	34(4)	39(4)	29(3)
N(12)	51(4)	27(3)	34(3)	8(3)	28(3)	13(3)	C(25)	78(6)	51(5)	60(5)	37(4)	54(5)	37(4)
C(11)	42(4)	61(6)	51(5)	27(4)	29(4)	20(4)	C(26)	73(5)	31(4)	67(5)	23(4)	55(5)	22(4)
C(12)	42(4)	76(6)	51(5)	33(5)	29(3)	29(4)	C(27)	55(4)	39(4)	55(4)	31(4)	42(4)	24(3)
C(13)	52(4)	74(6)	60(5)	48(5)	38(4)	36(4)	C(28)	67(5)	27(4)	43(4)	7(3)	34(4)	5(3)
C(14)	54(5)	82(7)	64(5)	57(5)	44(4)	39(4)	C(29)	61(4)	30(4)	31(4)	5(3)	20(3)	8(3)
C(15)	78(5)	49(5)	71(5)	46(5)	57(5)	43(4)	C(210)	45(4)	41(5)	39(4)	17(4)	19(3)	12(3)
C(16)	83(6)	39(5)	66(6)	31(4)	50(5)	29(4)	C(211)	48(4)	25(4)	31(3)	10(3)	24(3)	13(3)
C(17)	81(5)	27(4)	50(4)	18(3)	50(4)	19(3)	C(212)	41(4)	51(5)	49(5)	33(4)	31(3)	24(4)
C(18)	83(6)	37(5)	62(5)	22(4)	55(5)	14(4)	C(213)	55(5)	101(8)	122(8)	86(8)	51(5)	48(5)
C(19)	69(5)	29(4)	50(4)	11(4)	39(4)	0(4)	N(23)	42(3)	31(3)	31(3)	14(2)	14(2)	14(2)
C(110)	55(4)	27(4)	32(4)	3(3)	21(3)	10(3)	N(24)	28(2)	36(3)	33(3)	13(2)	14(2)	10(2)
C(111)	60(5)	39(5)	47(4)	26(4)	40(4)	25(4)	C(214)	40(3)	18(2)	26(3)	5(2)	13(2)	8(2)
C(112)	56(4)	36(4)	48(4)	25(4)	41(4)	25(4)	C(215)	38(3)	31(3)	34(3)	14(3)	12(3)	14(3)
C(113)	58(5)	80(7)	74(6)	40(5)	36(4)	33(5)	C(216)	42(3)	32(4)	57(5)	12(3)	18(3)	12(3)
N(13)	37(3)	25(3)	28(3)	6(2)	4(2)	6(2)	C(217)	45(3)	27(3)	63(4)	9(3)	17(3)	4(3)
N(14)	27(2)	41(3)	32(3)	20(3)	10(2)	6(2)	C(218)	42(3)	19(3)	46(4)	4(3)	11(3)	2(2)
C(114)	36(3)	29(3)	24(3)	10(2)	13(2)	8(2)	C(219)	35(3)	32(3)	42(3)	20(3)	18(2)	10(2)
C(115)	43(3)	37(4)	30(3)	11(3)	9(3)	16(3)	Cl(2)	32(1)	36(1)	34(1)	16(1)	13(1)	7(1)
C(116)	59(4)	32(3)	43(4)	12(3)	10(3)	16(3)	O(21)	33(3)	55(4)	35(3)	18(3)	14(2)	-2(2)
C(117)	66(4)	27(3)	38(3)	7(3)	19(3)	15(3)	O(22)	53(3)	83(5)	44(3)	14(3)	26(3)	-9(3)
C(118)	47(4)	33(3)	33(3)	9(3)	14(3)	1(3)	O(23)	38(3)	63(4)	79(4)	43(3)	3(3)	8(3)
C(119)	30(2)	31(3)	26(3)	10(2)	7(2)	3(2)	O(24)	88(4)	26(3)	66(4)	10(3)	42(3)	9(3)
Cl(1)	40(1)	31(1)	34(1)	13(1)	16(1)	9(1)	Cl(3)	63(1)	75(2)	56(1)	46(1)	36(1)	29(1)
O(11)	47(3)	53(3)	35(3)	20(3)	17(2)	15(3)	O(31)	58(3)	82(5)	55(3)	33(3)	24(3)	-3(3)
O(12)	43(3)	88(5)	41(3)	12(3)	23(2)	-5(3)	O(32)	102(4)	44(3)	55(3)	29(3)	49(3)	40(3)
O(13)	50(3)	48(3)	58(3)	28(3)	11(2)	12(2)	O(33)	98(4)	121(5)	38(3)	40(3)	0(3)	-33(4)
O(14)	67(4)	39(4)	78(4)	26(3)	22(3)	20(3)	O(34)	127(6)	39(3)	149(6)	41(4)	96(5)	37(3)
Cu(2)	38(1)	27(1)	31(1)	12(1)	14(1)	13(1)	Cl(4)	56(1)	39(1)	57(1)	24(1)	33(1)	16(1)
N(21)	31(3)	26(3)	45(4)	18(3)	21(3)	13(2)	O(41)	74(4)	103(6)	82(5)	54(4)	54(3)	31(4)
N(22)	45(3)	30(3)	39(3)	19(3)	25(3)	18(3)	O(42)	98(4)	71(4)	77(4)	42(4)	55(4)	19(3)
C(21)	43(4)	48(5)	54(5)	33(4)	28(4)	20(4)	O(43)	112(5)	130(6)	81(5)	16(4)	35(4)	-59(4)
C(22)	37(4)	59(6)	60(5)	37(5)	24(3)	14(4)	O(44)	107(5)	107(6)	236(9)	72(6)	100(6)	56(4)

Table S7. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for [Cu(*RR*-dach)(4mephen)]$(ClO_4)_2$.

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
H(11)	-293	7460	2324	68	H(11E)	6585	6058	4714	57	H(21B)	6383	2078	9693	111
H(12)	-1971	8711	1600	75	H(11F)	6519	3750	4340	72	H(21C)	5731	2051	10686	111
H(15)	393	13282	4178	75	H(11G)	4950	3542	4479	72	H(23A)	-338	6778	7300	51
H(16)	2551	14313	5881	80	H(11H)	4466	2617	2425	68	H(23B)	-1182	6133	7841	51
H(18)	5089	14103	7243	78	H(11I)	5411	3989	2521	68	H(24A)	2382	7977	10635	48
H(19)	6640	12640	7678	70	H(11J)	2883	3972	1654	60	H(24B)	3303	8167	9949	48
H(110)	5787	10245	6605	59	H(11K)	2572	3721	2733	60	H(214)	-493	7953	9536	43
H(11A)	-2642	10795	1578	96	H(119)	4330	6139	2955	45	H(21D)	-2249	8421	8002	51
H(11B)	-1316	12142	2229	96	H(21)	4698	6649	10656	62	H(21E)	-928	9075	7730	51
H(11C)	-2262	11804	2951	96	H(22)	6410	5366	11231	70	H(21F)	-1604	10880	8979	68
H(13A)	5548	7986	5103	51	H(25)	3818	786	8449	75	H(21G)	-1424	10173	9931	68
H(13B)	4854	7877	5958	51	H(26)	1557	-133	6909	71	H(21H)	956	11405	9508	73
H(14A)	1554	5808	3093	48	H(28)	-905	221	5639	66	H(21I)	686	11921	10745	73
H(14B)	1969	6328	2263	48	H(29)	-2342	1785	5201	63	H(21J)	2670	10722	10853	60
H(114)	3732	5713	4888	44	H(210)	-1462	4110	6373	61	H(21K)	1384	10041	11141	60
H(11D)	6264	5776	5776	57	H(21A)	7127	3243	11038	111	H(219)	1715	9042	8871	51

Table S8. Hydrogen bonds for [Cu(*RR*-dach)(4mephen)]$(ClO_4)_2$ (**4**$_{Cu}$) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(13)-H(13A)...O(13)	0.92	2.34	3.093(8)	139.4
N(13)-H(13B)...O(32)	0.92	2.07	2.981(8)	168.8
N(13)-H(13B)...Cl(3)	0.92	2.98	3.845(6)	157.9
N(14)-H(14A)...O(43)#1	0.92	2.4	3.223(9)	149.3
N(14)-H(14B)...O(21)#2	0.92	2.23	3.114(7)	161.2
N(23)-H(23A)...O(42)#1	0.92	2.19	3.012(9)	148.4
N(23)-H(23B)...O(23)	0.92	2.47	3.128(8)	128.9
N(24)-H(24A)...O(11)#3	0.92	2.33	3.163(8)	150.6
N(24)-H(24B)...O(33)	0.92	2.26	3.135(9)	159.3
N(24)-H(24B)...O(12)#3	0.92	2.57	3.146(8)	121.3
N(24)-H(24B)...Cl(3)	0.92	2.92	3.616(6)	133.4

Table S9. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for [Cu(56me$_2$phen)(*RR*-dach)(H_2O)]$(ClO_4)_2$.1.5H_2O (**10**$_{Cu}$). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
Cu(1)	1054(1)	6583(1)	7386(1)	21(1)	C(27)	5482(16)	-1717(8)	3679(8)	24(3)
N(11)	1393(13)	6235(6)	5929(6)	20(2)	C(28)	5671(16)	-2605(8)	3084(8)	25(3)
N(12)	954(13)	7963(7)	6978(6)	20(2)	C(29)	5582(16)	-2608(8)	2048(8)	25(3)
N(13)	541(15)	6925(7)	8799(6)	28(3)	C(210)	5284(16)	-1755(8)	1692(9)	23(3)
N(14)	1438(16)	5234(7)	7812(7)	29(2)	C(211)	5151(16)	-871(8)	3232(8)	19(2)
OW1	-2088(12)	6038(6)	6936(6)	34(2)	C(212)	4892(16)	23(8)	3791(8)	23(3)
C(11)	1721(17)	5388(8)	5450(8)	27(3)	C(213)	5488(18)	-606(9)	6427(8)	32(3)
C(12)	1745(17)	5257(9)	4420(8)	30(3)	C(214)	5963(18)	-2561(8)	5234(8)	33(3)
C(13)	1389(18)	5975(8)	3899(9)	34(3)	C(215)	4948(14)	987(6)	-147(6)	26(2)
C(14)	1071(16)	6930(8)	4371(8)	23(3)	C(216)	5622(17)	989(8)	-1153(8)	32(3)
C(15)	619(17)	7775(8)	3860(8)	28(3)	C(217)	5144(17)	1877(7)	-1647(7)	42(2)
C(16)	398(17)	8664(8)	4393(8)	27(3)	C(218)	5834(16)	2876(7)	-1003(7)	40(2)
C(17)	591(17)	8772(8)	5456(8)	26(3)	C(219)	5147(18)	2866(8)	30(8)	37(3)
C(18)	370(17)	9652(9)	6072(8)	27(3)	C(220)	5631(14)	1994(6)	490(6)	30(2)
C(19)	534(16)	9678(8)	7072(8)	26(3)	Cl(1)	5651(4)	-2451(2)	8647(2)	25(1)
C(110)	763(17)	8792(8)	7535(8)	23(3)	O(11)	4757(12)	-3049(6)	7745(6)	39(2)
C(111)	814(16)	7958(8)	5980(8)	21(2)	O(12)	4405(13)	-1857(7)	9057(7)	45(3)
C(112)	1079(15)	7007(7)	5411(7)	18(2)	O(13)	7278(12)	-1826(6)	8425(6)	36(2)
C(113)	560(20)	7650(9)	2754(9)	38(3)	O(14)	6128(15)	-3107(7)	9369(7)	51(3)
C(114)	-23(18)	9560(8)	3902(8)	33(3)	Cl(2)	424(4)	9589(2)	584(2)	28(1)
C(115)	206(15)	5963(7)	9266(6)	31(2)	O(21)	1425(12)	10199(6)	1465(6)	39(2)
C(116)	169(18)	6136(8)	10371(8)	35(3)	O(22)	1598(14)	8936(7)	164(7)	47(3)
C(117)	-15(17)	5117(7)	10766(7)	41(2)	O(23)	-1208(13)	9021(7)	829(7)	45(2)
C(118)	1397(18)	4436(8)	10410(8)	50(3)	O(24)	-106(15)	10252(7)	-73(8)	60(3)
C(119)	1346(16)	4306(8)	9291(7)	33(3)	Cl(3)	6061(5)	4501(2)	2865(2)	45(1)
C(120)	1584(13)	5331(6)	8908(6)	27(2)	O(31)	6476(12)	5107(6)	3786(6)	51(2)
Cu(2)	5050(1)	502(1)	1828(1)	23(1)	O(32)	7247(14)	3752(7)	2622(7)	64(2)
N(21)	4567(14)	782(7)	3255(7)	25(2)	O(33)	4149(14)	3977(7)	2759(6)	68(2)
N(22)	5147(14)	-887(7)	2244(6)	22(2)	O(34)	6130(15)	5081(7)	2036(7)	73(3)
N(23)	5455(13)	163(6)	404(6)	20(2)	Cl(4)	-250(5)	2462(3)	6443(3)	51(1)
N(24)	4797(16)	1876(7)	1468(7)	31(3)	O(41)	-1090(20)	1796(11)	5590(11)	126(5)
OW2	8243(12)	1034(6)	2266(7)	37(2)	O(42)	-630(30)	3386(12)	6390(11)	134(6)
C(21)	4189(17)	1628(8)	3738(8)	27(3)	O(43)	1541(15)	2298(7)	6701(7)	81(3)
C(22)	4114(17)	1759(8)	4766(8)	31(3)	O(44)	-1340(40)	1851(17)	6929(17)	219(9)
C(23)	4536(16)	975(7)	5320(8)	25(2)	OW3	-3284(13)	4324(6)	5564(6)	54(2)
C(24)	4953(17)	92(8)	4816(8)	26(3)	OW4	9827(15)	2674(7)	3575(7)	64(3)
C(25)	5286(16)	-753(8)	5293(8)	24(3)	OW5	-5854(13)	4067(7)	6996(6)	69(2)
C(26)	5557(15)	-1655(7)	4759(7)	20(2)					

Table S10. Bond lengths [Å] and angles [°] for [Cu(56me$_2$phen)(*RR*-dach)(H_2O)](ClO_4)$_2$.1.5H_2O (**10$_{Cu}$**).

Bond	Length [Å]	Bond	Length [Å]	Bond	Length [Å]	Bond	Length [Å]
Cu(1)-N(13)	2.011(9)	C(19)-C(110)	1.440(15)	N(22)-C(210)	1.342(14)	C(214)-H(21E)	0.96
Cu(1)-N(12)	2.014(9)	C(19)-H(19)	0.93	N(22)-C(211)	1.347(13)	C(214)-H(21F)	0.96
Cu(1)-N(14)	2.026(9)	C(110)-H(110)	0.93	N(23)-C(215)	1.486(11)	C(215)-C(216)	1.496(14)
Cu(1)-N(11)	2.037(9)	C(111)-C(112)	1.471(15)	N(23)-H(23A)	0.9	C(215)-C(220)	1.527(12)
Cu(1)-OW1	2.339(9)	C(113)-H(11A)	0.96	N(23)-H(23B)	0.9	C(215)-H(215)	0.98
Cu(1)-O(11)#1	2.699(9)	C(113)-H(11B)	0.96	N(24)-C(220)	1.527(12)	C(216)-C(217)	1.513(14)
N(11)-C(11)	1.316(14)	C(113)-H(11C)	0.96	N(24)-H(24A)	0.9	C(216)-H(21G)	0.97
N(11)-C(112)	1.362(13)	C(114)-H(11D)	0.96	N(24)-H(24B)	0.9	C(216)-H(21H)	0.97
N(12)-C(110)	1.312(14)	C(114)-H(11E)	0.96	OW2-HW2A	0.85(2)	C(217)-C(218)	1.522(13)
N(12)-C(111)	1.358(13)	C(114)-H(11F)	0.96	OW2-HW2B	0.85(2)	C(217)-H(21I)	0.97
N(13)-C(115)	1.506(12)	C(115)-C(120)	1.495(13)	C(21)-C(22)	1.402(15)	C(217)-H(21J)	0.97
N(13)-H(13A)	0.9	C(115)-C(116)	1.504(14)	C(21)-H(21)	0.93	C(218)-C(219)	1.536(14)
N(13)-H(13B)	0.9	C(115)-H(115)	0.98	C(22)-C(23)	1.425(14)	C(218)-H(21K)	0.97
N(14)-C(120)	1.483(12)	C(116)-C(117)	1.526(14)	C(22)-H(22)	0.93	C(218)-H(21L)	0.97
N(14)-H(14A)	0.9	C(116)-H(11G)	0.97	C(23)-C(24)	1.396(15)	C(219)-C(220)	1.471(14)
N(14)-H(14B)	0.9	C(116)-H(11H)	0.97	C(23)-H(23)	0.93	C(219)-H(21M)	0.97
OW1-HW1A	0.85(2)	C(117)-C(118)	1.556(16)	C(24)-C(212)	1.390(15)	C(219)-H(21N)	0.97
OW1-HW1B	0.85(2)	C(117)-H(11I)	0.97	C(24)-C(25)	1.418(15)	C(220)-H(220)	0.98
C(11)-C(12)	1.400(15)	C(117)-H(11J)	0.97	C(25)-C(26)	1.397(14)	Cl(1)-O(12)	1.412(9)
C(11)-H(11)	0.93	C(118)-C(119)	1.515(14)	C(25)-C(213)	1.533(15)	Cl(1)-O(13)	1.435(8)
C(12)-C(13)	1.311(15)	C(118)-H(11K)	0.97	C(26)-C(27)	1.464(14)	Cl(1)-O(11)	1.451(8)
C(12)-H(12)	0.93	C(118)-H(11L)	0.97	C(26)-C(214)	1.505(15)	Cl(1)-O(14)	1.455(9)
C(13)-C(14)	1.434(15)	C(119)-C(120)	1.526(12)	C(27)-C(211)	1.397(14)	Cl(2)-O(24)	1.412(10)
C(13)-H(13)	0.93	C(119)-H(11M)	0.97	C(27)-C(28)	1.402(15)	Cl(2)-O(23)	1.413(9)
C(14)-C(112)	1.413(14)	C(119)-H(11N)	0.97	C(28)-C(29)	1.412(15)	Cl(2)-O(22)	1.429(10)
C(14)-C(15)	1.468(15)	C(120)-H(120)	0.98	C(28)-H(28)	0.93	Cl(2)-O(21)	1.462(8)
C(15)-C(16)	1.371(15)	Cu(2)-N(24)	2.002(9)	C(29)-C(210)	1.341(15)	Cl(3)-O(31)	1.409(8)
C(15)-C(113)	1.498(16)	Cu(2)-N(23)	2.003(8)	C(29)-H(29)	0.93	Cl(3)-O(34)	1.448(9)
C(16)-C(17)	1.437(15)	Cu(2)-N(21)	2.013(10)	C(210)-H(210)	0.93	Cl(3)-O(32)	1.458(10)
C(16)-C(114)	1.508(16)	Cu(2)-N(22)	2.029(9)	C(211)-C(212)	1.401(15)	Cl(3)-O(33)	1.471(10)
C(17)-C(111)	1.400(15)	Cu(2)-OW2	2.369(9)	C(213)-H(21A)	0.96	Cl(4)-O(42)	1.328(15)
C(17)-C(18)	1.414(15)	Cu(2)-O(21)#2	2.644(9)	C(213)-H(21B)	0.96	Cl(4)-O(44)	1.33(2)
C(18)-C(19)	1.359(15)	N(21)-C(21)	1.331(14)	C(213)-H(21C)	0.96	Cl(4)-O(43)	1.397(11)
C(18)-H(18)	0.93	N(21)-C(212)	1.362(13)	C(214)-H(21D)	0.96	Cl(4)-O(41)	1.429(15)

Bond	Angle [°]	Bond	Angle [°]	Bond	Angle [°]
N(13)-Cu(1)-N(12)	96.5(4)	C(116)-C(115)-H(115)	107	C(28)-C(27)-C(26)	122.0(10)
N(13)-Cu(1)-N(14)	84.4(4)	N(13)-C(115)-H(115)	107	C(27)-C(28)-C(29)	118.9(10)
N(12)-Cu(1)-N(14)	174.2(5)	C(115)-C(116)-C(117)	108.6(9)	C(27)-C(28)-H(28)	120.6
N(13)-Cu(1)-N(11)	176.2(4)	C(115)-C(116)-H(11G)	110	C(29)-C(28)-H(28)	120.6
N(12)-Cu(1)-N(11)	82.6(4)	C(117)-C(116)-H(11G)	110	C(210)-C(29)-C(28)	117.3(10)
N(14)-Cu(1)-N(11)	96.8(4)	C(115)-C(116)-H(11H)	110	C(210)-C(29)-H(29)	121.4
N(13)-Cu(1)-OW1	90.3(4)	C(117)-C(116)-H(11H)	110	C(28)-C(29)-H(29)	121.4
N(12)-Cu(1)-OW1	93.1(3)	H(11G)-C(116)-H(11H)	108.3	C(29)-C(210)-N(22)	125.1(10)
N(14)-Cu(1)-OW1	92.7(4)	C(116)-C(117)-C(118)	114.5(10)	C(29)-C(210)-H(210)	117.4
N(11)-Cu(1)-OW1	86.0(3)	C(116)-C(117)-H(11I)	108.6	N(22)-C(210)-H(210)	117.4
N(13)-Cu(1)-O(11)#1	95.6(3)	C(118)-C(117)-H(11I)	108.6	N(22)-C(211)-C(27)	120.2(10)
N(12)-Cu(1)-O(11)#1	92.6(3)	C(116)-C(117)-H(11J)	108.6	N(22)-C(211)-C(212)	118.1(9)
N(14)-Cu(1)-O(11)#1	81.6(4)	C(118)-C(117)-H(11J)	108.6	C(27)-C(211)-C(212)	121.6(10)
N(11)-Cu(1)-O(11)#1	88.1(3)	H(11I)-C(117)-H(11J)	107.6	N(21)-C(212)-C(24)	124.4(10)
OW1-Cu(1)-O(11)#1	171.3(3)	C(119)-C(118)-C(117)	110.9(9)	N(21)-C(212)-C(211)	115.1(10)
C(11)-N(11)-C(112)	119.2(9)	C(119)-C(118)-H(11K)	109.5	C(24)-C(212)-C(211)	120.5(10)
C(11)-N(11)-Cu(1)	129.9(7)	C(117)-C(118)-H(11K)	109.5	C(25)-C(213)-H(21A)	109.5
C(112)-N(11)-Cu(1)	110.7(7)	C(119)-C(118)-H(11L)	109.5	C(25)-C(213)-H(21B)	109.5
C(110)-N(12)-C(111)	118.5(9)	C(117)-C(118)-H(11L)	109.5	H(21A)-C(213)-H(21B)	109.5
C(110)-N(12)-Cu(1)	128.1(7)	H(11K)-C(118)-H(11L)	108.1	C(25)-C(213)-H(21C)	109.5
C(111)-N(12)-Cu(1)	112.7(7)	C(118)-C(119)-C(120)	110.4(8)	H(21A)-C(213)-H(21C)	109.5
C(115)-N(13)-Cu(1)	108.7(6)	C(118)-C(119)-H(11M)	109.6	H(21B)-C(213)-H(21C)	109.5
C(115)-N(13)-H(13A)	109.9	C(120)-C(119)-H(11M)	109.6	C(26)-C(214)-H(21D)	109.5
Cu(1)-N(13)-H(13A)	109.9	C(118)-C(119)-H(11N)	109.6	C(26)-C(214)-H(21E)	109.5
C(115)-N(13)-H(13B)	109.9	C(120)-C(119)-H(11N)	109.6	H(21D)-C(214)-H(21E)	109.5

Table S10. Cont.

Cu(1)-N(13)-H(13B)	109.9	H(11M)-C(119)-H(11N)	108.1	C(26)-C(214)-H(21F)	109.5
H(13A)-N(13)-H(13B)	108.3	N(14)-C(120)-C(115)	108.4(8)	H(21D)-C(214)-H(21F)	109.5
C(120)-N(14)-Cu(1)	108.4(6)	N(14)-C(120)-C(119)	112.0(7)	H(21E)-C(214)-H(21F)	109.5
C(120)-N(14)-H(14A)	110	C(115)-C(120)-C(119)	112.1(8)	N(23)-C(215)-C(216)	114.8(8)
Cu(1)-N(14)-H(14A)	110	N(14)-C(120)-H(120)	108	N(23)-C(215)-C(220)	108.5(7)
C(120)-N(14)-H(14B)	110	C(115)-C(120)-H(120)	108	C(216)-C(215)-C(220)	110.8(8)
Cu(1)-N(14)-H(14B)	110	C(119)-C(120)-H(120)	108	N(23)-C(215)-H(215)	107.4
H(14A)-N(14)-H(14B)	108.4	N(24)-Cu(2)-N(23)	85.4(3)	C(216)-C(215)-H(215)	107.4
Cu(1)-OW1-HW1A	124(7)	N(24)-Cu(2)-N(21)	96.5(4)	C(220)-C(215)-H(215)	107.4
Cu(1)-OW1-HW1B	123(7)	N(23)-Cu(2)-N(21)	177.4(4)	C(215)-C(216)-C(217)	111.9(9)
HW1A-OW1-HW1B	113(4)	N(24)-Cu(2)-N(22)	176.0(4)	C(215)-C(216)-H(21G)	109.2
N(11)-C(11)-C(12)	121.8(10)	N(23)-Cu(2)-N(22)	97.4(3)	C(217)-C(216)-H(21G)	109.2
N(11)-C(11)-H(11)	119.1	N(21)-Cu(2)-N(22)	80.6(3)	C(215)-C(216)-H(21H)	109.2
C(12)-C(11)-H(11)	119.1	N(24)-Cu(2)-OW2	90.1(4)	C(217)-C(216)-H(21H)	109.2
C(13)-C(12)-C(11)	120.4(11)	N(23)-Cu(2)-OW2	91.8(4)	H(21G)-C(216)-H(21H)	107.9
C(13)-C(12)-H(12)	119.8	N(21)-Cu(2)-OW2	90.0(4)	C(216)-C(217)-C(218)	111.8(8)
C(11)-C(12)-H(12)	119.8	N(22)-Cu(2)-OW2	92.7(4)	C(216)-C(217)-H(21I)	109.2
C(12)-C(13)-C(14)	121.0(11)	N(24)-Cu(2)-O(21)#2	82.7(4)	C(218)-C(217)-H(21I)	109.2
C(12)-C(13)-H(13)	119.5	N(23)-Cu(2)-O(21)#2	93.3(3)	C(216)-C(217)-H(21J)	109.2
C(14)-C(13)-H(13)	119.5	N(21)-Cu(2)-O(21)#2	85.2(3)	C(218)-C(217)-H(21J)	109.2
C(112)-C(14)-C(13)	115.3(9)	N(22)-Cu(2)-O(21)#2	94.2(3)	H(21I)-C(217)-H(21J)	107.9
C(112)-C(14)-C(15)	119.1(9)	OW2-Cu(2)-O(21)#2	170.9(3)	C(217)-C(218)-C(219)	110.9(9)
C(13)-C(14)-C(15)	125.5(10)	C(21)-N(21)-C(212)	118.0(10)	C(217)-C(218)-H(21K)	109.5
C(16)-C(15)-C(14)	120.2(10)	C(21)-N(21)-Cu(2)	128.7(7)	C(219)-C(218)-H(21K)	109.5
C(16)-C(15)-C(113)	122.1(10)	C(212)-N(21)-Cu(2)	112.9(8)	C(217)-C(218)-H(21L)	109.5
C(14)-C(15)-C(113)	117.6(10)	C(210)-N(22)-C(211)	118.9(9)	C(219)-C(218)-H(21L)	109.5
C(15)-C(16)-C(17)	120.2(10)	C(210)-N(22)-Cu(2)	129.5(7)	H(21K)-C(218)-H(21L)	108
C(15)-C(16)-C(114)	122.1(10)	C(211)-N(22)-Cu(2)	111.6(7)	C(220)-C(219)-C(218)	111.0(9)
C(17)-C(16)-C(114)	117.7(10)	C(215)-N(23)-Cu(2)	108.4(6)	C(220)-C(219)-H(21M)	109.4
C(111)-C(17)-C(18)	113.1(10)	C(215)-N(23)-H(23A)	110	C(218)-C(219)-H(21M)	109.4
C(111)-C(17)-C(16)	121.9(10)	Cu(2)-N(23)-H(23A)	110	C(220)-C(219)-H(21N)	109.4
C(18)-C(17)-C(16)	124.6(10)	C(215)-N(23)-H(23B)	110	C(218)-C(219)-H(21N)	109.4
C(19)-C(18)-C(17)	120.5(11)	Cu(2)-N(23)-H(23B)	110	H(21M)-C(219)-H(21N)	108
C(19)-C(18)-H(18)	119.7	H(23A)-N(23)-H(23B)	108.4	C(219)-C(220)-C(215)	113.3(8)
C(17)-C(18)-H(18)	119.7	C(220)-N(24)-Cu(2)	108.4(6)	C(219)-C(220)-N(24)	113.4(8)
C(18)-C(19)-C(110)	121.4(11)	C(220)-N(24)-H(24A)	110	C(215)-C(220)-N(24)	104.2(7)
C(18)-C(19)-H(19)	119.3	Cu(2)-N(24)-H(24A)	110	C(219)-C(220)-H(220)	108.6
C(110)-C(19)-H(19)	119.3	C(220)-N(24)-H(24B)	110	C(215)-C(220)-H(220)	108.6
N(12)-C(110)-C(19)	118.9(10)	Cu(2)-N(24)-H(24B)	110	N(24)-C(220)-H(220)	108.6
N(12)-C(110)-H(110)	120.5	H(24A)-N(24)-H(24B)	108.4	O(12)-Cl(1)-O(13)	110.8(6)
C(19)-C(110)-H(110)	120.5	Cu(2)-OW2-HW2A	119(7)	O(12)-Cl(1)-O(11)	108.8(6)
N(12)-C(111)-C(17)	127.1(10)	Cu(2)-OW2-HW2B	127(7)	O(13)-Cl(1)-O(11)	109.3(5)
N(12)-C(111)-C(112)	115.1(9)	HW2A-OW2-HW2B	111(4)	O(12)-Cl(1)-O(14)	107.6(6)
C(17)-C(111)-C(112)	117.6(10)	N(21)-C(21)-C(22)	122.4(10)	O(13)-Cl(1)-O(14)	110.1(6)
N(11)-C(112)-C(14)	122.3(9)	N(21)-C(21)-H(21)	118.8	O(11)-Cl(1)-O(14)	110.2(6)
N(11)-C(112)-C(111)	117.4(9)	C(22)-C(21)-H(21)	118.8	O(24)-Cl(2)-O(23)	107.1(6)
C(14)-C(112)-C(111)	120.3(9)	C(21)-C(22)-C(23)	118.9(11)	O(24)-Cl(2)-O(22)	112.3(7)
C(15)-C(113)-H(11A)	109.5	C(21)-C(22)-H(22)	120.6	O(23)-Cl(2)-O(22)	110.4(6)
C(15)-C(113)-H(11B)	109.5	C(23)-C(22)-H(22)	120.6	O(24)-Cl(2)-O(21)	107.9(6)
H(11A)-C(113)-H(11B)	109.5	C(24)-C(23)-C(22)	118.8(10)	O(23)-Cl(2)-O(21)	110.6(6)
C(15)-C(113)-H(11C)	109.5	C(24)-C(23)-H(23)	120.6	O(22)-Cl(2)-O(21)	108.5(6)
H(11A)-C(113)-H(11C)	109.5	C(22)-C(23)-H(23)	120.6	O(31)-Cl(3)-O(34)	112.9(5)
H(11B)-C(113)-H(11C)	109.5	C(212)-C(24)-C(23)	117.4(10)	O(31)-Cl(3)-O(32)	117.3(6)
C(16)-C(114)-H(11D)	109.5	C(212)-C(24)-C(25)	119.4(10)	O(34)-Cl(3)-O(32)	103.4(6)
C(16)-C(114)-H(11E)	109.5	C(23)-C(24)-C(25)	123.0(10)	O(31)-Cl(3)-O(33)	111.0(5)
H(11D)-C(114)-H(11E)	109.5	C(26)-C(25)-C(24)	121.6(10)	O(34)-Cl(3)-O(33)	103.3(6)
C(16)-C(114)-H(11F)	109.5	C(26)-C(25)-C(213)	121.2(9)	O(32)-Cl(3)-O(33)	107.8(6)
H(11D)-C(114)-H(11F)	109.5	C(24)-C(25)-C(213)	116.9(9)	O(42)-Cl(4)-O(44)	117.9(14)
H(11E)-C(114)-H(11F)	109.5	C(25)-C(26)-C(27)	118.3(9)	O(42)-Cl(4)-O(43)	121.3(9)
C(120)-C(115)-C(116)	115.3(8)	C(25)-C(26)-C(214)	123.5(10)	O(44)-Cl(4)-O(43)	105.7(12)
C(120)-C(115)-N(13)	106.5(8)	C(27)-C(26)-C(214)	118.1(9)	O(42)-Cl(4)-O(41)	110.4(10)
C(116)-C(115)-N(13)	113.5(8)	C(211)-C(27)-C(28)	119.3(10)	O(44)-Cl(4)-O(41)	83.9(12)
C(120)-C(115)-H(115)	107	C(211)-C(27)-C(26)	118.6(10)	O(43)-Cl(4)-O(41)	111.5(8)

1 Symmetry transformations used to generate equivalent atoms: #1 x,y+1,z #2 x,y-1,z

Table S11. Anisotropic displacement parameters ($Å^2 \times 10^3$) for [Cu(56me$_2$phen)(*RR*-dach)(H_2O)](ClO_4)$_2$.1.5H_2O (**10$_{Cu}$**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}	Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	24(1)	22(1)	19(1)	4(1)	4(1)	5(1)	Cl(1)	23(2)	29(1)	20(1)	-1(1)	3(1)	1(1)
N(11)	14(5)	25(5)	22(5)	1(4)	2(4)	7(4)	O(11)	27(5)	48(5)	31(5)	-24(4)	4(4)	-7(4)
N(12)	18(5)	24(5)	19(5)	5(4)	-8(4)	7(4)	O(12)	21(5)	54(6)	51(6)	-33(5)	3(4)	4(4)
N(13)	27(6)	30(5)	22(5)	-2(4)	-8(4)	-4(5)	O(13)	19(5)	43(4)	45(5)	9(4)	7(4)	-5(4)
N(14)	42(7)	20(5)	28(5)	5(4)	3(4)	12(4)	O(14)	57(7)	60(6)	40(5)	17(5)	-4(5)	16(5)
OW1	30(5)	41(5)	28(4)	-12(4)	9(4)	5(4)	Cl(2)	19(2)	32(1)	31(2)	-3(1)	6(1)	5(1)
Cu(2)	32(1)	21(1)	18(1)	5(1)	5(1)	6(1)	O(21)	36(6)	51(5)	26(5)	-13(4)	-9(4)	19(4)
N(21)	33(6)	19(4)	24(5)	1(4)	1(4)	6(4)	O(22)	40(7)	39(5)	58(6)	-17(5)	18(5)	6(4)
N(22)	24(6)	22(5)	20(5)	1(4)	20(4)	-2(4)	O(23)	27(6)	59(5)	44(5)	0(4)	9(4)	-6(4)
N(23)	27(6)	14(4)	20(5)	7(4)	3(4)	6(4)	O(24)	57(8)	58(6)	63(7)	27(5)	-12(6)	-2(5)
N(24)	45(7)	27(5)	26(5)	3(4)	21(5)	13(5)	Cl(3)	70(3)	26(1)	43(2)	5(1)	14(2)	18(1)
OW2	27(5)	36(5)	45(6)	-6(4)	-9(4)	9(4)	Cl(4)	43(2)	47(2)	68(2)	15(2)	8(2)	14(2)

Table S12. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for [Cu(56me$_2$phen)(*RR*-dach)(H_2O)](ClO_4)$_2$.1.5H_2O (**10$_{Cu}$**).

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
H(13A)	1507	7343	9133	42	H(23A)	6643	103	348	30
H(13B)	-456	7237	8821	42	H(23B)	4755	-427	153	30
H(14A)	484	4757	7560	44	H(24A)	3601	1947	1407	46
H(14B)	2474	5053	7588	44	H(24B)	5388	2352	1946	46
HW1A	-2530(130)	5480(40)	6590(70)	51	HW2A	9000(110)	940(80)	1840(60)	55
HW1B	-2890(100)	6410(60)	7050(80)	51	HW2B	8740(130)	1470(60)	2740(50)	55
H(11)	1943	4862	5805	41	H(21)	3967	2152	3381	40
H(12)	2015	4657	4104	45	H(22)	3795	2347	5081	47
H(13)	1342	5864	3212	51	H(23)	4533	1051	6005	37
H(18)	111	10217	5790	40	H(28)	5853	-3182	3368	37
H(19)	498	10281	7466	39	H(29)	5725	-3179	1630	37
H(110)	775	8806	8218	34	H(210)	5163	-1765	1008	35
H(11A)	60	8200	2504	57	H(21A)	5498	-1247	6666	49
H(11B)	-205	7025	2489	57	H(21B)	4473	-309	6665	49
H(11C)	1783	7645	2560	57	H(21C)	6621	-168	6662	49
H(11D)	-728	9330	3278	49	H(21D)	4987	-3116	5029	50
H(11E)	1109	9969	3797	49	H(21E)	6055	-2404	5940	50
H(11F)	-716	9953	4319	49	H(21F)	7104	-2742	5035	50
H(115)	-1013	5609	8992	47	H(215)	3601	904	-233	39
H(11G)	-862	6473	10536	53	H(21G)	5077	368	-1563	48
H(11H)	1295	6561	10668	53	H(21H)	6947	1014	-1096	48
H(11I)	-1248	4757	10567	61	H(21I)	3818	1804	-1786	63
H(11J)	130	5232	11483	61	H(21J)	5686	1881	-2272	63
H(11K)	2625	4739	10693	76	H(21K)	5404	3420	-1315	59
H(11L)	1113	3781	10637	76	H(21L)	7170	2997	-942	59
H(11M)	180	3913	9009	50	H(21M)	5694	3484	445	56
H(11N)	2323	3942	9088	50	H(21N)	3821	2839	-22	56
H(120)	2816	5689	9155	41	H(220)	6974	2074	612	44

Table S13. Torsion angles [Cu(56me$_2$phen)(*RR*-dach)(H_2O)](ClO_4)$_2$.1.5H_2O (**10$_{Cu}$**) [Å and °].

Bond	Angle	Bond	Angle
N(13)-Cu(1)-N(11)-C(11)	-108(6)	N(24)-Cu(2)-N(21)-C(21)	0.8(11)
N(12)-Cu(1)-N(11)-C(11)	175.2(10)	N(23)-Cu(2)-N(21)-C(21)	-135(9)
N(14)-Cu(1)-N(11)-C(11)	1.0(10)	N(22)-Cu(2)-N(21)-C(21)	-176.4(11)
OW1-Cu(1)-N(11)-C(11)	-91.2(10)	OW2-Cu(2)-N(21)-C(21)	90.9(10)
O(11)#1-Cu(1)-N(11)-C(11)	82.3(10)	O(21)#2-Cu(2)-N(21)-C(21)	-81.3(10)
N(13)-Cu(1)-N(11)-C(112)	67(6)	N(24)-Cu(2)-N(21)-C(212)	-171.1(8)
N(12)-Cu(1)-N(11)-C(112)	-10.0(7)	N(23)-Cu(2)-N(21)-C(212)	53(10)
N(14)-Cu(1)-N(11)-C(112)	175.8(7)	N(22)-Cu(2)-N(21)-C(212)	11.7(8)
OW1-Cu(1)-N(11)-C(112)	83.6(7)	OW2-Cu(2)-N(21)-C(212)	-81.0(8)
O(11)#1-Cu(1)-N(11)-C(112)	-102.9(7)	O(21)#2-Cu(2)-N(21)-C(212)	106.8(8)
N(13)-Cu(1)-N(12)-C(110)	4.9(10)	N(24)-Cu(2)-N(22)-C(210)	129(6)
N(14)-Cu(1)-N(12)-C(110)	-94(4)	N(23)-Cu(2)-N(22)-C(210)	-4.9(11)
N(11)-Cu(1)-N(12)-C(110)	-178.8(10)	N(21)-Cu(2)-N(22)-C(210)	173.4(11)
OW1-Cu(1)-N(12)-C(110)	95.6(10)	OW2-Cu(2)-N(22)-C(210)	-97.0(10)
O(11)#1-Cu(1)-N(12)-C(110)	-91.0(10)	O(21)#2-Cu(2)-N(22)-C(210)	89.0(10)
N(13)-Cu(1)-N(12)-C(111)	-165.2(8)	N(24)-Cu(2)-N(22)-C(211)	-54(7)
N(14)-Cu(1)-N(12)-C(111)	96(4)	N(23)-Cu(2)-N(22)-C(211)	171.9(8)
N(11)-Cu(1)-N(12)-C(111)	11.0(8)	N(21)-Cu(2)-N(22)-C(211)	-9.9(8)
OW1-Cu(1)-N(12)-C(111)	-74.6(8)	OW2-Cu(2)-N(22)-C(211)	79.7(8)
O(11)#1-Cu(1)-N(12)-C(111)	98.8(8)	O(21)#2-Cu(2)-N(22)-C(211)	-94.3(8)
N(12)-Cu(1)-N(13)-C(115)	170.3(7)	N(24)-Cu(2)-N(23)-C(215)	-12.2(7)
N(14)-Cu(1)-N(13)-C(115)	-15.4(7)	N(21)-Cu(2)-N(23)-C(215)	124(9)
N(11)-Cu(1)-N(13)-C(115)	93(6)	N(22)-Cu(2)-N(23)-C(215)	164.9(7)
OW1-Cu(1)-N(13)-C(115)	77.2(7)	OW2-Cu(2)-N(23)-C(215)	-102.2(7)
O(11)#1-Cu(1)-N(13)-C(115)	-96.4(7)	O(21)#2-Cu(2)-N(23)-C(215)	70.2(6)
N(13)-Cu(1)-N(14)-C(120)	-13.4(7)	N(23)-Cu(2)-N(24)-C(220)	-17.8(7)
N(12)-Cu(1)-N(14)-C(120)	87(4)	N(21)-Cu(2)-N(24)-C(220)	164.0(7)
N(11)-Cu(1)-N(14)-C(120)	170.3(7)	N(22)-Cu(2)-N(24)-C(220)	-152(6)
OW1-Cu(1)-N(14)-C(120)	-103.4(7)	OW2-Cu(2)-N(24)-C(220)	73.9(7)
O(11)#1-Cu(1)-N(14)-C(120)	83.2(7)	O(21)#2-Cu(2)-N(24)-C(220)	-111.7(7)
C(112)-N(11)-C(11)-C(12)	-0.4(16)	C(212)-N(21)-C(21)-C(22)	-0.1(17)
Cu(1)-N(11)-C(11)-C(12)	174.0(9)	Cu(2)-N(21)-C(21)-C(22)	-171.6(9)
N(11)-C(11)-C(12)-C(13)	-1.8(18)	N(21)-C(21)-C(22)-C(23)	2.8(18)
C(11)-C(12)-C(13)-C(14)	3.6(18)	C(21)-C(22)-C(23)-C(24)	-2.0(16)
C(12)-C(13)-C(14)-C(112)	-3.1(17)	C(22)-C(23)-C(24)-C(212)	-1.4(16)
C(12)-C(13)-C(14)-C(15)	-178.4(12)	C(22)-C(23)-C(24)-C(25)	-176.2(11)
C(112)-C(14)-C(15)-C(16)	6.7(17)	C(212)-C(24)-C(25)-C(26)	0.1(17)
C(13)-C(14)-C(15)-C(16)	-178.1(12)	C(23)-C(24)-C(25)-C(26)	174.9(11)
C(112)-C(14)-C(15)-C(113)	-177.9(10)	C(212)-C(24)-C(25)-C(213)	175.4(10)
C(13)-C(14)-C(15)-C(113)	-2.7(18)	C(23)-C(24)-C(25)-C(213)	-9.9(17)
C(14)-C(15)-C(16)-C(17)	-0.5(17)	C(24)-C(25)-C(26)-C(27)	-0.3(16)
C(113)-C(15)-C(16)-C(17)	-175.7(12)	C(213)-C(25)-C(26)-C(27)	-175.3(10)
C(14)-C(15)-C(16)-C(114)	178.5(11)	C(24)-C(25)-C(26)-C(214)	178.3(11)
C(113)-C(15)-C(16)-C(114)	3.4(19)	C(213)-C(25)-C(26)-C(214)	3.3(17)
C(15)-C(16)-C(17)-C(111)	-6.8(18)	C(25)-C(26)-C(27)-C(211)	0.3(16)
C(114)-C(16)-C(17)-C(111)	174.0(11)	C(214)-C(26)-C(27)-C(211)	-178.5(10)
C(15)-C(16)-C(17)-C(18)	-179.3(12)	C(25)-C(26)-C(27)-C(28)	-177.6(11)
C(114)-C(16)-C(17)-C(18)	1.6(18)	C(214)-C(26)-C(27)-C(28)	3.7(16)
C(111)-C(17)-C(18)-C(19)	5.3(16)	C(211)-C(27)-C(28)-C(29)	2.1(17)
C(16)-C(17)-C(18)-C(19)	178.3(11)	C(26)-C(27)-C(28)-C(29)	179.9(10)
C(17)-C(18)-C(19)-C(110)	-5.9(18)	C(27)-C(28)-C(29)-C(210)	-1.2(16)
C(111)-N(12)-C(110)-C(19)	-4.0(16)	C(28)-C(29)-C(210)-N(22)	3.1(18)
Cu(1)-N(12)-C(110)-C(19)	-173.7(8)	C(211)-N(22)-C(210)-C(29)	-5.9(18)
C(18)-C(19)-C(110)-N(12)	5.1(18)	Cu(2)-N(22)-C(210)-C(29)	170.7(9)
C(110)-N(12)-C(111)-C(17)	4.2(18)	C(210)-N(22)-C(211)-C(27)	6.5(16)
Cu(1)-N(12)-C(111)-C(17)	175.4(10)	Cu(2)-N(22)-C(211)-C(27)	-170.7(9)
C(110)-N(12)-C(111)-C(112)	178.9(10)	C(210)-N(22)-C(211)-C(212)	-176.1(11)
Cu(1)-N(12)-C(111)-C(112)	-9.9(12)	Cu(2)-N(22)-C(211)-C(212)	6.7(13)
C(18)-C(17)-C(111)-N(12)	-4.7(17)	C(28)-C(27)-C(211)-N(22)	-4.8(17)
C(16)-C(17)-C(111)-N(12)	-177.9(11)	C(26)-C(27)-C(211)-N(22)	177.3(10)
C(18)-C(17)-C(111)-C(112)	-179.2(10)	C(28)-C(27)-C(211)-C(212)	177.9(11)
C(16)-C(17)-C(111)-C(112)	7.6(17)	C(26)-C(27)-C(211)-C(212)	0.0(17)
C(11)-N(11)-C(112)-C(14)	0.8(16)	C(21)-N(21)-C(212)-C(24)	-3.7(17)
Cu(1)-N(11)-C(112)-C(14)	-174.6(8)	Cu(2)-N(21)-C(212)-C(24)	169.2(9)
C(11)-N(11)-C(112)-C(111)	-176.9(10)	C(21)-N(21)-C(212)-C(211)	175.6(11)
Cu(1)-N(11)-C(112)-C(111)	7.7(12)	Cu(2)-N(21)-C(212)-C(211)	-11.5(13)
C(13)-C(14)-C(112)-N(11)	0.9(16)	C(23)-C(24)-C(212)-N(21)	4.3(17)

Table S13. Cont.

C(15)-C(14)-C(112)-N(11)	176.5(10)	C(25)-C(24)-C(212)-N(21)	179.4(11)
C(13)-C(14)-C(112)-C(111)	178.5(10)	C(23)-C(24)-C(212)-C(211)	-174.9(11)
C(15)-C(14)-C(112)-C(111)	-5.8(16)	C(25)-C(24)-C(212)-C(211)	0.1(17)
N(12)-C(111)-C(112)-N(11)	1.4(14)	N(22)-C(211)-C(212)-N(21)	3.1(16)
C(17)-C(111)-C(112)-N(11)	176.6(10)	C(27)-C(211)-C(212)-N(21)	-179.5(11)
N(12)-C(111)-C(112)-C(14)	-176.3(10)	N(22)-C(211)-C(212)-C(24)	-177.5(10)
C(17)-C(111)-C(112)-C(14)	-1.1(16)	C(27)-C(211)-C(212)-C(24)	-0.2(18)
Cu(1)-N(13)-C(115)-C(120)	40.9(9)	Cu(2)-N(23)-C(215)-C(216)	164.8(7)
Cu(1)-N(13)-C(115)-C(116)	168.8(8)	Cu(2)-N(23)-C(215)-C(220)	40.2(9)
C(120)-C(115)-C(116)-C(117)	-52.1(12)	N(23)-C(215)-C(216)-C(217)	-177.0(9)
N(13)-C(115)-C(116)-C(117)	-175.3(9)	C(220)-C(215)-C(216)-C(217)	-53.6(12)
C(115)-C(116)-C(117)-C(118)	50.7(13)	C(215)-C(216)-C(217)-C(218)	54.5(13)
C(116)-C(117)-C(118)-C(119)	-53.4(13)	C(216)-C(217)-C(218)-C(219)	-53.8(13)
C(117)-C(118)-C(119)-C(120)	53.1(12)	C(217)-C(218)-C(219)-C(220)	54.0(13)
Cu(1)-N(14)-C(120)-C(115)	40.0(9)	C(218)-C(219)-C(220)-C(215)	-54.9(12)
Cu(1)-N(14)-C(120)-C(119)	164.3(7)	C(218)-C(219)-C(220)-N(24)	-173.4(9)
C(116)-C(115)-C(120)-N(14)	179.9(8)	N(23)-C(215)-C(220)-C(219)	-178.0(9)
N(13)-C(115)-C(120)-N(14)	-53.3(10)	C(216)-C(215)-C(220)-C(219)	55.0(12)
C(116)-C(115)-C(120)-C(119)	55.7(11)	N(23)-C(215)-C(220)-N(24)	-54.3(10)
N(13)-C(115)-C(120)-C(119)	-177.5(8)	C(216)-C(215)-C(220)-N(24)	178.7(9)
C(118)-C(119)-C(120)-N(14)	-176.8(9)	Cu(2)-N(24)-C(220)-C(219)	166.4(8)
C(118)-C(119)-C(120)-C(115)	-54.6(11)	Cu(2)-N(24)-C(220)-C(215)	42.7(9)

Symmetry transformations used to generate equivalent atoms: #1 x,y+1,z #2 x,y-1,z.

Table S14. Hydrogen bonds for [Cu(56me$_2$phen)(*RR*-dach)(H_2O)](ClO_4)$_2$.1.5H_2O (**10$_{Cu}$**) [Å and °].

D-H...A	**d(D-H)**	**d(H...A)**	**d(D...A)**	**<(DHA)**
N(13)-H(13A)...O(12)#1	0.9	2.26	3.048(13)	145.5
N(13)-H(13A)...O(22)#3	0.9	2.42	3.080(13)	129.8
N(13)-H(13B)...O(13)#4	0.9	2.31	3.177(15)	162.5
N(14)-H(14A)...O(42)	0.9	2.31	3.112(19)	147.8
N(14)-H(14B)...OW5#5	0.9	2.08	2.928(15)	156.2
OW1-HW1A...OW3	0.85(2)	1.96(3)	2.797(12)	167(11)
OW1-HW1B...O(11)#4	0.85(2)	2.21(5)	3.013(13)	157(10)
N(23)-H(23A)...O(23)#6	0.9	2.41	3.142(14)	138.4
N(23)-H(23A)...O(24)#6	0.9	2.49	3.372(15)	166.3
N(23)-H(23B)...O(12)#7	0.9	2.28	3.077(12)	147.9
N(23)-H(23B)...O(22)#2	0.9	2.36	3.049(13)	133.2
N(24)-H(24B)...O(32)	0.9	2.23	3.082(14)	158.3
OW2-HW2A...O(21)#6	0.85(2)	2.23(7)	2.975(13)	146(11)
OW2-HW2B...OW4	0.85(2)	1.91(4)	2.741(13)	166(11)

Symmetry transformations used to generate equivalent atoms: #1 x,y+1,z #2 x,y-1,z #3 x,y,z+1 #4 x-1,y+1,z #5 x+1,y,z #6 x+1,y-1,z #7 x,y,z-1

Table S15. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for [Cu(56me$_2$phen)$_3$](ClO$_4$)$_2$.56me$_2$phen.2H$_2$O (**21$_{Cu}$**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
Cu(1)	1541(1)	1632(1)	-2028(1)	36(1)	C(33)	1138(12)	1333(11)	-5014(8)	42(4)
N(1)	899(9)	-47(9)	-1919(6)	36(3)	C(34)	89(13)	1619(12)	-5015(9)	51(4)
N(2)	661(9)	1940(8)	-1233(6)	31(2)	C(35)	-315(12)	1649(11)	-4342(8)	43(4)
C(1)	1040(12)	-991(11)	-2231(8)	39(3)	C(36)	-1430(14)	1816(13)	-4316(10)	57(4)
C(2)	439(12)	-1991(12)	-2178(8)	44(4)	C(37)	-1701(15)	1855(13)	-3618(9)	60(4)
C(3)	-349(11)	-1909(11)	-1746(8)	37(3)	C(38)	-909(14)	1770(13)	-2970(10)	57(4)
C(4)	-549(11)	-931(10)	-1401(7)	32(3)	C(39)	440(11)	1515(10)	-3650(7)	32(3)
C(5)	-1368(11)	-786(11)	-978(8)	36(3)	C(40)	1527(12)	1300(11)	-3619(8)	40(3)
C(6)	-1501(11)	196(11)	-627(7)	35(3)	C(41)	1549(13)	1243(12)	-5734(8)	50(4)
C(7)	-772(12)	1200(11)	-658(8)	37(3)	C(42)	-684(14)	1866(13)	-5703(9)	56(4)
C(8)	-783(11)	2226(11)	-301(8)	36(3)	Cl(1)	3952(4)	8346(3)	-1919(3)	55(1)
C(9)	-127(12)	3111(12)	-383(8)	43(4)	O(12)	3496(12)	8662(11)	-1260(8)	88(4)
C(10)	576(11)	2906(11)	-885(8)	37(3)	O(11)	4998(9)	8006(9)	-1669(6)	59(3)
C(11)	-5(11)	1046(11)	-1131(8)	36(3)	O(13)	3066(12)	7491(11)	-2565(8)	92(4)
C(12)	134(11)	16(11)	-1494(8)	36(3)	O(14)	4166(14)	9259(14)	-2179(10)	119(5)
C(13)	-2081(12)	-1788(11)	-910(8)	41(3)	Cl(2)	803(3)	5002(3)	1831(2)	48(1)
C(14)	-2415(11)	374(11)	-231(8)	40(3)	O(22)	-222(10)	4823(9)	1157(7)	67(3)
N(4)	2298(9)	3478(9)	-1838(6)	34(3)	O(21)	1588(9)	4364(8)	1613(6)	54(3)
N(6)	3179(8)	2009(8)	-1209(6)	27(2)	O(23)	1364(13)	6116(12)	2090(9)	104(5)
C(15)	1813(12)	4201(11)	-2090(8)	39(3)	O(24)	421(11)	4696(11)	2430(8)	84(4)
C(16)	2471(12)	5255(11)	-1958(8)	40(3)	N(7)	5290(12)	3186(12)	-4307(8)	67(4)
C(17)	3677(12)	5504(12)	-1554(8)	44(4)	N(8)	4849(12)	3370(11)	-5833(8)	64(4)
C(18)	4222(11)	4775(10)	-1269(7)	31(3)	C(43)	5522(16)	3170(14)	-3578(10)	66(5)
C(19)	5500(12)	4968(11)	-884(8)	36(3)	C(44)	4868(15)	3506(14)	-3083(11)	66(5)
C(20)	5938(12)	4215(11)	-623(8)	40(3)	C(45)	3938(14)	3839(13)	-3382(9)	54(4)
C(21)	5180(11)	3204(10)	-684(8)	34(3)	C(46)	3589(13)	3888(12)	-4179(9)	46(4)
C(22)	5583(12)	2462(11)	-335(8)	40(3)	C(47)	2604(15)	4281(14)	-4543(10)	61(5)
C(23)	4812(12)	1512(11)	-419(8)	38(3)	C(48)	2409(14)	4398(14)	-5261(10)	59(4)
C(24)	3626(12)	1337(11)	-869(8)	37(3)	C(49)	3155(13)	4098(12)	-5711(9)	48(4)
C(25)	3962(11)	2987(10)	-1095(7)	32(3)	C(50)	2977(15)	4163(13)	-6488(10)	60(4)
C(26)	3461(11)	3758(10)	-1416(7)	30(3)	C(51)	3687(14)	3852(13)	-6897(10)	60(4)
C(27)	6290(12)	6061(11)	-805(8)	41(3)	C(52)	4619(14)	3454(13)	-6570(9)	55(4)
C(28)	7305(11)	4366(11)	-291(8)	42(3)	C(53)	4101(13)	3666(12)	-5419(9)	49(4)
N(3)	2221(9)	1194(9)	-2940(6)	36(3)	C(54)	4351(14)	3581(13)	-4580(9)	54(4)
N(5)	152(9)	1590(8)	-2964(6)	34(3)	C(55)	1881(16)	4612(15)	-4030(11)	75(5)
C(29)	3229(12)	944(11)	-2901(8)	41(3)	C(56)	1420(16)	4870(15)	-5626(11)	79(6)
C(30)	3614(14)	773(12)	-3577(9)	53(4)	W(1)	6540(20)	1326(19)	-2119(13)	71(7)
C(31)	2944(13)	842(12)	-4269(9)	51(4)	W(2)	6563(18)	2186(17)	-5791(12)	55(5)
C(32)	1871(12)	1142(11)	-4327(8)	40(3)					

Table S16. Bond lengths [Å] and angles [°] for $[Cu(56me_2phen)_3](ClO_4)_2.56me_2phen.2H_2O$ (**21**$_{Cu}$).

Bond	Length [Å]	Bond	Length [Å]	Bond	Length [Å]	Bond	Length [Å]
Cu(1)-N(6)	2.024(10)	C(14)-H(14B)	0.96	N(5)-C(38)	1.346(18)	Cl(2)-O(22)	1.428(11)
Cu(1)-N(5)	2.032(10)	C(14)-H(14C)	0.96	N(5)-C(39)	1.380(16)	Cl(2)-O(21)	1.445(11)
Cu(1)-N(2)	2.029(10)	N(4)-C(15)	1.320(16)	C(29)-C(30)	1.42(2)	N(7)-C(43)	1.295(19)
Cu(1)-N(3)	2.057(11)	N(4)-C(26)	1.343(15)	C(29)-H(29)	0.93	N(7)-C(54)	1.358(19)
Cu(1)-N(1)	2.301(10)	N(6)-C(24)	1.317(15)	C(30)-C(31)	1.341(19)	N(8)-C(52)	1.340(18)
Cu(1)-N(4)	2.355(10)	N(6)-C(25)	1.397(15)	C(30)-H(30)	0.93	N(8)-C(53)	1.377(19)
N(1)-C(1)	1.294(16)	C(15)-C(16)	1.407(18)	C(31)-C(32)	1.41(2)	C(43)-C(44)	1.40(2)
N(1)-C(12)	1.365(16)	C(15)-H(15)	0.93	C(31)-H(31)	0.93	C(43)-H(43)	0.93
N(2)-C(10)	1.310(16)	C(16)-C(17)	1.384(18)	C(32)-C(40)	1.444(19)	C(44)-C(45)	1.31(2)
N(2)-C(11)	1.398(15)	C(16)-H(16)	0.93	C(32)-C(33)	1.438(18)	C(44)-H(44)	0.93
C(1)-C(2)	1.436(18)	C(17)-C(18)	1.387(18)	C(33)-C(34)	1.39(2)	C(45)-C(46)	1.43(2)
C(1)-H(1)	0.93	C(17)-H(17)	0.93	C(33)-C(41)	1.519(19)	C(45)-H(45)	0.93
C(2)-C(3)	1.399(19)	C(18)-C(26)	1.410(17)	C(34)-C(35)	1.44(2)	C(46)-C(54)	1.38(2)
C(2)-H(2)	0.93	C(18)-C(19)	1.463(17)	C(34)-C(42)	1.499(19)	C(46)-C(47)	1.45(2)
C(3)-C(4)	1.380(18)	C(19)-C(20)	1.337(18)	C(35)-C(39)	1.419(18)	C(47)-C(48)	1.33(2)
C(3)-H(3)	0.93	C(19)-C(27)	1.541(17)	C(35)-C(36)	1.42(2)	C(47)-C(55)	1.49(2)
C(4)-C(12)	1.454(17)	C(20)-C(21)	1.446(17)	C(36)-C(37)	1.40(2)	C(48)-C(49)	1.42(2)
C(4)-C(5)	1.425(18)	C(20)-C(28)	1.559(18)	C(36)-H(36)	0.93	C(48)-C(56)	1.52(2)
C(5)-C(6)	1.353(18)	C(21)-C(22)	1.387(18)	C(37)-C(38)	1.35(2)	C(49)-C(53)	1.41(2)
C(5)-C(13)	1.507(17)	C(21)-C(25)	1.404(16)	C(37)-H(37)	0.93	C(49)-C(50)	1.41(2)
C(6)-C(7)	1.487(17)	C(22)-C(23)	1.377(18)	C(38)-H(38)	0.93	C(50)-C(51)	1.34(2)
C(6)-C(14)	1.501(18)	C(22)-H(22)	0.93	C(39)-C(40)	1.384(18)	C(50)-H(50)	0.93
C(7)-C(8)	1.351(18)	C(23)-C(24)	1.395(17)	C(41)-H(41A)	0.96	C(51)-C(52)	1.38(2)
C(7)-C(11)	1.440(18)	C(23)-H(23)	0.93	C(41)-H(41B)	0.96	C(51)-H(51)	0.93
C(8)-C(9)	1.364(18)	C(24)-H(24)	0.93	C(41)-H(41C)	0.96	C(52)-H(52)	0.93
C(8)-H(8)	0.93	C(25)-C(26)	1.441(17)	C(42)-H(42A)	0.96	C(53)-C(54)	1.52(2)
C(9)-C(10)	1.424(19)	C(27)-H(27A)	0.96	C(42)-H(42B)	0.96	C(55)-H(55A)	0.96
C(9)-H(9)	0.93	C(27)-H(27B)	0.96	C(42)-H(42C)	0.96	C(55)-H(55B)	0.96
C(10)-H(10)	0.93	C(27)-H(27C)	0.96	Cl(1)-O(14)	1.417(16)	C(55)-H(55C)	0.96
C(11)-C(12)	1.414(19)	C(28)-H(28A)	0.96	Cl(1)-O(11)	1.416(11)	C(56)-H(56A)	0.96
C(13)-H(13A)	0.96	C(28)-H(28B)	0.96	Cl(1)-O(13)	1.428(14)	C(56)-H(56B)	0.96
C(13)-H(13B)	0.96	C(28)-H(28C)	0.96	Cl(1)-O(12)	1.457(14)	C(56)-H(56C)	0.96
C(13)-H(13C)	0.96	N(3)-C(29)	1.308(16)	Cl(2)-O(23)	1.407(15)		
C(14)-H(14A)	0.96	N(3)-C(40)	1.356(16)	Cl(2)-O(24)	1.424(13)		

Bond	Angle [°]	Bond	Angle [°]	Bond	Angle [°]
N(6)-Cu(1)-N(5)	162.7(4)	C(15)-C(16)-H(16)	121.7	N(5)-C(39)-C(35)	122.8(12)
N(6)-Cu(1)-N(2)	96.6(4)	C(18)-C(17)-C(16)	122.7(13)	C(40)-C(39)-C(35)	121.9(13)
N(5)-Cu(1)-N(2)	93.4(4)	C(18)-C(17)-H(17)	118.7	N(3)-C(40)-C(39)	119.5(13)
N(6)-Cu(1)-N(3)	90.4(4)	C(16)-C(17)-H(17)	118.7	N(3)-C(40)-C(32)	121.3(13)
N(5)-Cu(1)-N(3)	80.5(4)	C(17)-C(18)-C(26)	115.4(12)	C(39)-C(40)-C(32)	119.1(12)
N(2)-Cu(1)-N(3)	172.4(4)	C(17)-C(18)-C(19)	125.1(12)	C(33)-C(41)-H(41A)	109.5
N(6)-Cu(1)-N(1)	96.1(4)	C(26)-C(18)-C(19)	119.4(11)	C(33)-C(41)-H(41B)	109.5
N(5)-Cu(1)-N(1)	99.8(4)	C(20)-C(19)-C(18)	120.5(12)	H(41A)-C(41)-H(41B)	109.5
N(2)-Cu(1)-N(1)	77.1(4)	C(20)-C(19)-C(27)	122.8(12)	C(33)-C(41)-H(41C)	109.5
N(3)-Cu(1)-N(1)	99.4(4)	C(18)-C(19)-C(27)	116.7(11)	H(41A)-C(41)-H(41C)	109.5
N(6)-Cu(1)-N(4)	76.5(4)	C(19)-C(20)-C(21)	122.0(13)	H(41B)-C(41)-H(41C)	109.5
N(5)-Cu(1)-N(4)	88.8(4)	C(19)-C(20)-C(28)	120.7(12)	C(34)-C(42)-H(42A)	109.5
N(2)-Cu(1)-N(4)	93.7(4)	C(21)-C(20)-C(28)	117.2(11)	C(34)-C(42)-H(42B)	109.5
N(3)-Cu(1)-N(4)	90.7(4)	C(22)-C(21)-C(25)	118.5(11)	H(42A)-C(42)-H(42B)	109.5
N(1)-Cu(1)-N(4)	167.6(4)	C(22)-C(21)-C(20)	123.7(12)	C(34)-C(42)-H(42C)	109.5
C(1)-N(1)-C(12)	118.0(11)	C(25)-C(21)-C(20)	117.7(11)	H(42A)-C(42)-H(42C)	109.5
C(1)-N(1)-Cu(1)	133.0(9)	C(23)-C(22)-C(21)	120.7(13)	H(42B)-C(42)-H(42C)	109.5
C(12)-N(1)-Cu(1)	108.7(9)	C(23)-C(22)-H(22)	119.6	O(14)-Cl(1)-O(11)	111.6(8)
C(10)-N(2)-C(11)	118.5(11)	C(21)-C(22)-H(22)	119.6	O(14)-Cl(1)-O(13)	108.2(9)
C(10)-N(2)-Cu(1)	123.9(9)	C(22)-C(23)-C(24)	117.0(13)	O(11)-Cl(1)-O(13)	110.1(8)
C(11)-N(2)-Cu(1)	117.1(9)	C(22)-C(23)-H(23)	121.5	O(14)-Cl(1)-O(12)	106.9(9)
N(1)-C(1)-C(2)	125.3(13)	C(24)-C(23)-H(23)	121.5	O(11)-Cl(1)-O(12)	110.7(7)
N(1)-C(1)-H(1)	117.4	N(6)-C(24)-C(23)	125.6(12)	O(13)-Cl(1)-O(12)	109.3(8)
C(2)-C(1)-H(1)	117.4	N(6)-C(24)-H(24)	117.2	O(23)-Cl(2)-O(24)	111.6(9)
C(3)-C(2)-C(1)	115.8(14)	C(23)-C(24)-H(24)	117.2	O(23)-Cl(2)-O(22)	106.0(8)
C(3)-C(2)-H(2)	122.1	N(6)-C(25)-C(21)	121.2(11)	O(24)-Cl(2)-O(22)	108.2(7)
C(1)-C(2)-H(2)	122.1	N(6)-C(25)-C(26)	117.0(11)	O(23)-Cl(2)-O(21)	110.8(8)

Table S16. Cont.

C(4)-C(3)-C(2)	122.1(13)	C(21)-C(25)-C(26)	121.8(11)	O(24)-Cl(2)-O(21)	109.3(7)
C(4)-C(3)-H(3)	118.9	N(4)-C(26)-C(18)	123.1(11)	O(22)-Cl(2)-O(21)	110.9(7)
C(2)-C(3)-H(3)	118.9	N(4)-C(26)-C(25)	118.8(11)	C(43)-N(7)-C(54)	115.5(16)
C(3)-C(4)-C(12)	116.0(12)	C(18)-C(26)-C(25)	118.1(11)	C(52)-N(8)-C(53)	117.6(14)
C(3)-C(4)-C(5)	125.5(12)	C(19)-C(27)-H(27A)	109.5	N(7)-C(43)-C(44)	124.6(18)
C(12)-C(4)-C(5)	118.5(12)	C(19)-C(27)-H(27B)	109.5	N(7)-C(43)-H(43)	117.7
C(6)-C(5)-C(4)	123.1(12)	H(27A)-C(27)-H(27B)	109.5	C(44)-C(43)-H(43)	117.7
C(6)-C(5)-C(13)	119.7(12)	C(19)-C(27)-H(27C)	109.5	C(45)-C(44)-C(43)	118.0(17)
C(4)-C(5)-C(13)	117.1(12)	H(27A)-C(27)-H(27C)	109.5	C(45)-C(44)-H(44)	121
C(5)-C(6)-C(7)	120.7(12)	H(27B)-C(27)-H(27C)	109.5	C(43)-C(44)-H(44)	121
C(5)-C(6)-C(14)	124.6(12)	C(20)-C(28)-H(28A)	109.5	C(44)-C(45)-C(46)	122.6(17)
C(7)-C(6)-C(14)	114.6(12)	C(20)-C(28)-H(28B)	109.5	C(44)-C(45)-H(45)	118.7
C(8)-C(7)-C(11)	117.8(12)	H(28A)-C(28)-H(28B)	109.5	C(46)-C(45)-H(45)	118.7
C(8)-C(7)-C(6)	126.3(13)	C(20)-C(28)-H(28C)	109.5	C(54)-C(46)-C(45)	112.7(14)
C(11)-C(7)-C(6)	115.9(12)	H(28A)-C(28)-H(28C)	109.5	C(54)-C(46)-C(47)	121.1(14)
C(7)-C(8)-C(9)	123.3(14)	H(28B)-C(28)-H(28C)	109.5	C(45)-C(46)-C(47)	126.1(15)
C(7)-C(8)-H(8)	118.4	C(29)-N(3)-C(40)	121.1(12)	C(48)-C(47)-C(46)	122.2(16)
C(9)-C(8)-H(8)	118.4	C(29)-N(3)-Cu(1)	128.1(9)	C(48)-C(47)-C(55)	122.6(16)
C(8)-C(9)-C(10)	116.5(14)	C(40)-N(3)-Cu(1)	110.5(9)	C(46)-C(47)-C(55)	115.0(14)
C(8)-C(9)-H(9)	121.8	C(38)-N(5)-C(39)	117.6(12)	C(47)-C(48)-C(49)	119.9(16)
C(10)-C(9)-H(9)	121.8	C(38)-N(5)-Cu(1)	129.2(10)	C(47)-C(48)-C(56)	122.5(16)
N(2)-C(10)-C(9)	123.9(13)	C(39)-N(5)-Cu(1)	112.5(8)	C(49)-C(48)-C(56)	117.6(14)
N(2)-C(10)-H(10)	118	N(3)-C(29)-C(30)	120.3(13)	C(53)-C(49)-C(48)	121.7(14)
C(9)-C(10)-H(10)	118	N(3)-C(29)-H(29)	119.9	C(53)-C(49)-C(50)	115.0(15)
N(2)-C(11)-C(12)	117.2(12)	C(30)-C(29)-H(29)	119.9	C(48)-C(49)-C(50)	123.2(15)
N(2)-C(11)-C(7)	119.9(12)	C(31)-C(30)-C(29)	120.8(15)	C(51)-C(50)-C(49)	121.2(16)
C(12)-C(11)-C(7)	122.9(12)	C(31)-C(30)-H(30)	119.6	C(51)-C(50)-H(50)	119.4
N(1)-C(12)-C(11)	118.7(12)	C(29)-C(30)-H(30)	119.6	C(49)-C(50)-H(50)	119.4
N(1)-C(12)-C(4)	122.7(12)	C(30)-C(31)-C(32)	120.6(15)	C(50)-C(51)-C(52)	120.9(16)
C(11)-C(12)-C(4)	118.6(12)	C(30)-C(31)-H(31)	119.7	C(50)-C(51)-H(51)	119.5
C(5)-C(13)-H(13A)	109.5	C(32)-C(31)-H(31)	119.7	C(52)-C(51)-H(51)	119.5
C(5)-C(13)-H(13B)	109.5	C(31)-C(32)-C(40)	115.8(12)	N(8)-C(52)-C(51)	121.5(16)
H(13A)-C(13)-H(13B)	109.5	C(31)-C(32)-C(33)	125.3(13)	N(8)-C(52)-H(52)	119.2
C(5)-C(13)-H(13C)	109.5	C(40)-C(32)-C(33)	118.9(13)	C(51)-C(52)-H(52)	119.2
H(13A)-C(13)-H(13C)	109.5	C(34)-C(33)-C(32)	121.0(13)	N(8)-C(53)-C(49)	123.7(14)
H(13B)-C(13)-H(13C)	109.5	C(34)-C(33)-C(41)	120.4(13)	N(8)-C(53)-C(54)	118.3(14)
C(6)-C(14)-H(14A)	109.5	C(32)-C(33)-C(41)	118.6(13)	C(49)-C(53)-C(54)	117.9(14)
C(6)-C(14)-H(14B)	109.5	C(33)-C(34)-C(35)	119.5(13)	N(7)-C(54)-C(46)	126.4(14)
H(14A)-C(14)-H(14B)	109.5	C(33)-C(34)-C(42)	123.1(14)	N(7)-C(54)-C(53)	116.6(14)
C(6)-C(14)-H(14C)	109.5	C(35)-C(34)-C(42)	117.4(14)	C(46)-C(54)-C(53)	117.0(14)
H(14A)-C(14)-H(14C)	109.5	C(39)-C(35)-C(36)	116.8(13)	C(47)-C(55)-H(55A)	109.5
H(14B)-C(14)-H(14C)	109.5	C(39)-C(35)-C(34)	119.0(13)	C(47)-C(55)-H(55B)	109.5
C(15)-N(4)-C(26)	119.4(11)	C(36)-C(35)-C(34)	124.2(13)	H(55A)-C(55)-H(55B)	109.5
C(15)-N(4)-Cu(1)	132.6(9)	C(37)-C(36)-C(35)	118.5(15)	C(47)-C(55)-H(55C)	109.5
C(26)-N(4)-Cu(1)	108.0(8)	C(37)-C(36)-H(36)	120.8	H(55A)-C(55)-H(55C)	109.5
C(24)-N(6)-C(25)	116.8(11)	C(35)-C(36)-H(36)	120.8	H(55B)-C(55)-H(55C)	109.5
C(24)-N(6)-Cu(1)	124.9(8)	C(38)-C(37)-C(36)	121.1(16)	C(48)-C(56)-H(56A)	109.5
C(25)-N(6)-Cu(1)	117.4(8)	C(38)-C(37)-H(37)	119.5	C(48)-C(56)-H(56B)	109.5
N(4)-C(15)-C(16)	122.8(13)	C(36)-C(37)-H(37)	119.5	H(56A)-C(56)-H(56B)	109.5
N(4)-C(15)-H(15)	118.6	N(5)-C(38)-C(37)	123.1(16)	C(48)-C(56)-H(56C)	109.5
C(16)-C(15)-H(15)	118.6	N(5)-C(38)-H(38)	118.5	H(56A)-C(56)-H(56C)	109.5
C(17)-C(16)-C(15)	116.5(13)	C(37)-C(38)-H(38)	118.5	H(56B)-C(56)-H(56C)	109.5
C(17)-C(16)-H(16)	121.7	N(5)-C(39)-C(40)	115.3(11)		

1

2

Table S17. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $[Cu(56me_2phen)_3](ClO_4)_2.56me_2phen.2H_2O$ (**21$_{Cu}$**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	28(1)	39(1)	46(1)	20(1)	17(1)	2(1)
Cl(1)	54(2)	51(2)	65(3)	27(2)	19(2)	17(2)
Cl(2)	46(2)	46(2)	55(2)	20(2)	19(2)	12(2)

Table S18. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for $[Cu(56me_2phen)_3](ClO_4)_2.56me_2phen.2H_2O$ (**21$_{Cu}$**).

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
H(1)	1573	-1024	-2511	47	H(29)	3695	879	-2428	49
H(2)	565	-2652	-2417	53	H(30)	4339	610	-3540	63
H(3)	-750	-2534	-1689	44	H(31)	3190	690	-4714	62
H(8)	-1263	2335	15	43	H(36)	-1968	1898	-4754	68
H(9)	-138	3811	-124	52	H(37)	-2439	1941	-3598	72
H(10)	1001	3495	-971	45	H(38)	-1107	1839	-2507	68
H(13A)	-2467	-1582	-523	49	H(41A)	871	1032	-6211	60
H(13B)	-1564	-2221	-744	49	H(41B)	1995	709	-5774	60
H(13C)	-2668	-2200	-1421	49	H(41C)	2040	1931	-5673	60
H(14A)	-2994	-299	-373	48	H(42A)	-249	1981	-6053	68
H(14B)	-2800	889	-406	48	H(42B)	-927	2506	-5504	68
H(14C)	-2038	647	339	48	H(42C)	-1373	1268	-5992	68
H(15)	1002	4005	-2366	47	H(43)	6168	2917	-3368	79
H(16)	2114	5759	-2132	48	H(44)	5086	3493	-2559	79
H(17)	4141	6187	-1471	52	H(45)	3488	4051	-3061	65
H(22)	6383	2607	-42	48	H(50)	2354	4427	-6721	73
H(23)	5071	1011	-185	46	H(51)	3552	3904	-7409	72
H(24)	3106	690	-936	44	H(52)	5097	3240	-6867	67
H(27A)	6700	6459	-249	50	H(55A)	2379	5175	-3546	91
H(27B)	5805	6471	-1045	50	H(55B)	1536	4000	-3901	91
H(27C)	6857	5935	-1072	50	H(55C)	1262	4875	-4313	91
H(28A)	7706	4942	-430	50	H(56A)	1179	5278	-5211	94
H(28B)	7494	3707	-520	50	H(56B)	757	4293	-6001	94
H(28C)	7556	4541	281	50	H(56C)	1700	5337	-5897	94

Table S19. Crystallographic data for previously characterised structures [Cu(*SS*-dach)(phen)(H_2O)](ClO_4)$_2$.H_2O (**1$_{Cu}$**),[6] [Cu(phen)$_3$](ClO_4)$_2$,[7] and [Cu(phen)$_2$Cl](ClO_4)$_2$.[8]

	1$_{Cu}$	**[Cu(phen)$_3$](ClO$_4$)$_2$**	**[Cu(phen)$_2$Cl]ClO$_4$**
Empirical formula	$C_{18}H_{26}Cl_2CuN_4O_{10}$	$C_{36}H_{24}Cl_2CuN_6O_8$	$C_{24}H_{16}Cl_2CuN_4O_4$
Formula weight	592.87	803.06	558.86
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	P1	$P2_1/n$	$P2_1/n$
Temperature (K)	296(2)	293(2) K	293(2) K
a (Å)	8.2004(6)	9.3102(7)	12.6522(9)
b (Å)	12.8438(9)	29.737(2)	11.0952(8)
c (Å)	12.9886(9)	12.9620(10)	17.1660(15)
α (˚)	65.9260(10)	90	90
β (˚)	89.5650(10)	110.8950(10)	111.5880(10)
γ (°)	72.4800(10)	90	90
V (Å3)	1180.61(14)	3352.7(4)3	2240.7(3)3
Z	2	4	4
D_c (mg/m^3)	1.668	1.591	1.657
Absorption coefficient (mm^{-1})	1.213	0.876	1.255
θ range for data collection (°)	1.73 to 28.	1.37 to 20.73	2.24 to 28.37
Reflections	9340	14951	17287
Independent reflections	7939 [$R_{(int)}$ = 0.0142]	3440 [$R_{(int)}$ = 0.0355]	5151 [$R_{(int)}$ = 0.0260]
GooF on F2	1.013	1.054	1.061
Final R [I>2σ(I)] R1	0.0306	0.0376	0.0477
Final R [I>2σ(I)] wR_2	0.078	0.0951	0.1321
R indices (all data) R1	0.0355	0.0481	0.061
R indices (all data) wR_2	0.0807	0.1078	0.142
Crystal size (mm)	0.25 x 0.25 x 0.10	0.10 x 0.10 x 0.10 mm3	0.10 x 0.10 x 0.20 mm3
F(000)	610	1636	1132
Completeness to θ = 28.30°	88.20%	98.90%	92.00%
Refinement method	Full-matrix least-squares on F2	Full-matrix least-squares on F2	Full-matrix least-squares on F2
Data	7939	3440	5151
Restraints	15	0	0
Parameters	655	478	316
Index ranges	$-8 \le h \le 10$ $-16 \le k \le 17$ $-17 \le l \le 17$	$-7 \le h \le 9$ $-29 \le k \le 29$ $-12 \le l \le 12$	$-13 \le h \le 16$ $-14 \le k \le 14$ $-22 \le l \le 21$
Min., max. Δρ/e-3	0.554, -0.348	0.600 and -0.403 e.Å-3	1.564 and -1.249 e.Å-3

Table S20. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for [Cu(*SS*-dach)(phen)(H_2O)](ClO_4)$_2$.H_2O (**1$_{Cu}$**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
Cu(1)	8191(1)	4817(1)	3545(1)	22(1)	C(29)	6360(7)	9618(5)	-2379(5)	33(1)
N(11)	8242(5)	3624(4)	5173(4)	22(1)	C(210)	7644(7)	8568(5)	-2236(5)	27(1)
N(12)	9937(5)	3348(4)	3495(4)	23(1)	C(211)	8044(7)	9425(4)	-4124(4)	22(1)
C(11)	7396(7)	3787(5)	6005(5)	26(1)	C(212)	8965(6)	9281(4)	-5019(4)	22(1)
C(12)	7689(7)	2873(5)	7100(5)	32(1)	C(213)	11146(5)	4577(3)	-1386(3)	22(1)
C(13)	8892(7)	1761(5)	7357(5)	33(1)	C(214)	10571(7)	3532(5)	-599(5)	35(1)
C(14)	9807(7)	1567(5)	6503(5)	25(1)	C(215)	12026(6)	2331(4)	-348(4)	39(1)
C(15)	11115(7)	431(5)	6692(5)	34(1)	C(216)	12534(7)	2216(4)	-1427(5)	36(1)
C(16)	11964(7)	299(5)	5848(5)	33(1)	C(217)	13020(7)	3305(4)	-2238(5)	30(1)
C(17)	11625(7)	1276(4)	4709(5)	29(1)	C(218)	11567(6)	4461(4)	-2490(3)	27(1)
C(18)	12447(7)	1208(5)	3787(5)	33(1)	N(23)	9846(5)	5779(3)	-1665(3)	22(1)
C(19)	12053(7)	2168(5)	2747(5)	33(1)	N(24)	11927(7)	5563(4)	-3247(4)	34(1)
C(110)	10747(7)	3239(5)	2645(5)	29(1)	OW2	12430(5)	7277(4)	-2225(3)	35(1)
C(111)	10354(6)	2370(4)	4521(4)	21(1)	Cl(1)	2479(1)	4791(1)	4284(1)	25(1)
C(112)	9445(6)	2518(4)	5438(4)	22(1)	O(11)	760(5)	5285(4)	4522(4)	34(1)
C(113)	7966(5)	7245(3)	2055(3)	24(1)	O(12)	3594(5)	5327(4)	4595(4)	38(1)
C(114)	7624(7)	8273(4)	894(4)	30(1)	O(13)	2456(5)	5067(4)	3092(3)	39(1)
C(115)	7068(6)	9480(4)	963(4)	34(1)	O(14)	3080(6)	3517(3)	4932(4)	44(1)
C(116)	5485(7)	9611(4)	1619(5)	39(1)	Cl(2)	15954(1)	7048(1)	-3869(1)	23(1)
C(117)	5824(7)	8543(4)	2764(5)	33(1)	O(21)	16002(5)	6802(4)	-2676(3)	35(1)
C(118)	6370(6)	7352(4)	2644(3)	26(1)	O(22)	17692(5)	6575(3)	-4075(3)	31(1)
N(13)	8548(6)	6021(3)	2067(4)	28(1)	O(23)	14882(5)	6473(3)	-4144(3)	36(1)
N(14)	6729(5)	6264(4)	3743(4)	24(1)	O(24)	15284(5)	8317(3)	-4559(4)	44(1)
OW1	5993(5)	4565(4)	2689(3)	33(1)	Cl(3)	6040(2)	3503(1)	363(1)	33(1)
Cu(2)	10289(1)	7008(1)	-3126(1)	21(1)	O(31)	7307(6)	3595(5)	1059(4)	56(1)
N(21)	10194(5)	8209(4)	-4764(4)	24(1)	O(32)	4513(5)	3513(4)	923(4)	47(1)
N(22)	8486(6)	8464(4)	-3086(4)	23(1)	O(33)	5699(6)	4486(4)	-745(4)	59(1)
C(21)	11070(7)	8062(5)	-5584(5)	29(1)	O(34)	6672(7)	2419(4)	225(5)	68(1)
C(22)	10749(8)	8964(5)	-6717(5)	32(1)	Cl(4)	2234(2)	8479(1)	10053(1)	36(1)
C(23)	9520(7)	10040(5)	-6982(5)	29(1)	O(41)	1086(6)	8334(5)	9337(4)	54(1)
C(24)	8551(7)	10247(5)	-6124(4)	26(1)	O(42)	3703(6)	8606(6)	9537(5)	86(2)
C(25)	7252(7)	11338(5)	-6308(5)	33(1)	O(43)	2628(10)	7497(6)	11085(5)	124(3)
C(26)	6378(7)	11483(5)	-5440(5)	34(1)	O(44)	1365(9)	9537(5)	10181(7)	109(2)
C(27)	6762(7)	10520(4)	-4336(4)	25(1)	OW3	11456(5)	5618(3)	502(3)	41(1)
C(28)	5882(7)	10613(5)	-3410(5)	29(1)	OW4	6698(6)	6347(4)	-86(4)	53(1)

Table S21. Bond lengths [Å] and angles [°] for [Cu(*SS*-dach)(phen)(H_2O)](ClO_4)$_2$.H_2O (**1$_{Cu}$**).

Bond	Length [Å]	Bond	Length [Å]	Bond	Length [Å]	Bond	Length [Å]
Cu(1)-N(14)	2.000(4)	C(113)-C(118)	1.510(6)	C(21)-C(22)	1.417(7)	C(216)-H(21F)	0.97
Cu(1)-N(13)	2.001(5)	C(113)-H(113)	0.98	C(21)-H(21)	0.93	C(217)-C(218)	1.509(6)
Cu(1)-N(12)	2.022(4)	C(114)-C(115)	1.519(7)	C(22)-C(23)	1.350(7)	C(217)-H(21G)	0.97
Cu(1)-N(11)	2.035(4)	C(114)-H(11A)	0.97	C(22)-H(22)	0.93	C(217)-H(21H)	0.97
Cu(1)-OW1	2.294(4)	C(114)-H(11B)	0.97	C(23)-C(24)	1.430(7)	C(218)-N(24)	1.473(6)
Cu(1)-O(11)#1	2.800(4)	C(115)-C(116)	1.551(8)	C(23)-H(23)	0.93	C(218)-H(218)	0.98
N(11)-C(11)	1.333(6)	C(115)-H(11C)	0.97	C(24)-C(25)	1.410(8)	N(23)-H(23A)	0.9
N(11)-C(112)	1.368(6)	C(115)-H(11D)	0.97	C(24)-C(212)	1.420(7)	N(23)-H(23B)	0.9
N(12)-C(110)	1.318(7)	C(116)-C(117)	1.511(7)	C(25)-C(26)	1.377(8)	N(24)-H(24A)	0.9
N(12)-C(111)	1.361(6)	C(116)-H(11E)	0.97	C(25)-H(25)	0.93	N(24)-H(24B)	0.9
C(11)-C(12)	1.389(8)	C(116)-H(11F)	0.97	C(26)-C(27)	1.417(7)	OW2-HW2A	0.891(18)
C(11)-H(11)	0.93	C(117)-C(118)	1.532(6)	C(26)-H(26)	0.93	OW2-HW2B	0.892(18)
C(12)-C(13)	1.376(7)	C(117)-H(11G)	0.97	C(27)-C(211)	1.400(6)	Cl(1)-O(14)	1.423(4)
C(12)-H(12)	0.93	C(117)-H(11H)	0.97	C(27)-C(28)	1.426(7)	Cl(1)-O(13)	1.439(4)
C(13)-C(14)	1.399(7)	C(118)-N(14)	1.486(6)	C(28)-C(29)	1.375(8)	Cl(1)-O(12)	1.444(4)
C(13)-H(13)	0.93	C(118)-H(118)	0.98	C(28)-H(28)	0.93	Cl(1)-O(11)	1.449(4)
C(14)-C(112)	1.380(7)	N(13)-H(13A)	0.9	C(29)-C(210)	1.380(7)	Cl(2)-O(24)	1.428(4)
C(14)-C(15)	1.452(7)	N(13)-H(13B)	0.9	C(29)-H(29)	0.93	Cl(2)-O(23)	1.434(4)
C(15)-C(16)	1.336(8)	N(14)-H(14A)	0.9	C(210)-H(210)	0.93	Cl(2)-O(22)	1.441(4)
C(15)-H(15)	0.93	N(14)-H(14B)	0.9	C(211)-C(212)	1.425(7)	Cl(2)-O(21)	1.448(4)
C(16)-C(17)	1.457(8)	OW1-HW1A	0.877(18)	C(213)-N(23)	1.487(5)	Cl(3)-O(34)	1.417(4)
C(16)-H(16)	0.93	OW1-HW1B	0.886(18)	C(213)-C(214)	1.524(7)	Cl(3)-O(33)	1.433(4)
C(17)-C(18)	1.391(8)	Cu(2)-N(24)	2.002(4)	C(213)-C(218)	1.528(5)	Cl(3)-O(32)	1.443(5)
C(17)-C(111)	1.401(6)	Cu(2)-N(22)	2.025(4)	C(213)-H(213)	0.98	Cl(3)-O(31)	1.445(4)
C(18)-C(19)	1.363(8)	Cu(2)-N(23)	2.029(4)	C(214)-C(215)	1.548(6)	Cl(4)-O(43)	1.368(6)
C(18)-H(18)	0.93	Cu(2)-N(21)	2.041(5)	C(214)-H(21A)	0.97	Cl(4)-O(42)	1.395(5)
C(19)-C(110)	1.423(7)	Cu(2)-OW2	2.302(4)	C(214)-H(21B)	0.97	Cl(4)-O(44)	1.408(6)
C(19)-H(19)	0.93	Cu(2)-O(22)#2	2.771(4)	C(215)-C(216)	1.510(7)	Cl(4)-O(41)	1.431(4)
C(110)-H(110)	0.93	N(21)-C(21)	1.326(7)	C(215)-H(21C)	0.97	OW3-HW3A	0.907(18)
C(111)-C(112)	1.447(7)	N(21)-C(212)	1.349(6)	C(215)-H(21D)	0.97	OW3-HW3B	0.916(19)
C(113)-N(13)	1.494(5)	N(22)-C(210)	1.329(7)	C(216)-C(217)	1.533(7)	OW4-HW4A	0.936(19)
C(113)-C(114)	1.502(6)	N(22)-C(211)	1.362(6)	C(216)-H(21E)	0.97	OW4-HW4B	0.934(19)

Bond	Angle [°]	Bond	Angle [°]	Bond	Angle [°]
N(14)-Cu(1)-N(13)	84.88(17)	C(116)-C(117)-C(118)	111.4(4)	N(21)-C(212)-C(24)	123.1(5)
N(14)-Cu(1)-N(12)	171.74(19)	C(116)-C(117)-H(11G)	109.4	N(21)-C(212)-C(211)	117.3(4)
N(13)-Cu(1)-N(12)	96.49(17)	C(118)-C(117)-H(11G)	109.4	C(24)-C(212)-C(211)	119.6(4)
N(14)-Cu(1)-N(11)	94.98(17)	C(116)-C(117)-H(11H)	109.4	N(23)-C(213)-C(214)	113.2(4)
N(13)-Cu(1)-N(11)	168.8(2)	C(118)-C(117)-H(11H)	109.4	N(23)-C(213)-C(218)	109.0(3)
N(12)-Cu(1)-N(11)	82.09(17)	H(11G)-C(117)-H(11H)	108	C(214)-C(213)-C(218)	110.5(4)
N(14)-Cu(1)-OW1	96.10(15)	N(14)-C(118)-C(113)	108.4(3)	N(23)-C(213)-H(213)	108
N(13)-Cu(1)-OW1	92.30(18)	N(14)-C(118)-C(117)	114.0(4)	C(214)-C(213)-H(213)	108
N(12)-Cu(1)-OW1	91.99(15)	C(113)-C(118)-C(117)	109.6(4)	C(218)-C(213)-H(213)	108
N(11)-Cu(1)-OW1	98.82(17)	N(14)-C(118)-H(118)	108.2	C(213)-C(214)-C(215)	108.9(4)
N(14)-Cu(1)-O(11)#1	80.79(15)	C(113)-C(118)-H(118)	108.2	C(213)-C(214)-H(21A)	109.9
N(13)-Cu(1)-O(11)#1	85.46(17)	C(117)-C(118)-H(118)	108.2	C(215)-C(214)-H(21A)	109.9
N(12)-Cu(1)-O(11)#1	91.19(14)	C(113)-N(13)-Cu(1)	109.6(3)	C(213)-C(214)-H(21B)	109.9
N(11)-Cu(1)-O(11)#1	83.49(15)	C(113)-N(13)-H(13A)	109.7	C(215)-C(214)-H(21B)	109.9
OW1-Cu(1)-O(11)#1	176.30(13)	Cu(1)-N(13)-H(13A)	109.7	H(21A)-C(214)-H(21B)	108.3
C(11)-N(11)-C(112)	117.5(4)	C(113)-N(13)-H(13B)	109.7	C(216)-C(215)-C(214)	111.9(4)
C(11)-N(11)-Cu(1)	130.2(3)	Cu(1)-N(13)-H(13B)	109.7	C(216)-C(215)-H(21C)	109.2
C(112)-N(11)-Cu(1)	112.1(3)	H(13A)-N(13)-H(13B)	108.2	C(214)-C(215)-H(21C)	109.2
C(110)-N(12)-C(111)	117.9(4)	C(118)-N(14)-Cu(1)	109.4(3)	C(216)-C(215)-H(21D)	109.2
C(110)-N(12)-Cu(1)	129.4(4)	C(118)-N(14)-H(14A)	109.8	C(214)-C(215)-H(21D)	109.2
C(111)-N(12)-Cu(1)	112.6(3)	Cu(1)-N(14)-H(14A)	109.8	H(21C)-C(215)-H(21D)	107.9
N(11)-C(11)-C(12)	122.1(4)	C(118)-N(14)-H(14B)	109.8	C(215)-C(216)-C(217)	111.6(4)
N(11)-C(11)-H(11)	119	Cu(1)-N(14)-H(14B)	109.8	C(215)-C(216)-H(21E)	109.3
C(12)-C(11)-H(11)	119	H(14A)-N(14)-H(14B)	108.2	C(217)-C(216)-H(21E)	109.3
C(13)-C(12)-C(11)	120.1(5)	Cu(1)-OW1-HW1A	140(3)	C(215)-C(216)-H(21F)	109.3
C(13)-C(12)-H(12)	119.9	Cu(1)-OW1-HW1B	111(3)	C(217)-C(216)-H(21F)	109.3
C(11)-C(12)-H(12)	119.9	HW1A-OW1-HW1B	109(3)	H(21E)-C(216)-H(21F)	108
C(12)-C(13)-C(14)	119.1(5)	N(24)-Cu(2)-N(22)	175.3(2)	C(218)-C(217)-C(216)	110.4(4)
C(12)-C(13)-H(13)	120.5	N(24)-Cu(2)-N(23)	84.48(17)	C(218)-C(217)-H(21G)	109.6
C(14)-C(13)-H(13)	120.5	N(22)-Cu(2)-N(23)	95.94(16)	C(216)-C(217)-H(21G)	109.6
C(112)-C(14)-C(13)	117.4(5)	N(24)-Cu(2)-N(21)	96.67(17)	C(218)-C(217)-H(21H)	109.6
C(112)-C(14)-C(15)	119.3(5)	N(22)-Cu(2)-N(21)	81.76(17)	C(216)-C(217)-H(21H)	109.6

C(13)-C(14)-C(15)	123.3(5)	N(23)-Cu(2)-N(21)	165.46(18)	H(21G)-C(217)-H(21H)	108.1
C(16)-C(15)-C(14)	120.8(5)	N(24)-Cu(2)-OW2	92.56(18)	N(24)-C(218)-C(217)	114.5(4)
C(16)-C(15)-H(15)	119.6	N(22)-Cu(2)-OW2	92.05(15)	N(24)-C(218)-C(213)	107.1(3)
C(14)-C(15)-H(15)	119.6	N(23)-Cu(2)-OW2	93.65(17)	C(217)-C(218)-C(213)	110.1(3)
C(15)-C(16)-C(17)	121.9(5)	N(21)-Cu(2)-OW2	100.76(16)	N(24)-C(218)-H(218)	108.3
C(15)-C(16)-H(16)	119.1	N(24)-Cu(2)-O(22)#2	87.01(17)	C(217)-C(218)-H(218)	108.3
C(17)-C(16)-H(16)	119.1	N(22)-Cu(2)-O(22)#2	88.43(14)	C(213)-C(218)-H(218)	108.3
C(18)-C(17)-C(111)	117.2(5)	N(23)-Cu(2)-O(22)#2	82.66(15)	C(213)-N(23)-Cu(2)	109.1(3)
C(18)-C(17)-C(16)	125.3(4)	N(21)-Cu(2)-O(22)#2	82.93(15)	C(213)-N(23)-H(23A)	109.9
C(111)-C(17)-C(16)	117.5(5)	OW2-Cu(2)-O(22)#2	176.31(14)	Cu(2)-N(23)-H(23A)	109.9
C(19)-C(18)-C(17)	121.6(5)	C(21)-N(21)-C(212)	118.1(5)	C(213)-N(23)-H(23B)	109.9
C(19)-C(18)-H(18)	119.2	C(21)-N(21)-Cu(2)	130.0(4)	Cu(2)-N(23)-H(23B)	109.9
C(17)-C(18)-H(18)	119.2	C(212)-N(21)-Cu(2)	111.8(4)	H(23A)-N(23)-H(23B)	108.3
C(18)-C(19)-C(110)	116.9(5)	C(210)-N(22)-C(211)	118.3(4)	C(218)-N(24)-Cu(2)	110.3(3)
C(18)-C(19)-H(19)	121.6	C(210)-N(22)-Cu(2)	129.5(4)	C(218)-N(24)-H(24A)	109.6
C(110)-C(19)-H(19)	121.6	C(211)-N(22)-Cu(2)	112.0(3)	Cu(2)-N(24)-H(24A)	109.6
N(12)-C(110)-C(19)	123.7(5)	N(21)-C(21)-C(22)	123.2(5)	C(218)-N(24)-H(24B)	109.6
N(12)-C(110)-H(110)	118.1	N(21)-C(21)-H(21)	118.4	Cu(2)-N(24)-H(24B)	109.6
C(19)-C(110)-H(110)	118.1	C(22)-C(21)-H(21)	118.4	H(24A)-N(24)-H(24B)	108.1
N(12)-C(111)-C(17)	122.7(5)	C(23)-C(22)-C(21)	119.1(5)	Cu(2)-OW2-HW2A	112(3)
N(12)-C(111)-C(112)	116.6(4)	C(23)-C(22)-H(22)	120.4	Cu(2)-OW2-HW2B	121(3)
C(17)-C(111)-C(112)	120.7(4)	C(21)-C(22)-H(22)	120.4	HW2A-OW2-HW2B	109(3)
N(11)-C(112)-C(14)	123.9(5)	C(22)-C(23)-C(24)	119.8(5)	O(14)-Cl(1)-O(13)	109.4(3)
N(11)-C(112)-C(111)	116.3(4)	C(22)-C(23)-H(23)	120.1	O(14)-Cl(1)-O(12)	110.2(3)
C(14)-C(112)-C(111)	119.8(4)	C(24)-C(23)-H(23)	120.1	O(13)-Cl(1)-O(12)	109.4(3)
N(13)-C(113)-C(114)	114.8(4)	C(25)-C(24)-C(212)	119.1(5)	O(14)-Cl(1)-O(11)	109.3(3)
N(13)-C(113)-C(118)	107.4(4)	C(25)-C(24)-C(23)	124.3(5)	O(13)-Cl(1)-O(11)	110.2(2)
C(114)-C(113)-C(118)	110.6(3)	C(212)-C(24)-C(23)	116.6(5)	O(12)-Cl(1)-O(11)	108.3(2)
N(13)-C(113)-H(113)	107.9	C(26)-C(25)-C(24)	121.4(5)	O(24)-Cl(2)-O(23)	109.1(2)
C(114)-C(113)-H(113)	107.9	C(26)-C(25)-H(25)	119.3	O(24)-Cl(2)-O(22)	109.8(3)
C(118)-C(113)-H(113)	107.9	C(24)-C(25)-H(25)	119.3	O(23)-Cl(2)-O(22)	109.7(2)
C(113)-C(114)-C(115)	111.2(4)	C(25)-C(26)-C(27)	120.2(5)	O(24)-Cl(2)-O(21)	110.3(3)
C(113)-C(114)-H(11A)	109.4	C(25)-C(26)-H(26)	119.9	O(23)-Cl(2)-O(21)	110.1(2)
C(115)-C(114)-H(11A)	109.4	C(27)-C(26)-H(26)	119.9	O(22)-Cl(2)-O(21)	108.0(2)
C(113)-C(114)-H(11B)	109.4	C(211)-C(27)-C(26)	119.9(5)	O(34)-Cl(3)-O(33)	107.5(3)
C(115)-C(114)-H(11B)	109.4	C(211)-C(27)-C(28)	117.5(4)	O(34)-Cl(3)-O(32)	109.4(3)
H(11A)-C(114)-H(11B)	108	C(26)-C(27)-C(28)	122.6(4)	O(33)-Cl(3)-O(32)	112.2(3)
C(114)-C(115)-C(116)	111.0(4)	C(29)-C(28)-C(27)	117.4(4)	O(34)-Cl(3)-O(31)	110.7(3)
C(114)-C(115)-H(11C)	109.4	C(29)-C(28)-H(28)	121.3	O(33)-Cl(3)-O(31)	109.0(3)
C(116)-C(115)-H(11C)	109.4	C(27)-C(28)-H(28)	121.3	O(32)-Cl(3)-O(31)	108.0(3)
C(114)-C(115)-H(11D)	109.4	C(28)-C(29)-C(210)	121.7(5)	O(43)-Cl(4)-O(42)	111.9(4)
C(116)-C(115)-H(11D)	109.4	C(28)-C(29)-H(29)	119.1	O(43)-Cl(4)-O(44)	110.3(5)
H(11C)-C(115)-H(11D)	108	C(210)-C(29)-H(29)	119.1	O(42)-Cl(4)-O(44)	109.2(4)
C(117)-C(116)-C(115)	110.9(4)	N(22)-C(210)-C(29)	121.9(5)	O(43)-Cl(4)-O(41)	108.2(4)
C(117)-C(116)-H(11E)	109.4	N(22)-C(210)-H(210)	119.1	O(42)-Cl(4)-O(41)	109.6(3)
C(115)-C(116)-H(11E)	109.5	C(29)-C(210)-H(210)	119.1	O(44)-Cl(4)-O(41)	107.5(4)
C(117)-C(116)-H(11F)	109.5	N(22)-C(211)-C(27)	123.2(5)	HW3A-OW3-HW3B	104(3)
C(115)-C(116)-H(11F)	109.5	N(22)-C(211)-C(212)	116.9(4)	HW4A-OW4-HW4B	100(2)
H(11E)-C(116)-H(11F)	108	C(27)-C(211)-C(212)	119.9(4)		

Symmetry transformations used to generate equivalent atoms: #1 x+1,y,z #2 x-1,y,z

Table S22. Anisotropic displacement parameters ($Å^2 \times 10^3$) for [Cu(*SS*-dach)(phen)(H_2O)](ClO_4)$_2$.H_2O (**1$_{Cu}$**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}	Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	20(1)	20(1)	19(1)	-6(1)	3(1)	-3(1)	C(29)	37(3)	35(3)	30(3)	-18(2)	14(2)	-13(2)
N(11)	21(2)	23(2)	20(2)	-9(2)	6(2)	-9(2)	C(210)	27(3)	27(2)	23(3)	-8(2)	4(2)	-8(2)
N(12)	18(2)	22(2)	26(2)	-11(2)	6(2)	-4(2)	C(211)	22(3)	19(2)	26(3)	-9(2)	1(2)	-9(2)
C(11)	20(3)	30(3)	28(3)	-14(2)	4(2)	-4(2)	C(212)	20(2)	26(2)	22(3)	-6(2)	1(2)	-15(2)
C(12)	23(3)	46(3)	27(3)	-14(3)	8(2)	-14(2)	C(213)	19(2)	24(2)	22(2)	-10(2)	0(2)	-4(2)
C(13)	34(3)	37(3)	24(3)	-8(2)	2(2)	-12(3)	C(214)	32(3)	31(2)	38(3)	-12(2)	10(2)	-11(2)
C(14)	24(3)	28(2)	25(3)	-8(2)	-2(2)	-13(2)	C(215)	35(3)	26(2)	43(3)	-6(2)	6(2)	-6(2)
C(15)	36(3)	27(3)	32(3)	-8(2)	-4(2)	-7(2)	C(216)	31(3)	23(2)	49(3)	-13(2)	-2(2)	-5(2)
C(16)	29(3)	23(2)	37(3)	-11(2)	-5(2)	2(2)	C(217)	30(3)	27(2)	32(2)	-15(2)	7(2)	-4(2)
C(17)	27(3)	20(2)	38(3)	-14(2)	-3(2)	-2(2)	C(218)	32(2)	26(2)	23(2)	-9(2)	5(2)	-10(2)
C(18)	27(3)	29(3)	38(3)	-16(2)	-1(2)	-1(2)	N(23)	17(2)	28(2)	17(2)	-8(2)	7(2)	-4(2)
C(19)	32(3)	29(3)	37(3)	-19(2)	7(2)	-2(2)	N(24)	48(3)	23(2)	26(2)	-10(2)	16(2)	-7(2)
C(110)	33(3)	28(3)	27(3)	-13(2)	9(2)	-9(2)	OW2	27(2)	47(2)	30(2)	-18(2)	3(2)	-7(2)
C(111)	18(2)	24(2)	21(3)	-9(2)	-1(2)	-8(2)	Cl(1)	19(1)	31(1)	26(1)	-15(1)	2(1)	-6(1)
C(112)	16(2)	21(2)	28(3)	-11(2)	-2(2)	-4(2)	O(11)	18(2)	46(2)	39(2)	-23(2)	4(2)	-5(2)
C(113)	21(2)	24(2)	24(2)	-7(2)	2(2)	-8(2)	O(12)	28(2)	55(2)	50(3)	-36(2)	10(2)	-21(2)
C(114)	27(2)	30(2)	24(2)	-5(2)	3(2)	-8(2)	O(13)	30(2)	61(3)	27(2)	-20(2)	4(2)	-15(2)
C(115)	38(3)	25(2)	33(2)	-4(2)	0(2)	-13(2)	O(14)	51(3)	26(2)	45(3)	-12(2)	-2(2)	-3(2)
C(116)	40(3)	24(2)	45(3)	-13(2)	0(2)	-2(2)	Cl(2)	18(1)	27(1)	24(1)	-14(1)	3(1)	-5(1)
C(117)	34(3)	27(2)	34(3)	-14(2)	4(2)	-5(2)	O(21)	29(2)	57(3)	26(2)	-21(2)	8(2)	-17(2)
C(118)	28(2)	22(2)	25(2)	-9(2)	2(2)	-4(2)	O(22)	18(2)	48(2)	35(2)	-27(2)	7(2)	-9(2)
N(13)	27(2)	19(2)	30(3)	-8(2)	0(2)	-1(2)	O(23)	23(2)	47(2)	48(3)	-30(2)	2(2)	-13(2)
N(14)	20(2)	26(2)	22(2)	-9(2)	3(2)	-5(2)	O(24)	44(3)	32(2)	44(3)	-11(2)	2(2)	-2(2)
OW1	22(2)	49(2)	41(2)	-31(2)	8(2)	-13(2)	Cl(3)	34(1)	34(1)	29(1)	-12(1)	1(1)	-11(1)
Cu(2)	23(1)	19(1)	17(1)	-6(1)	4(1)	-3(1)	O(31)	45(3)	99(4)	52(3)	-50(3)	16(2)	-37(3)
N(21)	19(2)	28(2)	23(2)	-8(2)	-1(2)	-7(2)	O(32)	31(2)	51(2)	48(2)	-14(2)	8(2)	-12(2)
N(22)	25(2)	24(2)	21(2)	-9(2)	1(2)	-10(2)	O(33)	60(3)	49(2)	41(2)	8(2)	2(2)	-17(2)
C(21)	29(3)	33(3)	24(3)	-9(2)	4(2)	-12(2)	O(34)	76(3)	51(2)	92(3)	-45(3)	17(2)	-19(2)
C(22)	38(3)	40(3)	20(3)	-12(2)	7(2)	-19(3)	Cl(4)	42(1)	38(1)	29(1)	-8(1)	3(1)	-21(1)
C(23)	33(3)	31(3)	18(3)	-3(2)	0(2)	-16(2)	O(41)	48(3)	93(3)	38(2)	-30(2)	13(2)	-45(3)
C(24)	28(3)	23(2)	23(3)	-3(2)	-2(2)	-11(2)	O(42)	45(3)	160(5)	76(3)	-54(3)	24(2)	-61(3)
C(25)	40(3)	21(2)	25(3)	2(2)	-6(2)	-8(2)	O(43)	152(6)	117(5)	55(3)	34(3)	-55(3)	-78(4)
C(26)	33(3)	20(2)	38(3)	-7(2)	-3(2)	-2(2)	O(44)	92(4)	81(4)	185(7)	-84(4)	41(4)	-34(3)
C(27)	23(3)	29(3)	26(3)	-12(2)	1(2)	-11(2)	OW3	52(2)	39(2)	34(2)	-16(2)	7(2)	-13(2)
C(28)	20(2)	25(2)	45(3)	-19(2)	6(2)	-6(2)	OW4	63(3)	54(3)	47(3)	-26(2)	4(2)	-22(2)

Table S23. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for [Cu(*SS*-dach)(phen)(H_2O)](ClO_4)$_2$.H_2O (**1$_{Cu}$**).

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
H(11)	6584	4535	5848	40	H(23)	9304	10644	-7719	43
H(12)	7070	3014	7659	47	H(25)	6978	11973	-7030	50
H(13)	9094	1147	8089	50	H(26)	5536	12213	-5578	50
H(15)	11364	-212	7409	51	H(28)	5018	11319	-3500	43
H(16)	12796	-438	5992	49	H(29)	5803	9653	-1762	49
H(18)	13286	490	3883	49	H(210)	7929	7915	-1524	40
H(19)	12611	2125	2133	49	H(213)	12202	4536	-1001	34
H(110)	10448	3900	1939	44	H(21A)	9525	3548	-958	52
H(113)	8869	7294	2507	35	H(21B)	10330	3604	106	52
H(11A)	6727	8246	432	45	H(21C)	13027	2288	81	58
H(11B)	8662	8188	529	45	H(21D)	11641	1661	116	58
H(11C)	6776	10128	201	51	H(21E)	11580	2150	-1805	54
H(11D)	8016	9547	1346	51	H(21F)	13507	1486	-1236	54
H(11E)	5234	10346	1727	59	H(21G)	14053	3322	-1896	45
H(11F)	4486	9673	1175	59	H(21H)	13264	3231	-2942	45
H(11G)	4787	8614	3132	49	H(218)	10542	4432	-2846	41
H(11H)	6727	8542	3243	49	H(23A)	9923	5997	-1094	33
H(118)	5438	7364	2167	40	H(23B)	8778	5746	-1751	33
H(13A)	9672	5813	1977	41	H(24A)	11818	5653	-3971	50
H(13B)	7943	6028	1487	41	H(24B)	13018	5497	-3056	50
H(14A)	5730	6158	3976	36	HW2A	12220(50)	7210(40)	-1530(20)	42
H(14B)	7280	6361	4277	36	HW2B	13540(30)	6870(40)	-2190(30)	42
HW1A	4880(30)	4680(40)	2690(40)	40	HW3A	11200(50)	6400(20)	380(40)	50
HW1B	6370(50)	4230(30)	2220(30)	40	HW3B	12560(30)	5420(30)	340(40)	50
H(21)	11938	7331	-5408	44	HW4A	6360(50)	5780(30)	-220(40)	63
H(22)	11376	8817	-7271	47	HW4B	5630(40)	6950(30)	-230(40)	63

Table S24. Hydrogen bonds for [Cu(*SS*-dach)(phen)(H_2O)](ClO_4)$_2$.H_2O (**1$_{Cu}$**) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(13)-H(13A)...O(13)#1	0.9	2.41	3.149(6)	139
N(13)-H(13A)...OW3	0.9	2.45	3.182(6)	138.7
N(13)-H(13B)...OW4	0.9	2.12	3.003(6)	168.1
N(14)-H(14A)...O(12)	0.9	2.29	3.164(6)	162.8
N(14)-H(14B)...O(22)#3	0.9	2.31	3.156(6)	157.4
N(14)-H(14B)...Cl(2)#3	0.9	2.98	3.629(4)	130.5
OW1-HW1A...O(13)	0.877(18)	2.02(2)	2.869(6)	163(4)
OW1-HW1A...Cl(1)	0.877(18)	2.86(3)	3.547(4)	136(3)
OW1-HW1B...O(31)	0.886(18)	2.032(19)	2.916(6)	175(4)
OW1-HW1B...Cl(3)	0.886(18)	2.96(3)	3.785(4)	155(3)
N(23)-H(23A)...OW3	0.9	2.23	3.021(6)	146.5
N(23)-H(23B)...O(21)#2	0.9	2.31	3.090(6)	145.6
N(24)-H(24A)...O(11)#4	0.9	2.42	3.244(6)	153.1
N(24)-H(24A)...O(12)#4	0.9	2.45	3.193(6)	140.4
N(24)-H(24A)...Cl(1)#4	0.9	2.89	3.710(5)	153.1
N(24)-H(24B)...O(23)	0.9	2.36	3.025(7)	130.4
OW2-HW2A...O(41)#4	0.891(18)	2.18(3)	2.913(6)	140(3)
OW2-HW2B...O(21)	0.892(18)	2.10(3)	2.913(6)	151(4)
OW2-HW2B...Cl(2)	0.892(18)	2.92(3)	3.592(4)	134(3)
OW3-HW3A...O(41)#4	0.907(18)	2.26(3)	3.100(6)	153(4)
OW3-HW3A...O(43)#4	0.907(18)	2.50(4)	3.196(8)	134(3)
OW3-HW3A...Cl(4)#4	0.907(18)	2.91(3)	3.729(4)	151(3)
OW3-HW3B...O(32)#1	0.916(19)	2.30(3)	2.938(5)	127(3)
OW4-HW4A...O(33)	0.936(19)	2.23(2)	3.159(7)	173(5)
OW4-HW4A...O(31)	0.936(19)	2.48(4)	3.101(7)	124(3)
OW4-HW4A...Cl(3)	0.936(19)	2.80(3)	3.663(5)	154(4)
OW4-HW4B...O(42)#5	0.934(19)	2.14(2)	3.043(7)	162(4)

Symmetry transformations used to generate equivalent atoms: #1 x+1,y,z #2 x-1,y,z #3 x-1,y,z+1 #4 x+1,y,z-1 #5 x,y,z-1

Table S25. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for [Cu(phen)$_2$Cl].ClO$_4$. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
Cu(1)	2828(1)	2342(1)	725(1)	31(1)	C(21)	3201(3)	4096(3)	-599(2)	35(1)
Cl(2)	2419(1)	356(1)	352(1)	34(1)	C(22)	2805(3)	4803(3)	-1317(2)	41(1)
N(11)	3502(2)	3039(2)	1926(2)	29(1)	C(23)	1659(3)	5040(3)	-1688(2)	41(1)
N(12)	4469(2)	2126(3)	924(2)	35(1)	C(24)	914(3)	4576(3)	-1323(2)	34(1)
C(11)	2997(3)	3489(3)	2417(2)	33(1)	C(25)	-296(3)	4752(3)	-1664(2)	41(1)
C(12)	3608(3)	3991(3)	3202(2)	37(1)	C(26)	-964(3)	4277(3)	-1285(2)	39(1)
C(13)	4763(3)	4025(3)	3488(2)	36(1)	C(27)	-500(3)	3577(3)	-533(2)	32(1)
C(14)	5335(3)	3536(3)	2990(2)	30(1)	C(28)	-1156(3)	3039(3)	-116(2)	37(1)
C(15)	6545(3)	3483(3)	3240(2)	34(1)	C(29)	-638(3)	2357(3)	575(2)	37(1)
C(16)	7037(3)	2942(3)	2749(2)	33(1)	C(210)	547(3)	2186(3)	872(2)	34(1)
C(17)	6361(3)	2449(3)	1951(2)	31(1)	C(211)	677(2)	3374(3)	-198(2)	29(1)
C(18)	6810(3)	1892(3)	1402(2)	39(1)	C(212)	1393(3)	3881(3)	-598(2)	29(1)
C(19)	6090(3)	1504(4)	632(2)	47(1)	Cl(1)	4610(1)	6812(1)	1756(1)	50(1)
C(110)	4921(3)	1630(4)	414(2)	46(1)	O(11)	5494(3)	6328(3)	2443(2)	77(1)
C(111)	5177(3)	2530(3)	1679(2)	28(1)	O(12)	3660(3)	7085(5)	1953(2)	99(2)
C(112)	4654(2)	3057(3)	2212(2)	27(1)	O(13)	5041(4)	7945(5)	1544(3)	107(2)
N(21)	2523(2)	3626(2)	-241(2)	29(1)	O(14)	4310(4)	6083(6)	1064(3)	139(2)
N(22)	1187(2)	2683(2)	492(2)	29(1)					

Table S26. Bond lengths [Å] and angles [°] for $[Cu(phen)_2Cl].ClO_4$

Bond	Length [Å]	Bond	Length [Å]	Bond	Length [Å]	Bond	Length [Å]
Cu(1)-N(12)	1.990(3)	C(14)-C(112)	1.401(4)	N(21)-C(212)	1.363(4)	C(27)-C(211)	1.403(4)
Cu(1)-N(22)	2.000(3)	C(14)-C(15)	1.431(4)	N(22)-C(210)	1.333(4)	C(27)-C(28)	1.412(5)
Cu(1)-N(11)	2.070(2)	C(15)-C(16)	1.357(5)	N(22)-C(211)	1.358(4)	C(28)-C(29)	1.356(5)
Cu(1)-N(21)	2.111(3)	C(15)-H(15)	0.93	C(21)-C(22)	1.391(5)	C(28)-H(28)	0.93
Cu(1)-Cl(2)	2.3000(9)	C(16)-C(17)	1.431(4)	C(21)-H(21)	0.93	C(29)-C(210)	1.409(4)
N(11)-C(11)	1.327(4)	C(16)-H(16)	0.93	C(22)-C(23)	1.377(5)	C(29)-H(29)	0.93
N(11)-C(112)	1.356(4)	C(17)-C(111)	1.398(4)	C(22)-H(22)	0.93	C(210)-H(210)	0.93
N(12)-C(110)	1.329(4)	C(17)-C(18)	1.409(4)	C(23)-C(24)	1.408(5)	C(211)-C(212)	1.437(4)
N(12)-C(111)	1.352(4)	C(18)-C(19)	1.370(5)	C(23)-H(23)	0.93	Cl(1)-O(14)	1.370(5)
C(11)-C(12)	1.398(4)	C(18)-H(18)	0.93	C(24)-C(212)	1.398(4)	Cl(1)-O(12)	1.396(3)
C(11)-H(11)	0.93	C(19)-C(110)	1.393(5)	C(24)-C(25)	1.437(5)	Cl(1)-O(11)	1.399(3)
C(12)-C(13)	1.361(5)	C(19)-H(19)	0.93	C(25)-C(26)	1.348(5)	Cl(1)-O(13)	1.470(5)
C(12)-H(12)	0.93	C(110)-H(110)	0.93	C(25)-H(25)	0.93		
C(13)-C(14)	1.415(4)	C(111)-C(112)	1.436(4)	C(26)-C(27)	1.435(5)		
C(13)-H(13)	0.93	N(21)-C(21)	1.330(4)	C(26)-H(26)	0.93		

Bond	Angle [°]	Bond	Angle [°]	Bond	Angle [°]
N(12)-Cu(1)-N(22)	175.69(11)	C(111)-C(17)-C(18)	116.8(3)	C(212)-C(24)-C(25)	119.0(3)
N(12)-Cu(1)-N(11)	81.50(10)	C(111)-C(17)-C(16)	119.0(3)	C(23)-C(24)-C(25)	123.8(3)
N(22)-Cu(1)-N(11)	98.38(10)	C(18)-C(17)-C(16)	124.2(3)	C(26)-C(25)-C(24)	120.9(3)
N(12)-Cu(1)-N(21)	95.38(11)	C(19)-C(18)-C(17)	119.6(3)	C(26)-C(25)-H(25)	119.5
N(22)-Cu(1)-N(21)	80.74(10)	C(19)-C(18)-H(18)	120.2	C(24)-C(25)-H(25)	119.5
N(11)-Cu(1)-N(21)	114.81(10)	C(17)-C(18)-H(18)	120.2	C(25)-C(26)-C(27)	121.6(3)
N(12)-Cu(1)-Cl(2)	92.64(9)	C(18)-C(19)-C(110)	119.4(3)	C(25)-C(26)-H(26)	119.2
N(22)-Cu(1)-Cl(2)	90.85(8)	C(18)-C(19)-H(19)	120.3	C(27)-C(26)-H(26)	119.2
N(11)-Cu(1)-Cl(2)	127.13(8)	C(110)-C(19)-H(19)	120.3	C(211)-C(27)-C(28)	117.3(3)
N(21)-Cu(1)-Cl(2)	118.05(7)	N(12)-C(110)-C(19)	122.4(3)	C(211)-C(27)-C(26)	118.4(3)
C(11)-N(11)-C(112)	118.0(3)	N(12)-C(110)-H(110)	118.8	C(28)-C(27)-C(26)	124.3(3)
C(11)-N(11)-Cu(1)	130.9(2)	C(19)-C(110)-H(110)	118.8	C(29)-C(28)-C(27)	119.6(3)
C(112)-N(11)-Cu(1)	111.09(18)	N(12)-C(111)-C(17)	123.4(3)	C(29)-C(28)-H(28)	120.2
C(110)-N(12)-C(111)	118.3(3)	N(12)-C(111)-C(112)	116.5(3)	C(27)-C(28)-H(28)	120.2
C(110)-N(12)-Cu(1)	127.7(2)	C(17)-C(111)-C(112)	120.1(3)	C(28)-C(29)-C(210)	120.0(3)
C(111)-N(12)-Cu(1)	114.0(2)	N(11)-C(112)-C(14)	123.5(3)	C(28)-C(29)-H(29)	120
N(11)-C(11)-C(12)	122.5(3)	N(11)-C(112)-C(111)	116.7(2)	C(210)-C(29)-H(29)	120
N(11)-C(11)-H(11)	118.8	C(14)-C(112)-C(111)	119.8(3)	N(22)-C(210)-C(29)	121.7(3)
C(12)-C(11)-H(11)	118.8	C(21)-N(21)-C(212)	117.3(3)	N(22)-C(210)-H(210)	119.2
C(13)-C(12)-C(11)	119.9(3)	C(21)-N(21)-Cu(1)	131.6(2)	C(29)-C(210)-H(210)	119.2
C(13)-C(12)-H(12)	120.1	C(212)-N(21)-Cu(1)	110.6(2)	N(22)-C(211)-C(27)	122.7(3)
C(11)-C(12)-H(12)	120.1	C(210)-N(22)-C(211)	118.8(3)	N(22)-C(211)-C(212)	117.2(3)
C(12)-C(13)-C(14)	119.4(3)	C(210)-N(22)-Cu(1)	126.6(2)	C(27)-C(211)-C(212)	120.1(3)
C(12)-C(13)-H(13)	120.3	C(211)-N(22)-Cu(1)	114.0(2)	N(21)-C(212)-C(24)	123.6(3)
C(14)-C(13)-H(13)	120.3	N(21)-C(21)-C(22)	123.2(3)	N(21)-C(212)-C(211)	116.5(3)
C(112)-C(14)-C(13)	116.7(3)	N(21)-C(21)-H(21)	118.4	C(24)-C(212)-C(211)	119.9(3)
C(112)-C(14)-C(15)	119.0(3)	C(22)-C(21)-H(21)	118.4	O(14)-Cl(1)-O(12)	110.5(3)
C(13)-C(14)-C(15)	124.3(3)	C(23)-C(22)-C(21)	119.4(3)	O(14)-Cl(1)-O(11)	112.6(3)
C(16)-C(15)-C(14)	121.2(3)	C(23)-C(22)-H(22)	120.3	O(12)-Cl(1)-O(11)	111.8(2)
C(16)-C(15)-H(15)	119.4	C(21)-C(22)-H(22)	120.3	O(14)-Cl(1)-O(13)	107.4(4)
C(14)-C(15)-H(15)	119.4	C(22)-C(23)-C(24)	119.2(3)	O(12)-Cl(1)-O(13)	107.8(3)
C(15)-C(16)-C(17)	120.9(3)	C(22)-C(23)-H(23)	120.4	O(11)-Cl(1)-O(13)	106.4(2)
C(15)-C(16)-H(16)	119.5	C(24)-C(23)-H(23)	120.4		
C(17)-C(16)-H(16)	119.5	C(212)-C(24)-C(23)	117.1(3)		

Table S27. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $[Cu(phen)_2Cl].ClO_4$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}	Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	20(1)	46(1)	28(1)	-6(1)	10(1)	5(1)	C(21)	30(2)	36(2)	43(2)	-5(1)	18(1)	-4(1)
Cl(2)	37(1)	35(1)	38(1)	5(1)	23(1)	6(1)	C(22)	46(2)	36(2)	50(2)	0(1)	29(2)	-5(2)
N(11)	25(1)	37(1)	26(1)	1(1)	11(1)	8(1)	C(23)	52(2)	33(2)	43(2)	5(1)	24(2)	6(2)
N(12)	26(1)	50(2)	31(1)	-9(1)	13(1)	5(1)	C(24)	38(2)	28(1)	37(2)	-1(1)	16(1)	6(1)
C(11)	31(2)	40(2)	31(2)	2(1)	16(1)	13(1)	C(25)	40(2)	40(2)	40(2)	4(1)	13(1)	14(1)
C(12)	44(2)	45(2)	28(2)	-1(1)	19(1)	12(2)	C(26)	28(2)	44(2)	43(2)	1(1)	10(1)	11(1)
C(13)	42(2)	40(2)	25(1)	-2(1)	11(1)	6(1)	C(27)	24(1)	34(2)	38(2)	-5(1)	12(1)	6(1)
C(14)	31(2)	31(2)	26(1)	4(1)	9(1)	4(1)	C(28)	22(2)	45(2)	46(2)	-8(1)	15(1)	3(1)
C(15)	30(2)	41(2)	26(1)	5(1)	6(1)	-3(1)	C(29)	28(2)	45(2)	46(2)	-4(1)	21(1)	1(1)
C(16)	23(1)	41(2)	34(2)	9(1)	9(1)	1(1)	C(210)	29(2)	40(2)	37(2)	0(1)	16(1)	5(1)
C(17)	25(2)	35(2)	33(2)	6(1)	12(1)	4(1)	C(211)	26(1)	30(1)	31(1)	-7(1)	11(1)	2(1)
C(18)	25(2)	52(2)	46(2)	2(2)	20(1)	7(1)	C(212)	27(2)	28(1)	33(2)	-7(1)	13(1)	1(1)
C(19)	32(2)	66(2)	49(2)	-14(2)	24(2)	7(2)	Cl(1)	27(1)	88(1)	35(1)	1(1)	12(1)	9(1)
C(110)	30(2)	70(2)	42(2)	-20(2)	17(2)	2(2)	O(11)	39(2)	98(3)	76(2)	20(2)	1(2)	5(2)
C(111)	24(1)	35(2)	28(1)	2(1)	12(1)	5(1)	O(12)	38(2)	195(5)	71(2)	-4(3)	29(2)	22(2)
C(112)	27(1)	30(1)	25(1)	2(1)	11(1)	6(1)	O(13)	72(3)	122(4)	104(3)	49(3)	5(2)	-12(3)
N(21)	24(1)	32(1)	32(1)	-7(1)	11(1)	-2(1)	O(14)	79(3)	221(6)	113(4)	-86(4)	30(3)	-18(3)
N(22)	23(1)	36(1)	31(1)	-3(1)	12(1)	4(1)							

Table S28. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for $[Cu(phen)_2Cl].ClO_4$.

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
H(11)	2208	3469	2232	49	H(19)	6379	1158	259	70	H(26)	-1744	4407	-1518	59
H(12)	3224	4300	3527	56	H(110)	4439	1357	-109	69	H(28)	-1940	3151	-315	55
H(13)	5174	4367	4006	54	H(21)	3977	3943	-356	52	H(29)	-1066	2003	853	56
H(15)	7002	3825	3746	51	H(22)	3310	5114	-1546	61	H(210)	892	1713	1346	51
H(16)	7825	2892	2935	50	H(23)	1381	5501	-2174	61					
H(18)	7591	1790	1562	58	H(25)	-623	5199	-2152	61					

Table S29. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $[Cu(phen)_3]ClO_4)_2$. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
Cu	297(1)	1397(1)	5959(1)	29(1)	C(211)	1882(6)	999(2)	8117(4)	30(1)
N(11)	-2263(4)	1674(1)	5244(3)	29(1)	C(212)	3067(5)	961(1)	7648(4)	28(1)
N(12)	512(4)	2056(1)	6404(3)	30(1)	N(31)	370(4)	1495(1)	4428(3)	25(1)
C(11)	-3592(6)	1489(2)	4649(4)	32(1)	N(32)	-622(4)	793(1)	5267(3)	26(1)
C(12)	-4947(6)	1736(2)	4177(4)	38(1)	C(31)	935(5)	1840(2)	4034(4)	30(1)
C(13)	-4905(6)	2188(2)	4347(4)	39(1)	C(32)	770(5)	1875(2)	2927(4)	33(1)
C(14)	-3525(6)	2399(2)	4972(4)	32(1)	C(33)	-11(6)	1549(2)	2200(4)	33(1)
C(15)	-3392(7)	2873(2)	5180(4)	43(1)	C(34)	-605(5)	1176(2)	2584(4)	30(1)
C(16)	-2045(7)	3057(2)	5793(4)	44(1)	C(35)	-1970(6)	467(2)	2317(4)	39(1)
C(17)	-676(6)	2790(2)	6244(4)	32(1)	C(36)	-1432(6)	815(2)	1896(4)	40(1)
C(18)	749(7)	2969(2)	6891(4)	41(1)	C(37)	-1714(5)	440(1)	3466(4)	27(1)
C(19)	1988(6)	2695(2)	7309(4)	42(1)	C(38)	-2236(5)	88(2)	3963(4)	33(1)
C(110)	1837(6)	2235(2)	7038(4)	38(1)	C(39)	-1946(6)	93(2)	5068(4)	33(1)
C(111)	-749(6)	2326(2)	6028(3)	28(1)	C(310)	-1121(5)	448(2)	5701(4)	31(1)
C(112)	-2211(5)	2128(2)	5396(3)	28(1)	C(311)	-910(5)	788(1)	4163(4)	25(1)
N(21)	2774(4)	1139(1)	6629(3)	30(1)	C(312)	-359(5)	1163(1)	3715(4)	24(1)
N(22)	533(5)	1201(1)	7506(3)	30(1)	Cl(1)	3371(2)	572(1)	2786(1)	40(1)
C(21)	3810(6)	1082(2)	6166(4)	36(1)	O(11)	3849(7)	643(2)	3923(3)	99(2)
C(22)	5188(6)	848(2)	6672(4)	42(1)	O(12)	2157(5)	242(2)	2429(4)	82(1)
C(23)	5509(6)	680(2)	7706(4)	39(1)	O(13)	2891(6)	976(1)	2186(3)	85(2)
C(24)	4439(6)	734(2)	8232(4)	32(1)	O(14)	4583(5)	386(2)	2503(4)	91(2)
C(25)	4659(6)	560(2)	9311(4)	40(1)	Cl(2)	6533(2)	1894(1)	9191(1)	40(1)
C(26)	3573(7)	601(2)	9760(4)	44(1)	O(21)	6725(5)	1463(1)	9710(3)	61(1)
C(27)	2127(6)	816(2)	9173(4)	36(1)	O(22)	7614(4)	2195(1)	9925(3)	67(1)
C(28)	916(7)	852(2)	9581(4)	45(1)	O(23)	5047(4)	2068(2)	8994(3)	68(1)
C(29)	-415(7)	1064(2)	8968(4)	44(1)	O(24)	6824(7)	1872(2)	8196(4)	111(2)
C(210)	-561(6)	1236(2)	7934(4)	39(1)					

1 Table S30. Bond lengths [Å] and angles [°] for $[Cu(phen)_3]ClO_4)_2$.

Bond	Length [Å]	Bond	Length [Å]	Bond	Length [Å]	Bond	Length [Å]
Cu-N(22)	2.023(4)	C(17)-C(18)	1.398(7)	C(26)-C(27)	1.437(7)	C(35)-C(36)	1.347(7)
Cu-N(31)	2.031(4)	C(17)-C(111)	1.406(6)	C(26)-H(26)	0.93	C(35)-C(37)	1.424(6)
Cu-N(12)	2.033(4)	C(18)-C(19)	1.358(7)	C(27)-C(28)	1.410(7)	C(35)-H(35)	0.93
Cu-N(32)	2.053(4)	C(18)-H(18)	0.93	C(27)-C(211)	1.414(6)	C(36)-H(36)	0.93
Cu-N(21)	2.287(4)	C(19)-C(110)	1.407(7)	C(28)-C(29)	1.366(7)	C(37)-C(311)	1.402(6)
Cu-N(11)	2.375(4)	C(19)-H(19)	0.93	C(28)-H(28)	0.93	C(37)-C(38)	1.404(6)
N(11)-C(11)	1.322(6)	C(110)-H(110)	0.93	C(29)-C(210)	1.394(7)	C(38)-C(39)	1.360(6)
N(11)-C(112)	1.363(6)	C(111)-C(112)	1.441(7)	C(29)-H(29)	0.93	C(38)-H(38)	0.93
N(12)-C(110)	1.325(6)	N(21)-C(21)	1.316(6)	C(210)-H(210)	0.93	C(39)-C(310)	1.387(6)
N(12)-C(111)	1.360(6)	N(21)-C(212)	1.358(6)	C(211)-C(212)	1.442(7)	C(39)-H(39)	0.93
C(11)-C(12)	1.398(7)	N(22)-C(210)	1.327(6)	N(31)-C(31)	1.334(6)	C(310)-H(310)	0.93
C(11)-H(11)	0.93	N(22)-C(211)	1.363(6)	N(31)-C(312)	1.358(6)	C(311)-C(312)	1.433(6)
C(12)-C(13)	1.360(7)	C(21)-C(22)	1.400(7)	N(32)-C(310)	1.332(6)	Cl(1)-O(11)	1.396(4)
C(12)-H(12)	0.93	C(21)-H(21)	0.93	N(32)-C(311)	1.359(5)	Cl(1)-O(13)	1.415(4)
C(13)-C(14)	1.400(7)	C(22)-C(23)	1.360(7)	C(31)-C(32)	1.391(6)	Cl(1)-O(14)	1.418(5)
C(13)-H(13)	0.93	C(22)-H(22)	0.93	C(31)-H(31)	0.93	Cl(1)-O(12)	1.443(4)
C(14)-C(112)	1.404(6)	C(23)-C(24)	1.403(7)	C(32)-C(33)	1.365(6)	Cl(2)-O(24)	1.410(4)
C(14)-C(15)	1.431(7)	C(23)-H(23)	0.93	C(32)-H(32)	0.93	Cl(2)-O(23)	1.414(4)
C(15)-C(16)	1.339(7)	C(24)-C(212)	1.403(7)	C(33)-C(34)	1.409(7)	Cl(2)-O(22)	1.427(4)
C(15)-H(15)	0.93	C(24)-C(25)	1.436(7)	C(33)-H(33)	0.93	Cl(2)-O(21)	1.429(4)
C(16)-C(17)	1.437(7)	C(25)-C(26)	1.340(7)	C(34)-C(312)	1.401(6)		
C(16)-H(16)	0.93	C(25)-H(25)	0.93	C(34)-C(36)	1.431(7)		

Bond	Angle [°]	Bond	Angle [°]	Bond	Angle [°]
N(22)-Cu-N(31)	168.60(15)	N(12)-C(111)-C(17)	122.3(4)	C(310)-N(32)-C(311)	118.0(4)
N(22)-Cu-N(12)	91.82(14)	N(12)-C(111)-C(112)	118.9(4)	C(310)-N(32)-Cu	130.1(3)
N(31)-Cu-N(12)	95.96(14)	C(17)-C(111)-C(112)	118.9(4)	C(311)-N(32)-Cu	111.4(3)
N(22)-Cu-N(32)	93.57(14)	N(11)-C(112)-C(14)	122.2(4)	N(31)-C(31)-C(32)	122.5(4)
N(31)-Cu-N(32)	81.54(14)	N(11)-C(112)-C(111)	117.7(4)	N(31)-C(31)-H(31)	118.7
N(12)-Cu-N(32)	161.96(15)	C(14)-C(112)-C(111)	120.2(4)	C(32)-C(31)-H(31)	118.7
N(22)-Cu-N(21)	77.82(15)	C(21)-N(21)-C(212)	117.9(4)	C(33)-C(32)-C(31)	119.7(4)
N(31)-Cu-N(21)	92.23(14)	C(21)-N(21)-Cu	132.3(3)	C(33)-C(32)-H(32)	120.1
N(12)-Cu-N(21)	103.42(14)	C(212)-N(21)-Cu	109.0(3)	C(31)-C(32)-H(32)	120.1
N(32)-Cu-N(21)	94.55(13)	C(210)-N(22)-C(211)	118.5(4)	C(32)-C(33)-C(34)	119.6(4)
N(22)-Cu-N(11)	103.03(14)	C(210)-N(22)-Cu	124.3(3)	C(32)-C(33)-H(33)	120.2
N(31)-Cu-N(11)	86.96(13)	C(211)-N(22)-Cu	117.1(3)	C(34)-C(33)-H(33)	120.2
N(12)-Cu-N(11)	76.10(14)	N(21)-C(21)-C(22)	123.2(4)	C(312)-C(34)-C(33)	116.9(4)
N(32)-Cu-N(11)	85.91(13)	N(21)-C(21)-H(21)	118.4	C(312)-C(34)-C(36)	118.9(4)
N(21)-Cu-N(11)	179.01(13)	C(22)-C(21)-H(21)	118.4	C(33)-C(34)-C(36)	124.3(4)
C(11)-N(11)-C(112)	118.2(4)	C(23)-C(22)-C(21)	119.2(5)	C(36)-C(35)-C(37)	121.3(4)
C(11)-N(11)-Cu	133.2(3)	C(23)-C(22)-H(22)	120.4	C(36)-C(35)-H(35)	119.4
C(112)-N(11)-Cu	107.9(3)	C(21)-C(22)-H(22)	120.4	C(37)-C(35)-H(35)	119.4
C(110)-N(12)-C(111)	118.7(4)	C(22)-C(23)-C(24)	119.5(5)	C(35)-C(36)-C(34)	121.2(4)
C(110)-N(12)-Cu	122.5(3)	C(22)-C(23)-H(23)	120.3	C(35)-C(36)-H(36)	119.4
C(111)-N(12)-Cu	118.8(3)	C(24)-C(23)-H(23)	120.3	C(34)-C(36)-H(36)	119.4
N(11)-C(11)-C(12)	123.2(4)	C(212)-C(24)-C(23)	117.4(4)	C(311)-C(37)-C(38)	116.6(4)
N(11)-C(11)-H(11)	118.4	C(212)-C(24)-C(25)	119.0(5)	C(311)-C(37)-C(35)	118.9(4)
C(12)-C(11)-H(11)	118.4	C(23)-C(24)-C(25)	123.6(5)	C(38)-C(37)-C(35)	124.5(4)
C(13)-C(12)-C(11)	118.7(5)	C(26)-C(25)-C(24)	121.5(5)	C(39)-C(38)-C(37)	120.3(4)
C(13)-C(12)-H(12)	120.7	C(26)-C(25)-H(25)	119.2	C(39)-C(38)-H(38)	119.9
C(11)-C(12)-H(12)	120.7	C(24)-C(25)-H(25)	119.2	C(37)-C(38)-H(38)	119.9
C(12)-C(13)-C(14)	120.3(5)	C(25)-C(26)-C(27)	121.3(5)	C(38)-C(39)-C(310)	119.4(4)
C(12)-C(13)-H(13)	119.9	C(25)-C(26)-H(26)	119.4	C(38)-C(39)-H(39)	120.3
C(14)-C(13)-H(13)	119.9	C(27)-C(26)-H(26)	119.4	C(310)-C(39)-H(39)	120.3
C(13)-C(14)-C(112)	117.4(4)	C(28)-C(27)-C(211)	117.3(5)	N(32)-C(310)-C(39)	122.7(4)
C(13)-C(14)-C(15)	123.4(5)	C(28)-C(27)-C(26)	123.9(5)	N(32)-C(310)-H(310)	118.7
C(112)-C(14)-C(15)	119.2(5)	C(211)-C(27)-C(26)	118.7(5)	C(39)-C(310)-H(310)	118.7
C(16)-C(15)-C(14)	120.9(5)	C(29)-C(28)-C(27)	119.9(5)	N(32)-C(311)-C(37)	123.0(4)
C(16)-C(15)-H(15)	119.5	C(29)-C(28)-H(28)	120.1	N(32)-C(311)-C(312)	117.0(4)
C(14)-C(15)-H(15)	119.5	C(27)-C(28)-H(28)	120.1	C(37)-C(311)-C(312)	119.9(4)
C(15)-C(16)-C(17)	121.5(5)	C(28)-C(29)-C(210)	119.1(5)	N(31)-C(312)-C(34)	123.2(4)
C(15)-C(16)-H(16)	119.3	C(28)-C(29)-H(29)	120.5	N(31)-C(312)-C(311)	117.0(4)
C(17)-C(16)-H(16)	119.3	C(210)-C(29)-H(29)	120.5	C(34)-C(312)-C(311)	119.8(4)
C(18)-C(17)-C(111)	117.5(5)	N(22)-C(210)-C(29)	123.2(5)	O(11)-Cl(1)-O(13)	111.8(3)
C(18)-C(17)-C(16)	123.2(5)	N(22)-C(210)-H(210)	118.4	O(11)-Cl(1)-O(14)	110.4(3)

Table S30. Cont.

C(111)-C(17)-C(16)	119.3(5)	C(29)-C(210)-H(210)	118.4	O(13)-Cl(1)-O(14)	108.4(3)
C(19)-C(18)-C(17)	120.0(5)	N(22)-C(211)-C(27)	122.0(5)	O(11)-Cl(1)-O(12)	111.1(3)
C(19)-C(18)-H(18)	120	N(22)-C(211)-C(212)	118.3(4)	O(13)-Cl(1)-O(12)	110.1(3)
C(17)-C(18)-H(18)	120	C(27)-C(211)-C(212)	119.7(4)	O(14)-Cl(1)-O(12)	104.8(3)
C(18)-C(19)-C(110)	119.3(5)	N(21)-C(212)-C(24)	122.8(4)	O(24)-Cl(2)-O(23)	110.3(3)
C(18)-C(19)-H(19)	120.3	N(21)-C(212)-C(211)	117.5(4)	O(24)-Cl(2)-O(22)	108.6(3)
C(110)-C(19)-H(19)	120.3	C(24)-C(212)-C(211)	119.7(4)	O(23)-Cl(2)-O(22)	107.6(3)
N(12)-C(110)-C(19)	122.2(5)	C(31)-N(31)-C(312)	117.9(4)	O(24)-Cl(2)-O(21)	110.9(3)
N(12)-C(110)-H(110)	118.9	C(31)-N(31)-Cu	129.8(3)	O(23)-Cl(2)-O(21)	111.4(3)
C(19)-C(110)-H(110)	118.9	C(312)-N(31)-Cu	112.2(3)	O(22)-Cl(2)-O(21)	108.0(2)

Table S31. Anisotropic displacement parameters ($Å^2 \times 10^3$)for $[Cu(phen)_3]ClO_4)_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Atom	**U^{11}**	**U^{22}**	**U^{33}**	**U^{23}**	**U^{13}**	**U^{12}**	**Atom**	**U^{11}**	**U^{22}**	**U^{33}**	**U^{23}**	**U^{13}**	**U^{12}**
Cu	31(1)	28(1)	24(1)	1(1)	7(1)	-1(1)	C(211)	33(3)	27(3)	23(3)	-3(2)	2(2)	-1(2)
N(11)	23(3)	33(3)	28(2)	-1(2)	6(2)	-1(2)	C(212)	26(3)	25(3)	24(3)	-4(2)	0(2)	-7(2)
N(12)	25(3)	35(2)	25(2)	-1(2)	4(2)	-3(2)	N(31)	16(2)	25(2)	32(2)	1(2)	4(2)	1(2)
C(11)	30(3)	34(3)	34(3)	1(2)	12(3)	-3(3)	N(32)	25(2)	27(2)	26(2)	4(2)	8(2)	3(2)
C(12)	27(3)	49(4)	36(3)	-7(3)	11(3)	0(3)	C(31)	21(3)	25(3)	38(3)	2(2)	6(2)	-2(2)
C(13)	28(3)	52(4)	36(3)	-1(3)	10(3)	7(3)	C(32)	29(3)	33(3)	39(3)	10(3)	15(2)	2(2)
C(14)	35(4)	34(3)	32(3)	0(2)	17(3)	6(3)	C(33)	33(3)	40(3)	27(3)	5(3)	12(2)	5(3)
C(15)	47(4)	40(3)	42(3)	-1(3)	15(3)	11(3)	C(34)	24(3)	33(3)	33(3)	4(2)	10(2)	1(2)
C(16)	60(4)	34(3)	43(3)	-6(3)	26(3)	4(3)	C(35)	40(3)	40(3)	33(3)	-8(2)	7(3)	-9(3)
C(17)	39(4)	32(3)	26(3)	-3(2)	15(3)	-3(3)	C(36)	48(4)	44(3)	25(3)	-4(3)	11(3)	-5(3)
C(18)	53(4)	40(3)	37(3)	-8(3)	23(3)	-11(3)	C(37)	24(3)	24(3)	30(3)	1(2)	7(2)	1(2)
C(19)	44(4)	50(4)	37(3)	-14(3)	19(3)	-22(3)	C(38)	32(3)	24(3)	38(3)	-6(2)	6(2)	-4(2)
C(110)	34(4)	48(4)	31(3)	0(2)	11(3)	-5(3)	C(39)	34(3)	27(3)	38(3)	4(2)	12(2)	-4(2)
C(111)	31(3)	33(3)	22(3)	-3(2)	12(2)	-5(3)	C(310)	31(3)	29(3)	31(3)	7(2)	11(2)	6(2)
C(112)	30(3)	30(3)	24(3)	-1(2)	11(2)	0(2)	C(311)	19(3)	27(3)	29(3)	3(2)	6(2)	3(2)
N(21)	33(3)	28(2)	27(2)	-1(2)	7(2)	-4(2)	C(312)	17(3)	27(3)	27(3)	4(2)	7(2)	5(2)
N(22)	31(3)	32(2)	26(2)	-1(2)	7(2)	0(2)	Cl(1)	41(1)	46(1)	33(1)	3(1)	13(1)	2(1)
C(21)	36(3)	43(3)	30(3)	4(2)	12(3)	-2(3)	O(11)	169(5)	94(3)	37(3)	-14(2)	42(3)	-74(3)
C(22)	33(4)	50(3)	45(4)	1(3)	16(3)	2(3)	O(12)	65(3)	82(3)	88(3)	-28(3)	12(3)	-30(3)
C(23)	26(3)	37(3)	43(3)	-1(3)	-1(3)	3(2)	O(13)	128(4)	51(3)	63(3)	7(2)	17(3)	25(3)
C(24)	31(3)	27(3)	30(3)	-2(2)	1(3)	-4(2)	O(14)	72(3)	108(4)	105(4)	34(3)	46(3)	39(3)
C(25)	36(4)	37(3)	34(3)	4(2)	-4(3)	3(3)	Cl(2)	46(1)	36(1)	40(1)	1(1)	18(1)	6(1)
C(26)	55(4)	43(3)	26(3)	5(2)	4(3)	2(3)	O(21)	81(3)	30(2)	66(3)	8(2)	20(2)	-5(2)
C(27)	45(4)	34(3)	24(3)	-2(2)	7(3)	-1(3)	O(22)	49(3)	41(2)	96(3)	12(2)	9(2)	-12(2)
C(28)	59(4)	48(3)	24(3)	0(2)	12(3)	-4(3)	O(23)	34(3)	97(3)	65(3)	17(2)	9(2)	9(2)
C(29)	54(4)	49(3)	34(3)	-2(3)	20(3)	-4(3)	O(24)	194(6)	104(4)	64(3)	26(3)	82(4)	79(4)
C(210)	40(4)	39(3)	36(3)	-7(2)	13(3)	-2(3)							

Table S32. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for $[Cu(phen)_3]ClO_4)_2$.

Atom	**x**	**y**	**z**	**U(eq)**	**Atom**	**x**	**y**	**z**	**U(eq)**	**Atom**	**x**	**y**	**z**	**U(eq)**
H(11)	-3629	1180	4538	49	H(21)	3617	1204	5468	55	H(31)	1459	2066	4518	44
H(12)	-5858	1595	3755	56	H(22)	5875	808	6306	63	H(32)	1190	2118	2683	49
H(13)	-5798	2358	4046	59	H(23)	6430	531	8062	59	H(33)	-150	1574	1455	50
H(15)	-4253	3055	4884	65	H(25)	5576	416	9708	61	H(35)	-2518	240	1849	59
H(16)	-1994	3365	5931	66	H(26)	3758	488	10465	66	H(36)	-1601	821	1144	60
H(18)	849	3276	7035	62	H(28)	1024	731	10267	67	H(38)	-2782	-149	3535	50
H(19)	2927	2809	7770	63	H(29)	-1213	1095	9237	66	H(39)	-2297	-139	5397	50
H(110)	2696	2050	7312	57	H(210)	-1470	1381	7525	58	H(310)	-908	444	6458	46

Turbidimetric evaluation of antimicrobial growth inhibition

Compound abbreviations are defined in Table S1. Error bars of line charts are representative of 1 ± SEM (Figure S10-Figure S14). For all growth inhibitory assays of $\mathbf{1_{Cu}}$-$\mathbf{21_{Cu}}$, $\mathbf{1_{IL}}$-$\mathbf{8_{IL}}$, and $\mathbf{10_{IL}}$ a final concentration of 0.4% DMSO was used. Data not shown in cases where change in turbidity of all compounds tested was considered to be insignificant (< 15% of control). Results are provided as an average of no less than 2 independent tests.

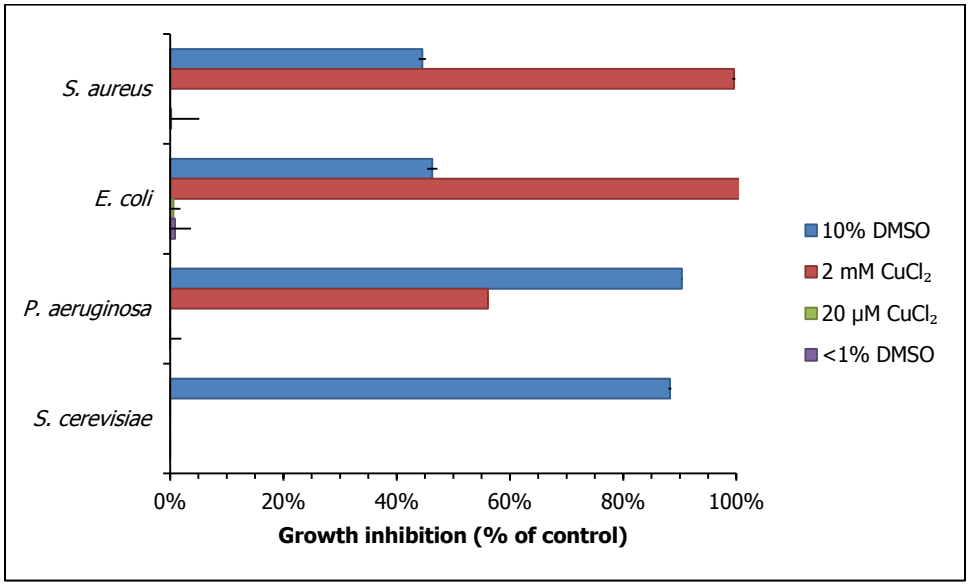
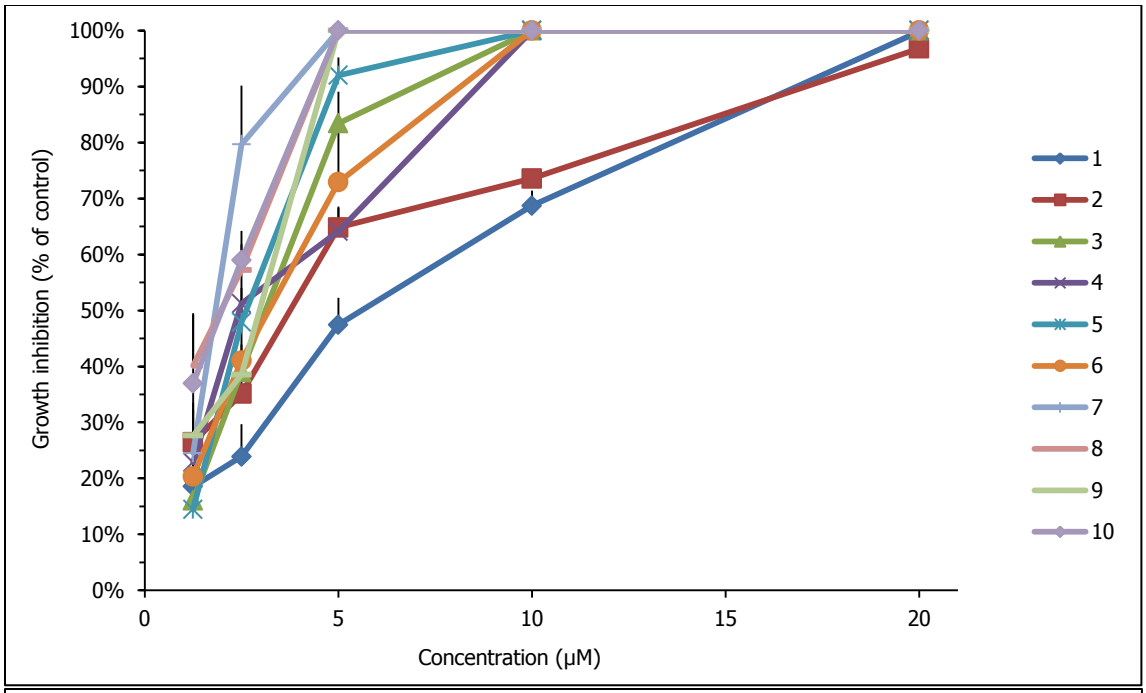


Figure S9. Preliminary DMSO and $CuCl_2$ growth inhibition (final concentrations) of *S. aureus*, *E. coli*, *P. aeruginosa* and *S. cerevisiae*. Tests are representative of a single experiment conducted with duplicate samples (10% DMSO and 2 mM $CuCl_2$), or 4 experiments conducted with triplicate samples (20 µM $CuCl_2$, <1% DMSO). Error bars are representative of 2 ± SEM.



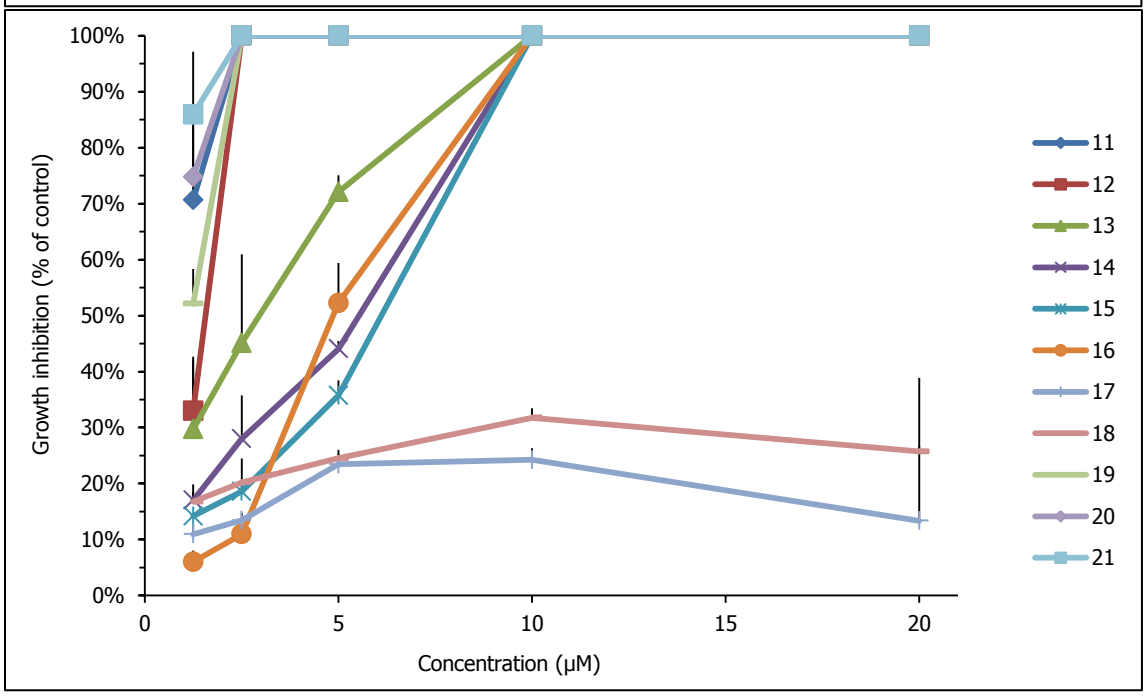
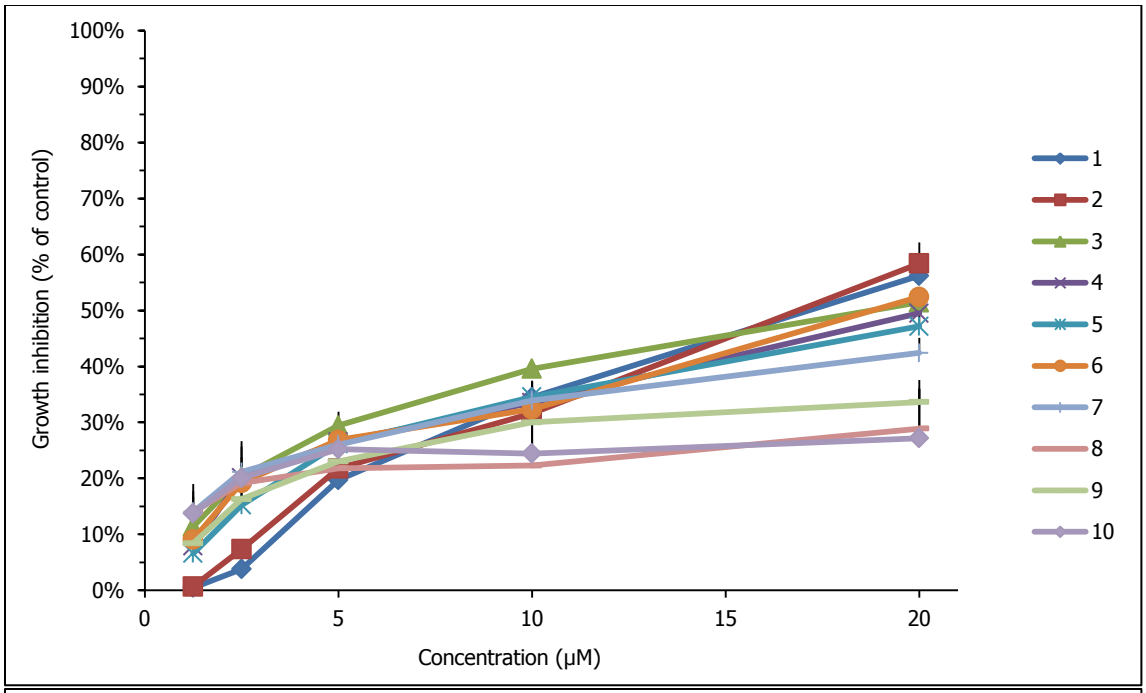


Figure S10. *S. aureus* growth inhibition at various concentrations of $\mathbf{1_{Cu}}$-$\mathbf{21_{Cu}}$.



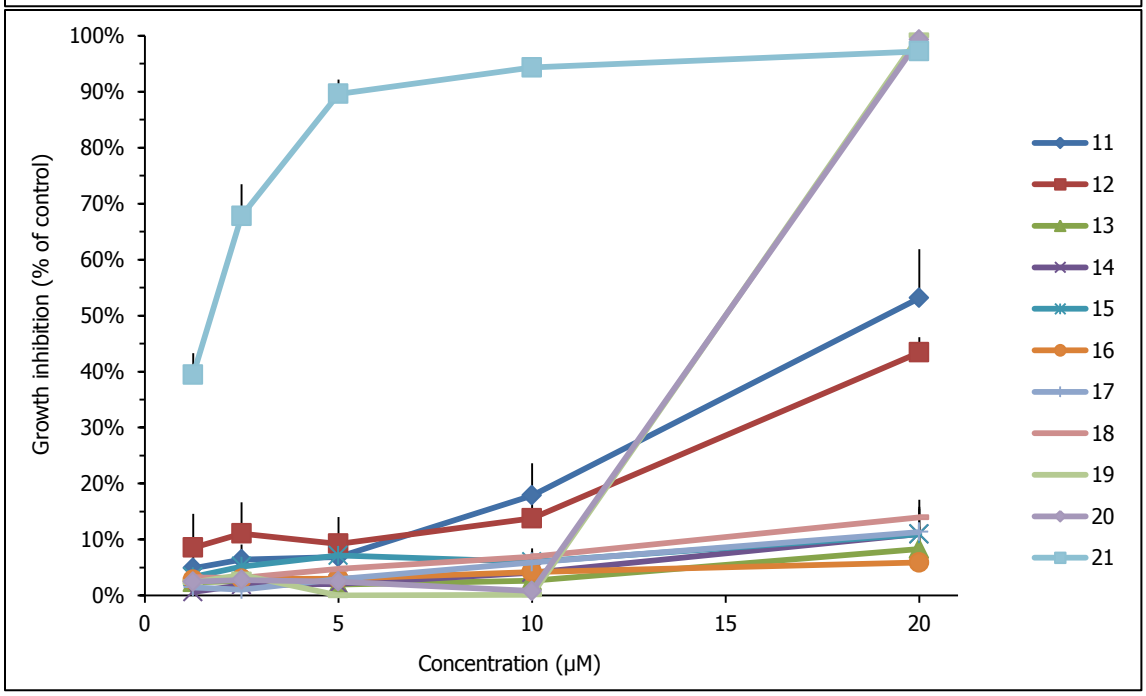


Figure S11. *E. coli* growth inhibition at various concentrations of $\mathbf{1}_{Cu}$-$\mathbf{21}_{Cu}$.

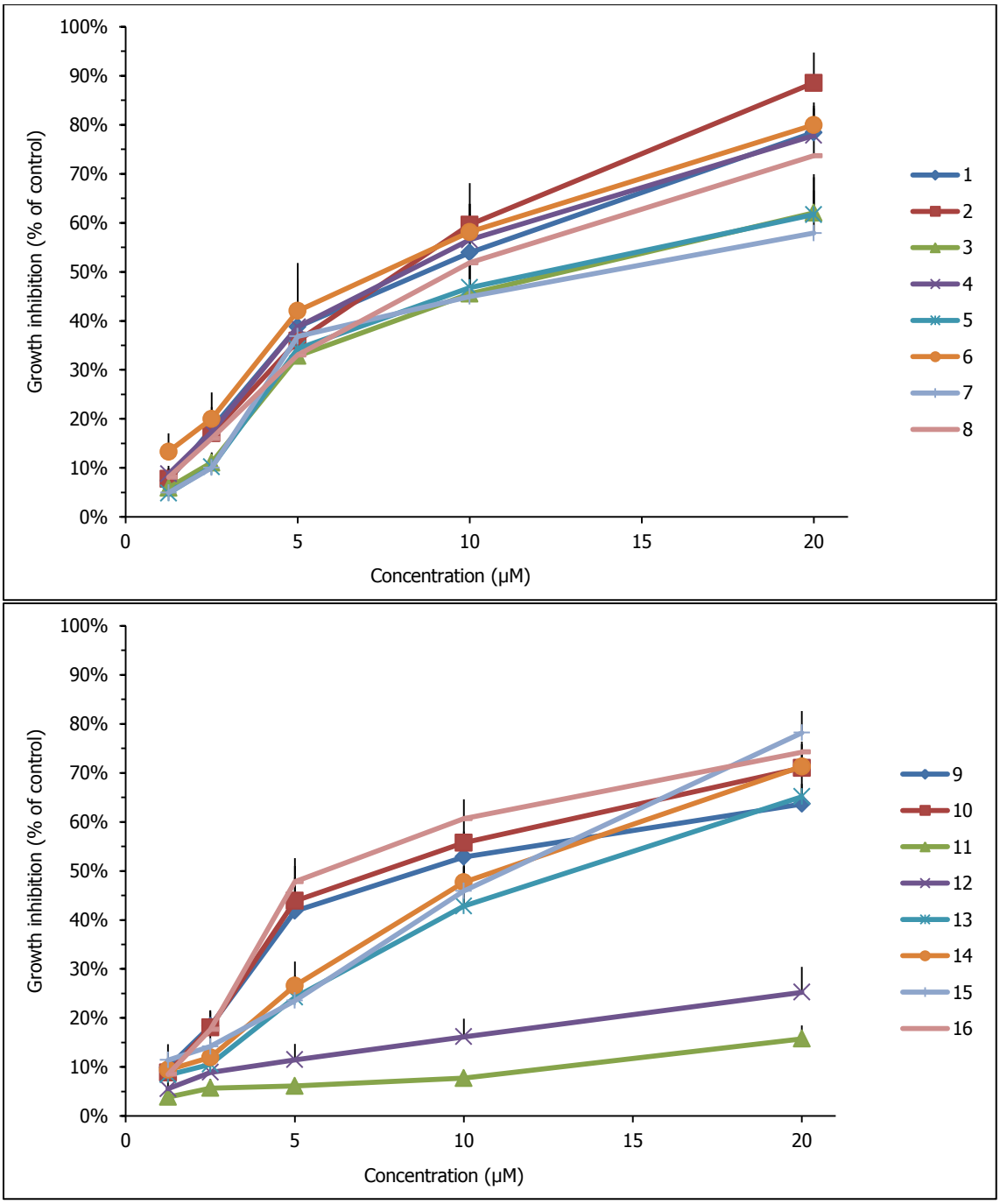


Figure S12. *E. coli* growth inhibition at various concentrations of $\mathbf{1_{Pt}}$-$\mathbf{16_{Pt}}$.

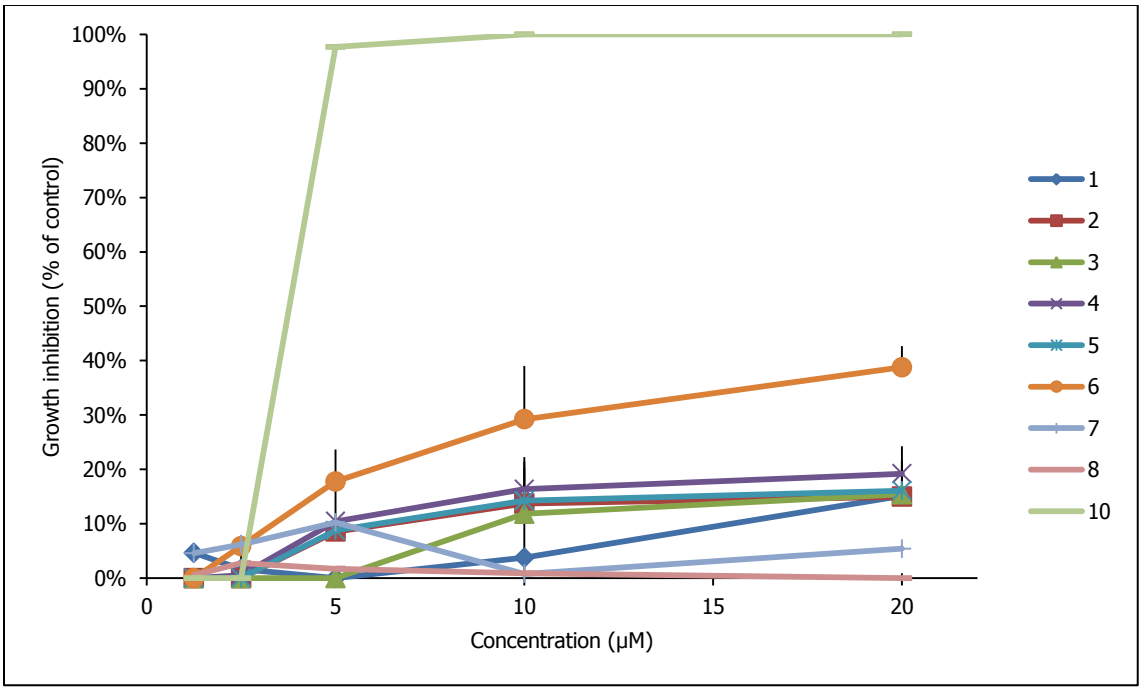


Figure S13. *S. aureus* growth inhibition at various concentrations of $\mathbf{1_{IL}}$-$\mathbf{8_{IL}}$, and$\mathbf{10_{IL}}$.

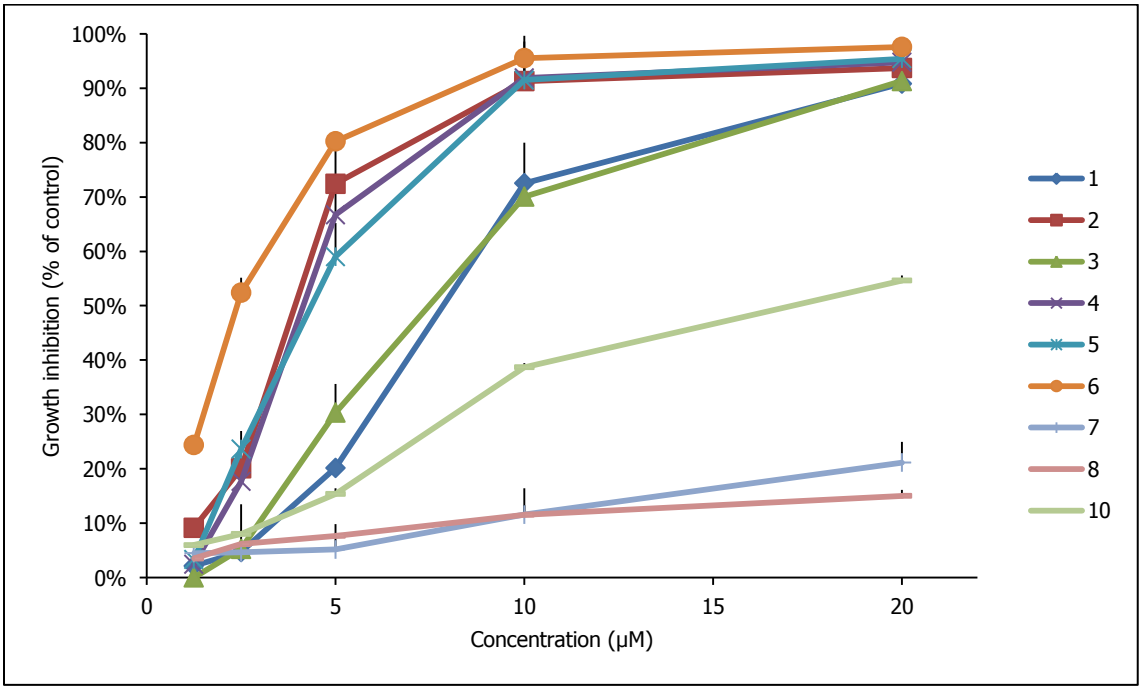


Figure S14. *E. coli* growth inhibition at various concentrations of $\mathbf{1_{IL}}$-$\mathbf{8_{IL}}$, and $\mathbf{10_{IL}}$.

Qualitative inference of membrane permeabilisation by fluorescent dyes

Compound abbreviations are defined in Table S1. In images below, PI emission is represented in the left-most window (>650 nm), SYTO9 fluorescence in the middle window (505-530 nm) and both filters active in the right window. Each image is representative of duplicate samples.

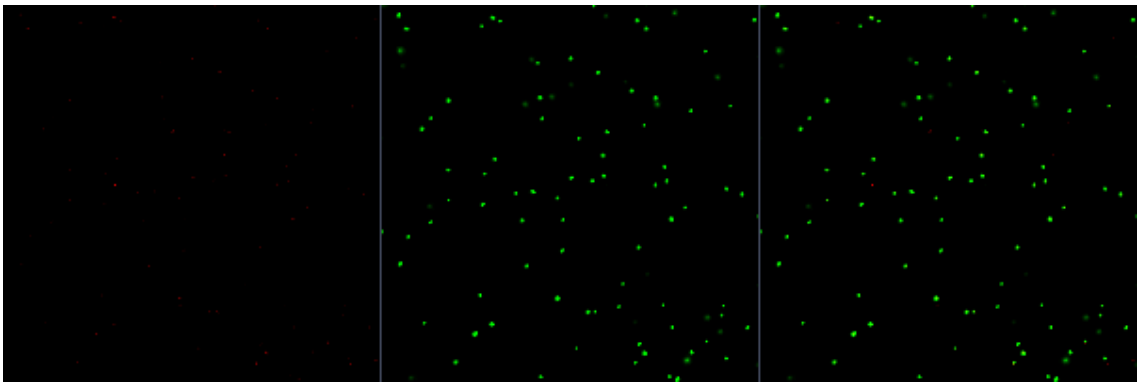


Figure S15. *S. aureus* solvent control (DMSO 0.3%)

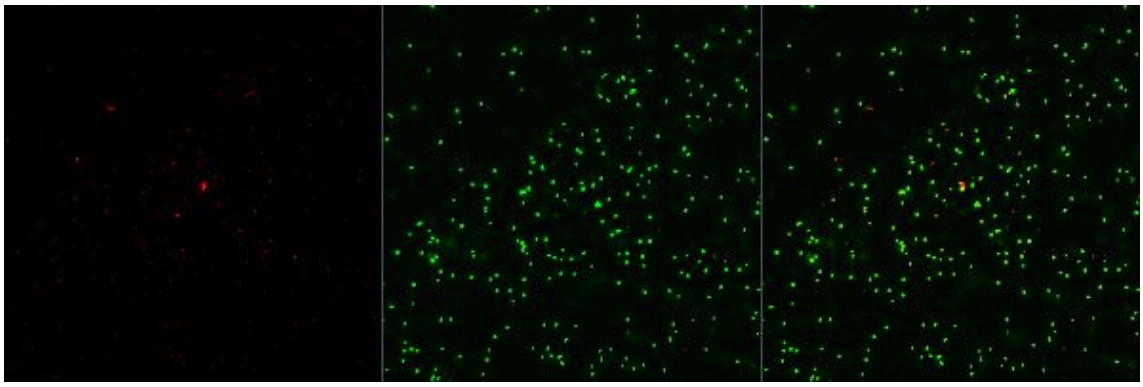


Figure S16. *S. aureus* treated with 15 µM $\mathbf{11_{Cu}}$.

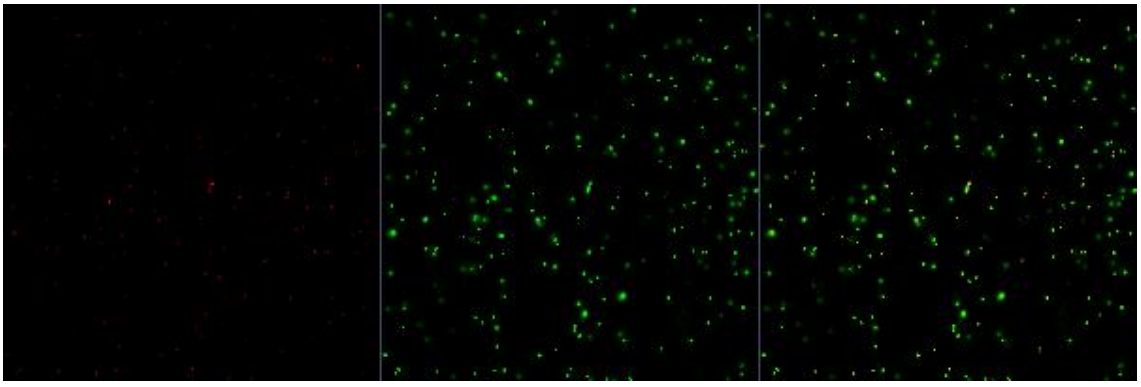


Figure S17. *S. aureus* treated with 15 µM $\mathbf{12_{Cu}}$.

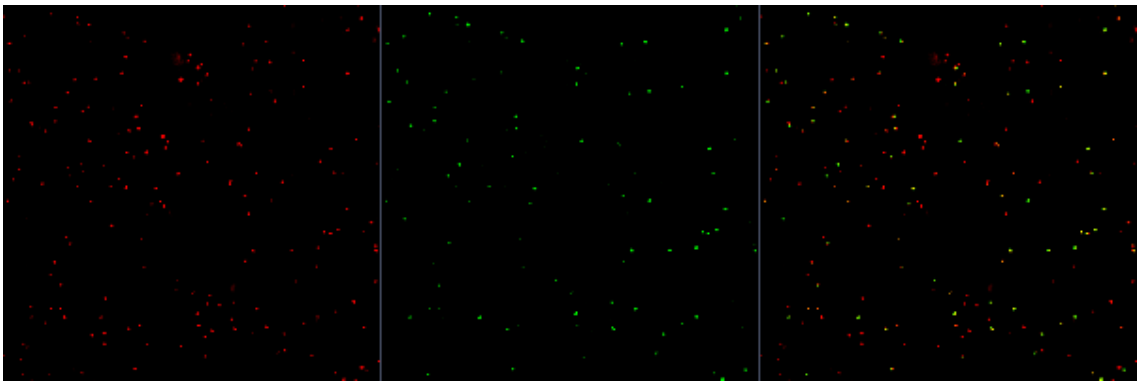


Figure S18. *S. aureus* treated with 15 µM **19$_{Cu}$**.

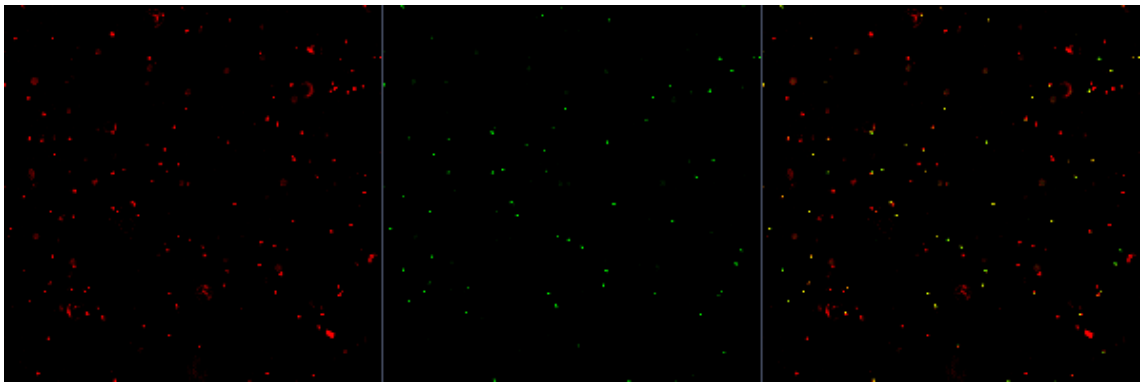


Figure S19. *S. aureus* treated with 15 µM **20$_{Cu}$**.

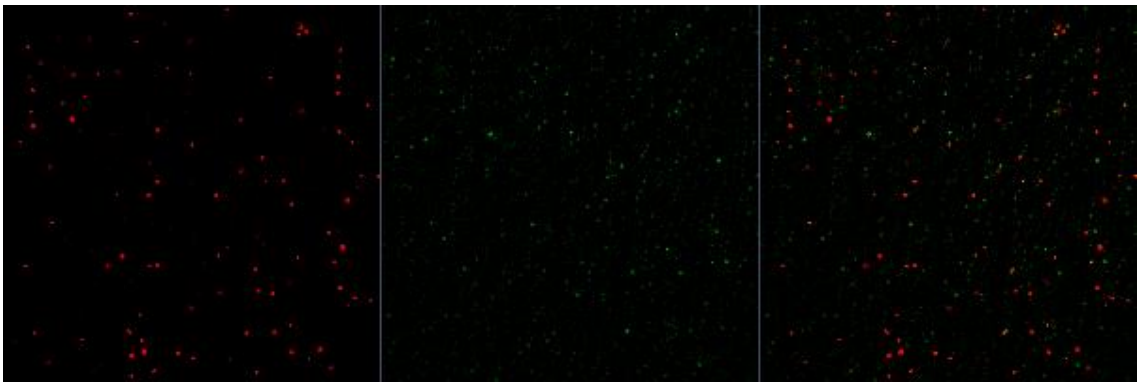


Figure S20. *S. aureus* treated with 15 µM **21$_{Cu}$**.

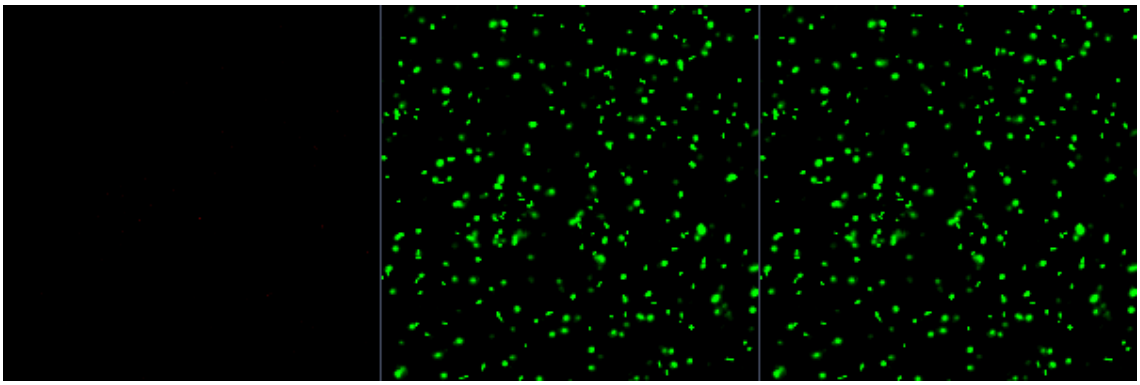


Figure S21. *E. coli* solvent control (H_2O)

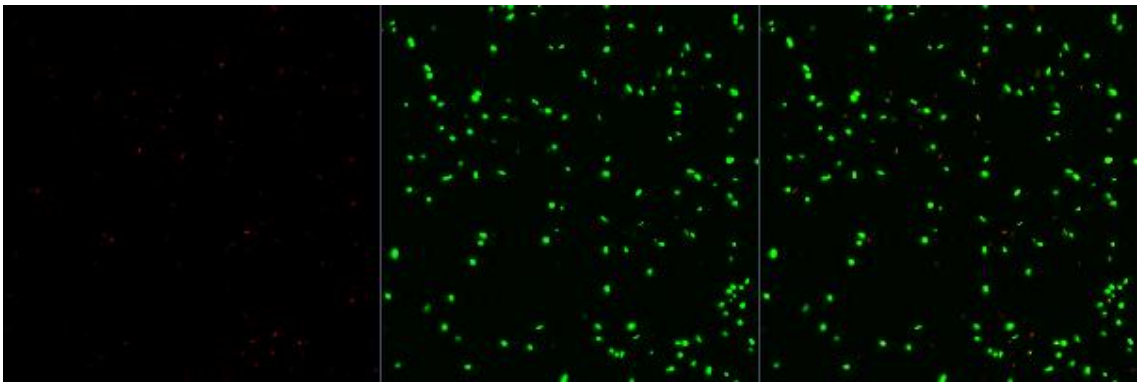


Figure S22. *E. coli* treated with 180 µM $\mathbf{1_{Pt}}$.

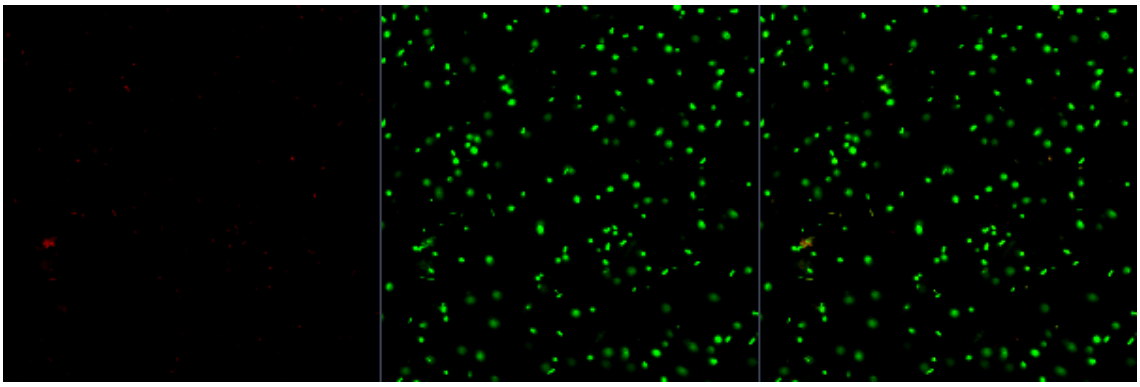


Figure S23. *E. coli* treated with 180 µM $\mathbf{2_{Pt}}$.

References

1. N. J. Wheate, R. I. Taleb, A. M. Krause-Heuer, R. L. Cook, S. Wang, V. J. Higgins and J. R. Aldrich-Wright, *Dalton Trans.*, 2007, 5055-5064.
2. D. M. Fisher, P. J. Bednarski, R. Grünert, P. Turner, R. R. Fenton and J. R. Aldrich-Wright, *ChemMedChem*, 2007, **2**, 488-495.
3. S. Kemp, N. J. Wheate, S. Wang, J. G. Collins, S. F. Ralph, A. I. Day, V. J. Higgins and J. R. Aldrich-Wright, *J. Biol. Inorg. Chem.*, 2007, **12**, 969-979.
4. C. R. Brodie, J. G. Collins and J. R. Aldrich-Wright, *Dalton Trans.*, 2004, 1145-1152.
5. R. M. Silverstein, G. C. Bassler and T. C. Morrill, *Spectrometric Identification of Organic Compounds*, John Wiley & Sons, Inc., Singapore, 1991.
6. A. M. Krause-Heuer, P. Leverett, A. Bolhuis and J. R. Aldrich-Wright, *Aust. J. Chem.*, 2012, **65**, 860-873.
7. O. P. Anderson, *Dalton Trans.*, 1973, 1237-1241.
8. Y. B. Wei and P. Yang, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2004, **60**, m429-m431.