Supplementary Materials: Cu^{II} Complexes and Coordination Polymers with Pyridine or Pyrazine Amides and Amino Benzamides—Structures and EPR Patterns

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contents:

Table S14. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for $(HIna)_2[CuCl_4]\cdot 2H_2O$ (**6**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Table S15. Anisotropic Displacement Parameters (Å²×10³) for $(HIna)_2[CuCl_4]\cdot 2H_2O$ (**6**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Table S16. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for $(HIna)[Cu(H_2O)Cl_3]$ (**7**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Table S17. Anisotropic Displacement Parameters (Å²×10³) for $(HIna)[Cu(H_2O)Cl_3]$ (**7**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Table S18. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for $[Cu(Ina)_2Br_2]$ (**5**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Table S19. Anisotropic Displacement Parameters (Å²×10³) for $^1_\infty[Cu(Ina)_2Br_2]$ (**5**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Table S20. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for $^2_\infty[Cu(Pya)_2](BF_4)_2$ (**9**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Table S21. Anisotropic Displacement Parameters (Å²×10³) for $^2_\infty[Cu(Pya)_2](BF_4)_2$ (**9**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Table S22. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for $[Cu(Pya)_2(H_2O)(NO_3)](NO_3)$ (**10**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Table S23. Anisotropic Displacement Parameters (Å²×10³) for $[Cu(Pya)_2(H_2O)(NO_3)](NO_3)$ (**10**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Table S24. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for $^1_\infty[Cu(Pya)(NO_3)_2]$ (**11**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Table S25. Anisotropic Displacement Parameters (Å²×10³) for $^1_\infty[Cu(Pya)(NO_3)_2]$ (**11**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Table S26. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for $^2_\infty[Cu(Pyc)(Tfa)]$ (**12**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Table S27. Anisotropic Displacement Parameters (Å²×10³) for $^2_\infty[Cu(Pyc)(Tfa)]$ (**12**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Table S28. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for $[Cu(2\text{-}Aba)_2(NO_3)_2]$ (**13**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Table S29. Anisotropic Displacement Parameters (Å²×10³) for $[Cu(_2\text{-}Aba)_2(NO_3)_2]$ (**13**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Table S30. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for $^1_\infty[Cu_2(4\text{-}Aba)_2(H_2O)_3(NO_3)_3](NO_3)$ (**14**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Table S31. Anisotropic Displacement Parameters (Å²×10³) for $^1_\infty[Cu_2(4\text{-}Aba)_2(H_2O)_3(NO_3)_3](NO_3)$ (**14**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Table S32. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for $^2_\infty[Cu(4\text{-}Aba)_2(EtOH)_2](ClO_4)_2$ (**15**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Table S33. Anisotropic Displacement Parameters (Å²×10³) for $^2_\infty[Cu(4\text{-}Aba)_2(EtOH)_2](ClO_4)_2$ (**15**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Table S34. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for $^2_\infty[Cu(4\text{-}Aba)_2(EtOH)_2](BF_4)_2$ (**16**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Table S35. Anisotropic Displacement Parameters (Å²×10³) for $^2_\infty[Cu(4\text{-}Aba)_2(EtOH)_2](BF_4)_2$ (**16**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Table S36. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for $[Cu(4\text{-}HAba)_2Cl_4]$ (**17**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Table S37. Anisotropic Displacement Parameters (Å²×10³) for $[Cu(4\text{-}HAba)_2Cl_4]$ (**17**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Table S38. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for [Cu(Tba)$_2$](ClO$_4$)$_2$ (**18**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.
Table S39. Anisotropic Displacement Parameters (Å^2×10^3) for [Cu(Tba)$_2$](ClO$_4$)$_2$ (**18**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.
Supplementary experimental information

Synthesis of picolinamide and nicotinamide – general description
12.31 g (100 mmol) of the acid were dissolved in 20 mL (12.20 g, 100 mmol) freshly distilled thionyl chloride ($SOCl_2$) and stirred at 80°C for 2 h. After removing all volatiles, the sticky residue was dissolved/suspended in 50 mL MeOH and heated to 80°C for 1 h. After cooling, all volatiles were evaporated and the residue treated with saturated aqueous Na_2CO_3 solution to achieve a pH of 6. The aqueous solution was extracted using ethyl acetate (3 x 100 mL), the organic phase was dried using $MgSO_4$. Evaporation of the volatiles allowed isolating the methyl esters. The esters were mixed with 20 mL of concentrated aqueous NH_3 solution and stirred for 2 h. The colourless precipitates were filtered off, washed subsequently with cold H_2O, EtOH and diethyl ether and dried in vacuo.
Picolinamide. Starting from picolinic acid, the first step yielded 11.54 g (84 mmol, 84%) yellowish methyl picolinate. The amination reaction gave 6.5 g (52.8 mmol, 52.8%) colourless solid. M: 122.12 g/mol; $C_6H_6N_2O$. Elemental analysis (%), found, (calculated): C 58.88 (59.01); H 5.01 (4.95); N 22.90 (22.94). ^{1}H NMR (300 MHz, DMSO-d$_6$): δ (ppm) = 8.08 (d, 1H, H3), 7.98 (t, 1H, H4), 7.60 (t, 1H, H5), 8.65 (d, 1H, H6), 8.16 (s, 1H, NH), 7.69 (s, 1H, NH'). ^{13}C NMR (75 MHz, DMSO-d$_6$): δ (ppm) = 122.3 (C3), 126.9 (C5), 138.1 (C4), 148.9 (C6), 150.8 (C7), 166.5 (C5).
Nicotinamide. Starting from nicotinic acid, the first reaction yielded 12.22 g (89 mmol, 89%) colourless methyl nicotinate. The second reaction gave 10.1 g (74 mmol, 74%) of a colourless solid. M: 122.12 g/mol; $C_6H_6N_2O$. Elemental analysis (%), found, (calculated): C 58.97 (59.01); H 5.02 (4.95); N 22.91 (22.94). ^{1}H NMR (300 MHz, DMSO-d$_6$): δ (ppm) = 7.52 (t, 1H, H5), 7.66 (s, 1H, NH), 8.20 (s, 1H, NH'), 8.24 (d, 1H, H4), 8.73 (d, 1H, H6), 9.08 (s, 1H, H2). ^{13}C NMR (75 MHz, DMSO-d$_6$): δ (ppm) = 123.8 (C5), 130.1 (C3), 135.6 (C4), 149.1 (C2), 152.3 (C6), 166.9 (C5).

Supplementary Figures

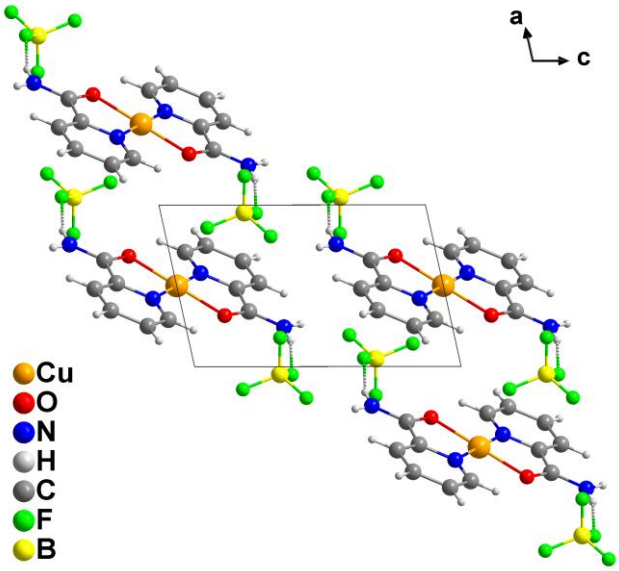

Figure S1. Crystal structure of [Cu(Pia)$_2$(BF$_4$)$_2$] (**8**) viewed along the *b* axis.

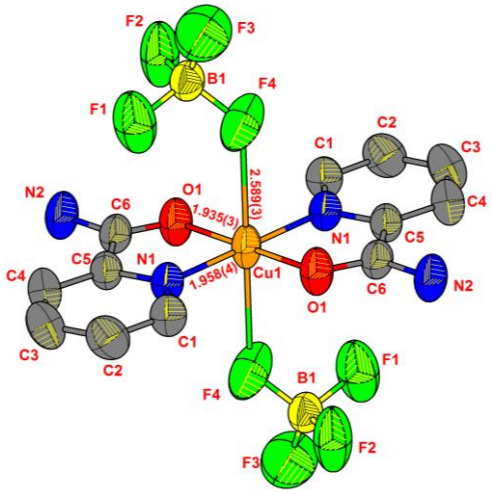

Figure S2. Molecular structure of $[Cu(Pia)_2(BF_4)_2]$ (**8**) at 50% probability level; protons were omitted for clarity, distances in Å.

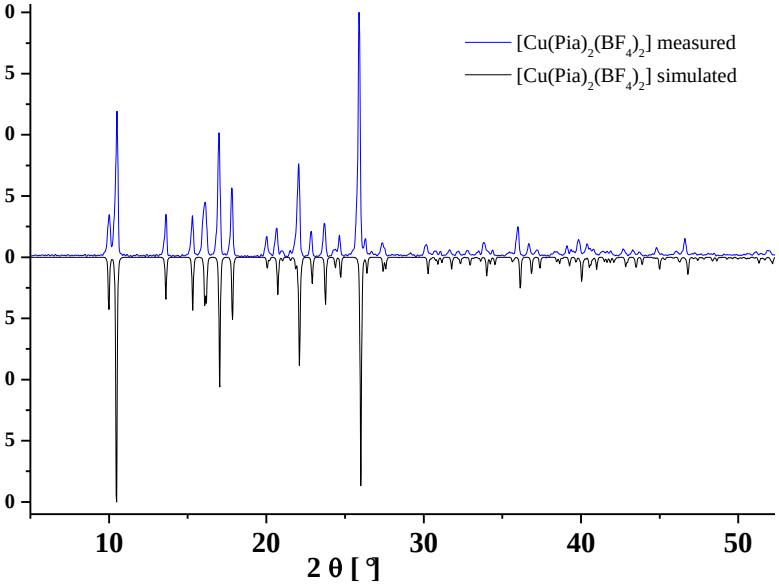

Figure S3. Powder XRD of $[Cu(Pia)_2(BF_4)_2]$ (**8**).

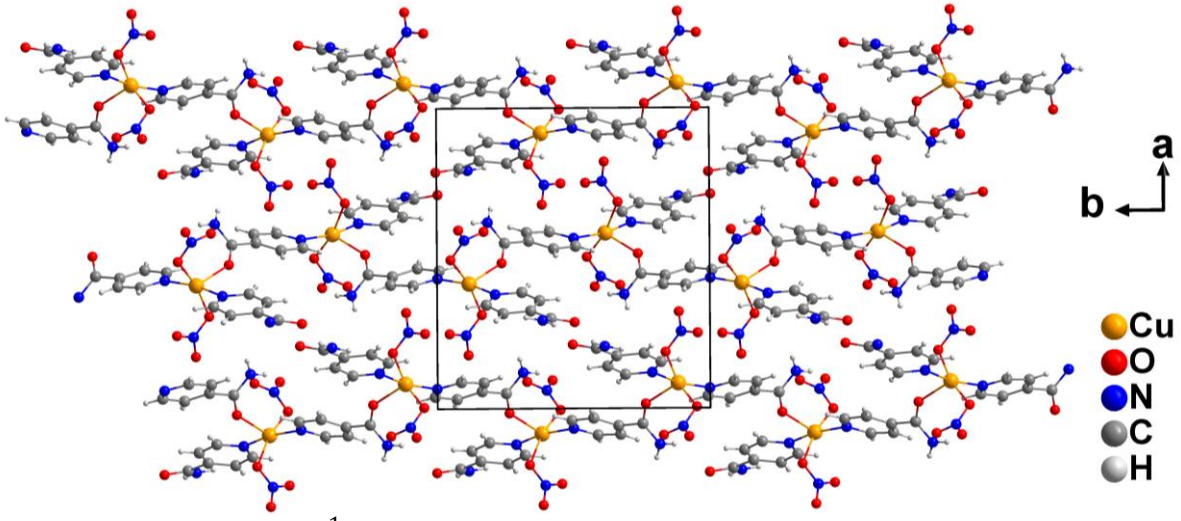

Figure S4. Crystal structure of $^{1}_{\infty}[Cu(Ina)_2(NO_3)_2]$ (**2**) viewed along the *c* axis.

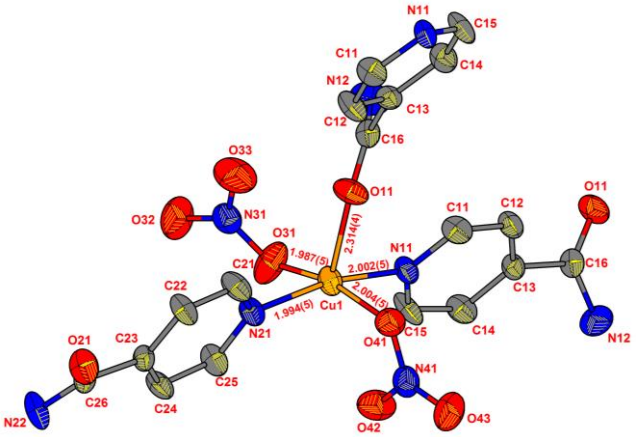

Figure S5. Molecular entity in the structure of $^{1}_{\infty}[Cu(Ina)_2(NO_3)_2]$ (**2**) at 50% probability level; protons were omitted for clarity, distances in Å.

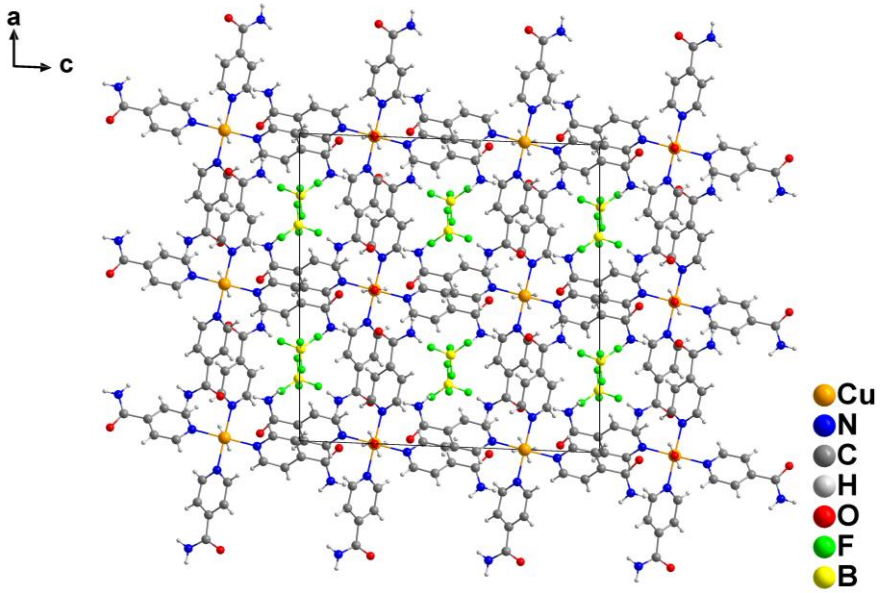

Figure S6. Crystal structure of $[Cu(Ina)_4(H_2O)_2](BF_4)_2$ (**1**) viewed along the *b* axis.

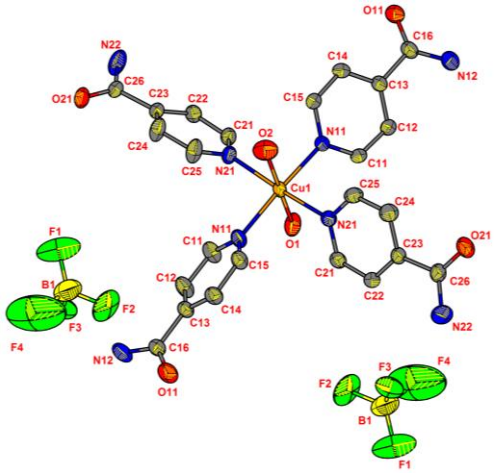

Figure S7. Molecular structure of $[Cu(Ina)_4(H_2O)_2](BF_4)_2$ (**1**) at 50% probability level; protons were omitted for clarity.

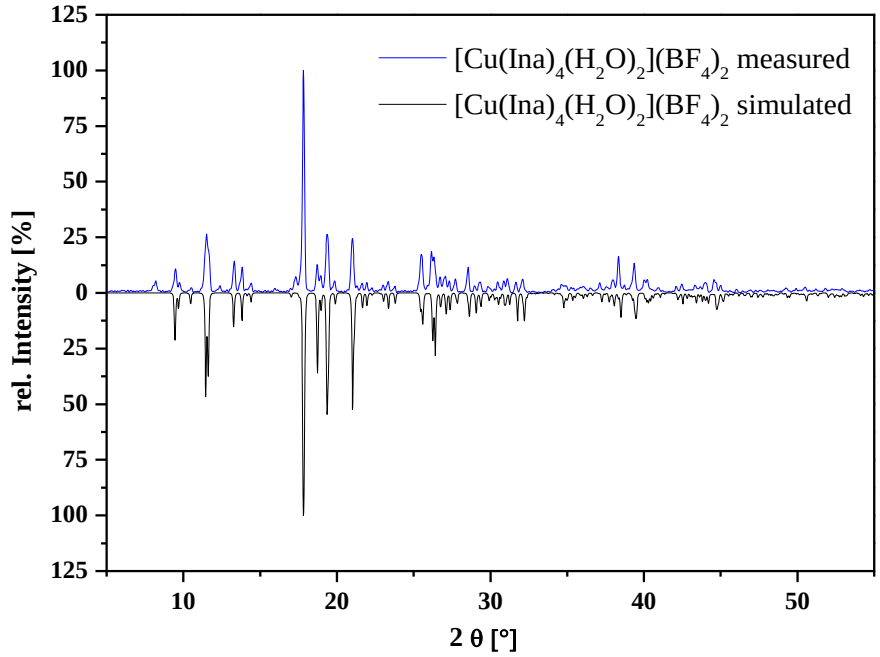

Figure S8. Powder XRD of $[Cu(Ina)_4(H_2O)_2](BF_4)_2$ (**1**).

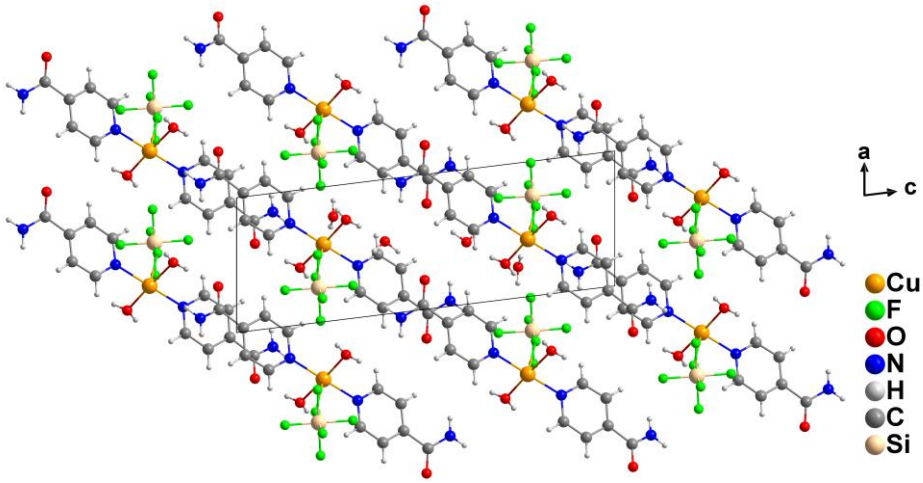

Figure S9. Crystal structure of $[Cu(Ina)_2(H_2O)_3(SiF_6)]\cdot H_2O$ (**4**) viewed along the *b* axis.

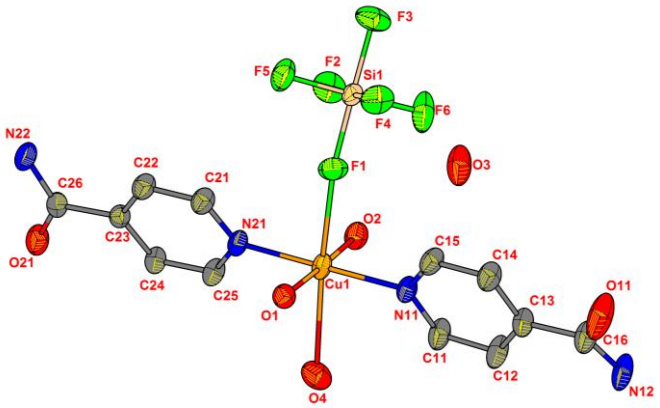

Figure S10. Molecular structure of $[Cu(Ina)_2(H_2O)_3(SiF_6)]\cdot H_2O$ (**4**) at 50% probability level; protons were omitted for clarity.

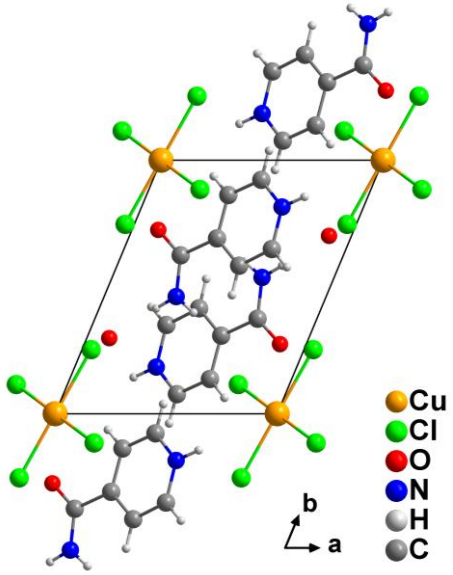

Figure S11. Crystal structure of $(HIna)_2[CuCl_4]\cdot 2H_2O$ (**6**) viewed along the *c* axis.

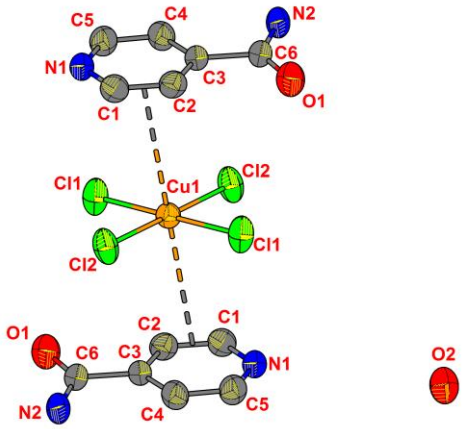

Figure S12. Molecular structure of $(HIna)_2[CuCl_4]\cdot 2H_2O$ (**6**) at 50% probability level.

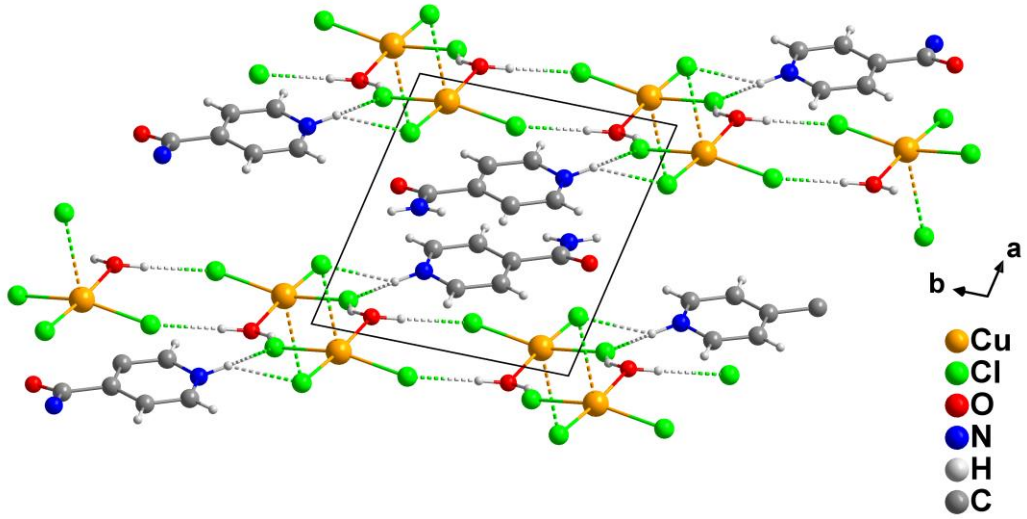

Figure S13. Crystal structure of $(HIna)[Cu(H_2O)Cl_3]$ (**7**) viewed along the *c* axis.

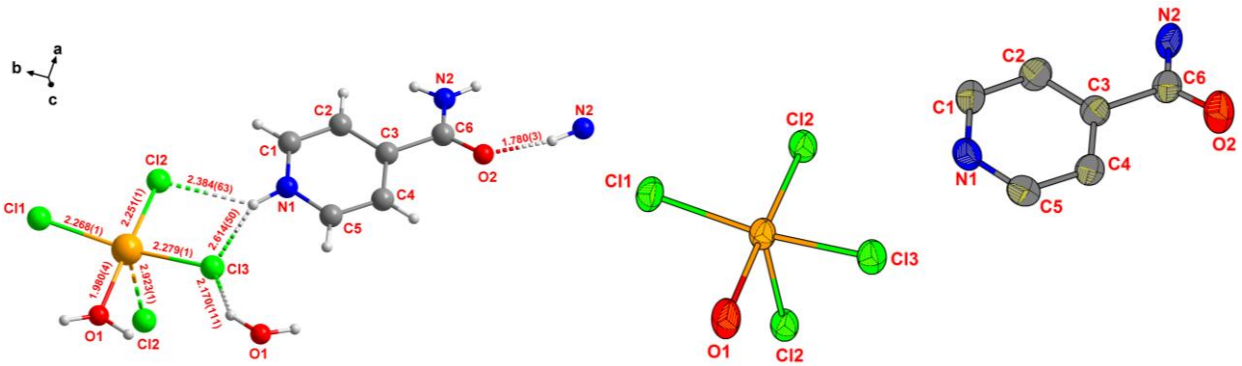

Figure S14. Molecular structure of (HIna)[Cu(H$_2$O)Cl$_3$] (**7**) at 50% probability level, distances in Å.

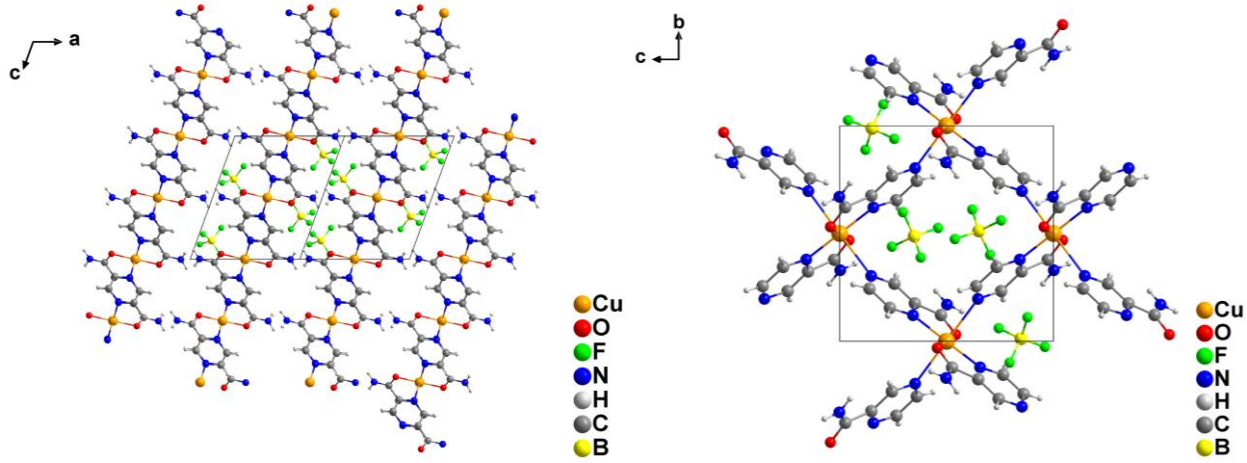

Figure S15. Crystal structure of $^{2}_{\infty}$[Cu(Pya)$_2$](BF$_4$)$_2$ (**9**) viewed along the *b* axis (left) and along the *a* axis (right).

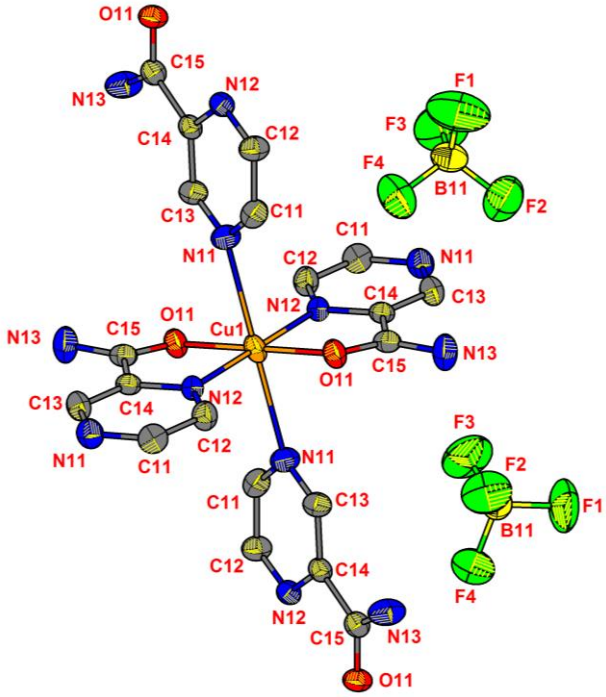

Figure S16. Molecular structure of $^{2}_{\infty}$[Cu(Pya)$_2$](BF$_4$)$_2$ (**9**) at 50% probability level; protons were omitted for clarity.

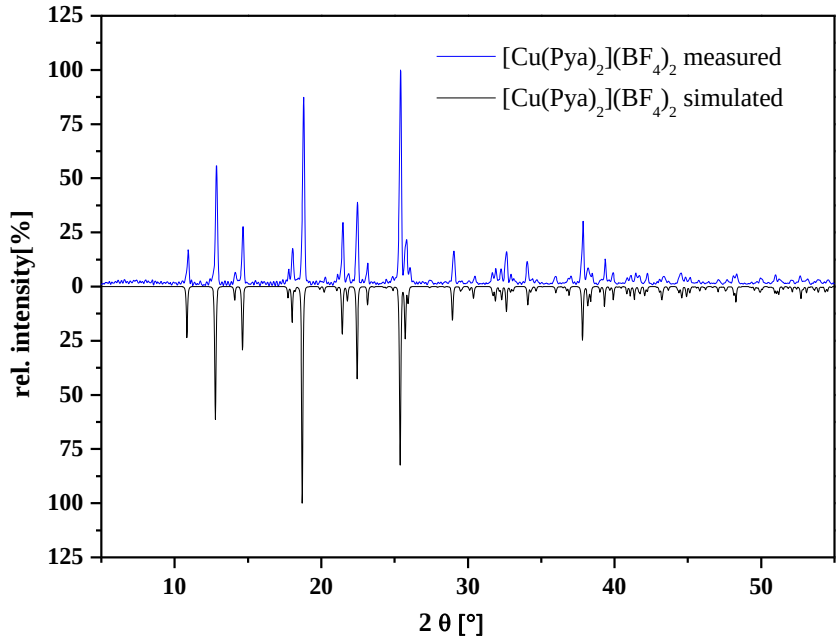

Figure S17. Powder XRD of $^{2}_{\infty}$[Cu(Pya)$_2$](BF$_4$)$_2$ (**9**).

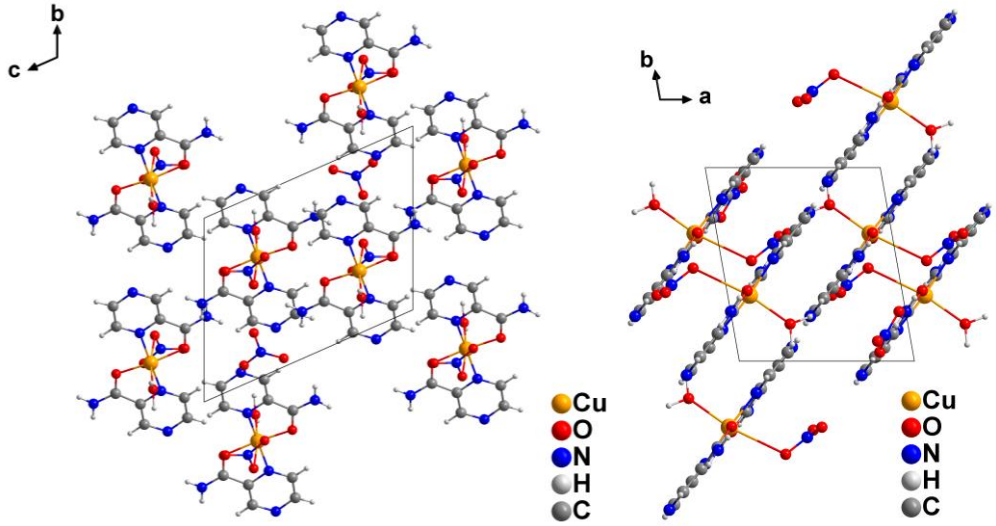

Figure S18. Crystal structure of [Cu(Pya)$_2$(H$_2$O)(NO$_3$)](NO$_3$) (**10**) viewed along the *a* axis (left) and *c* axes (right).

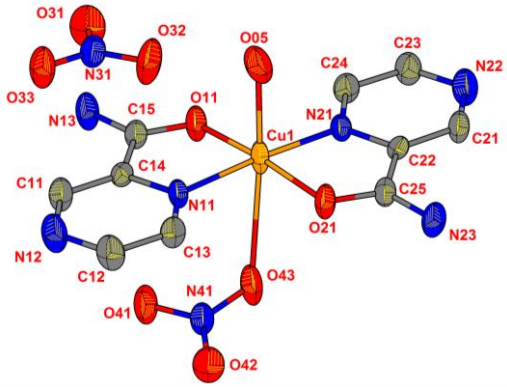

Figure S19. Molecular structure of [Cu(Pya)$_2$(H$_2$O)(NO$_3$)](NO$_3$) (**10**) at 50% probability level; protons were omitted for clarity.

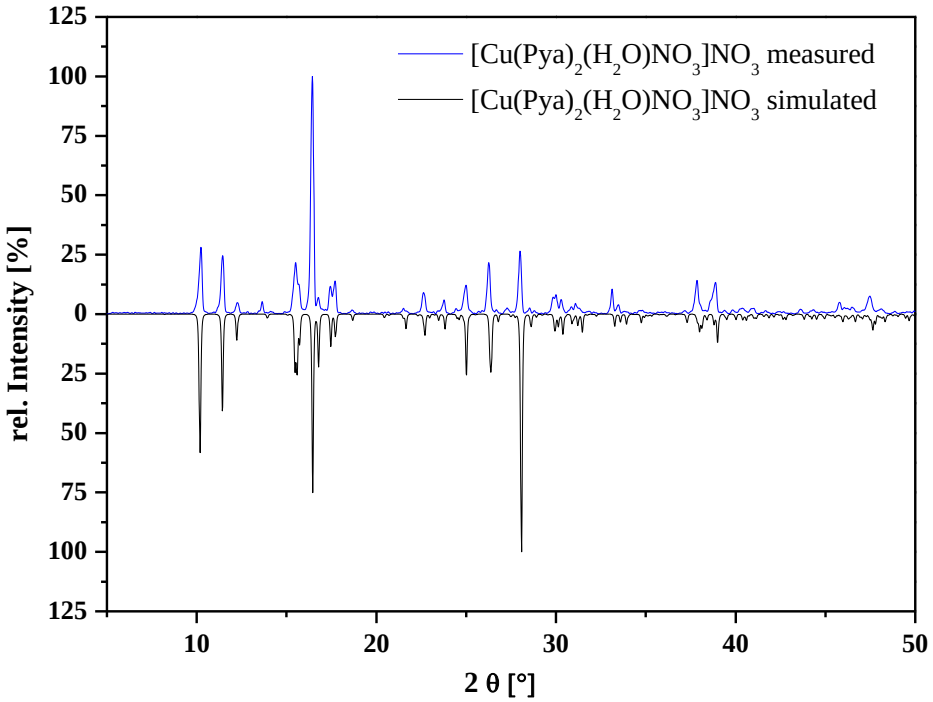

Figure S20. Powder XRD of $[Cu(Pya)_2(H_2O)(NO_3)](NO_3)$ (**10**).

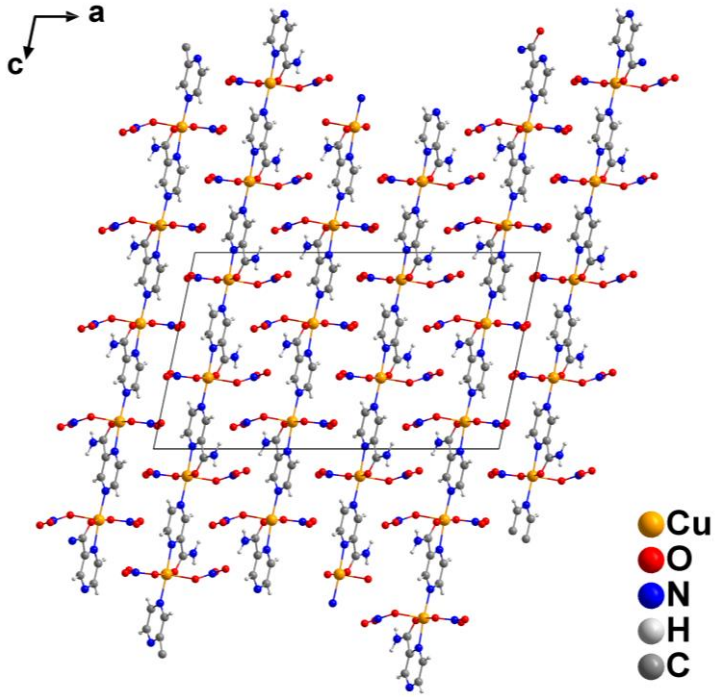

Figure S21. Crystal structure of $^{1}_{\infty}[Cu(Pya)(NO_3)_2]$ (**11**) along the *b* axis.

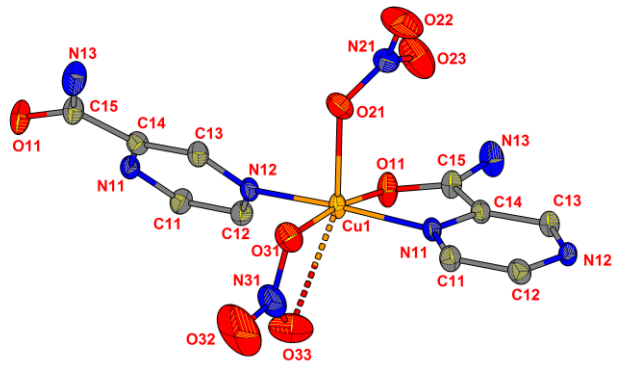

Figure S22. Molecular entity in the structure of $^{1}_{\infty}$[Cu(Pya)(NO_3)$_2$] (**11**) at 50% probability level; protons were omitted for clarity.

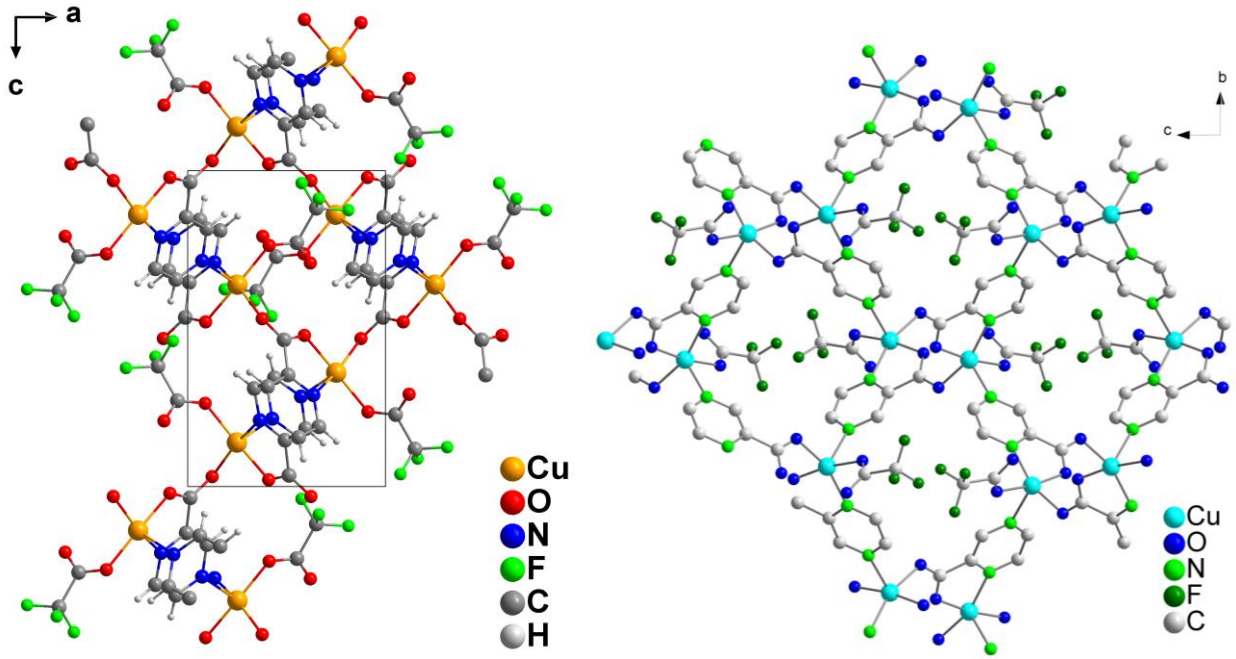

Figure S23. Crystal structure of $^{2}_{\infty}$[Cu(Pyc)(Tfa)] (**12**) viewed along the *b* axis (left) and the *a* axis (right). Note the different colour code.

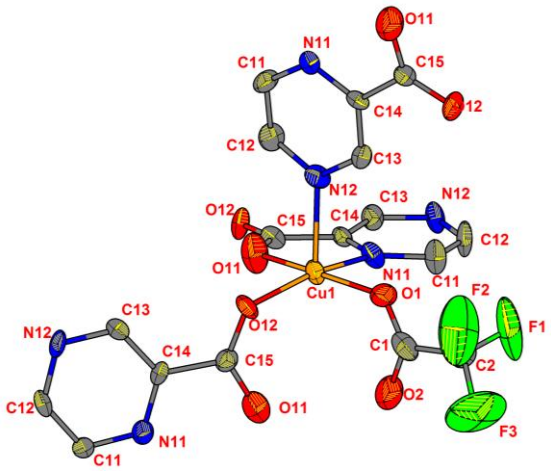

Figure S24. Molecular entity in the structure of $^{2}_{\infty}$[Cu(Pyc)(Tfa)] (**12**) at 50% probability level; protons were omitted for clarity.

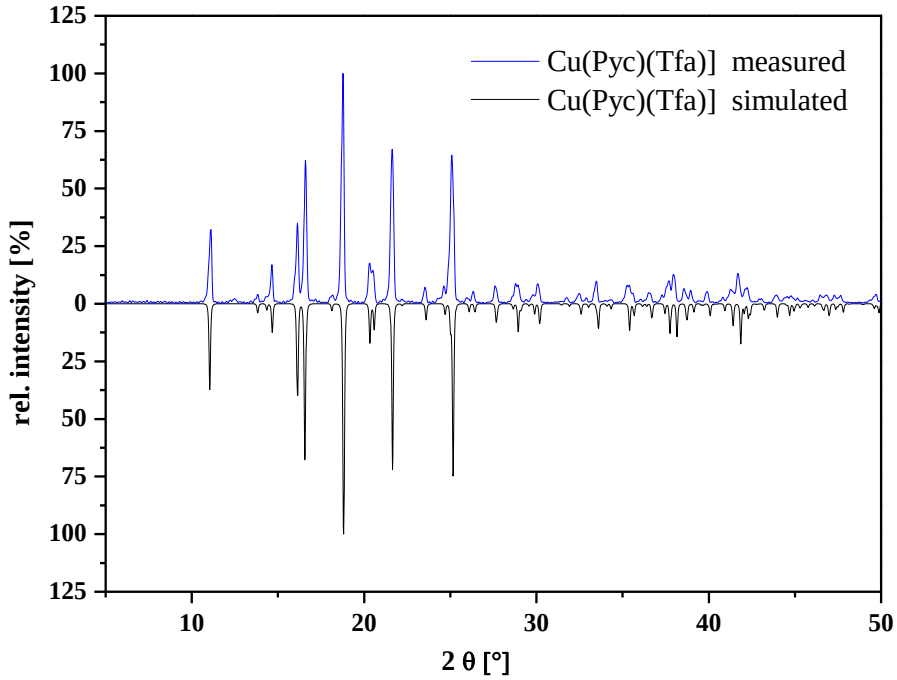

Figure S25. Powder XRD of $^{2}_{\infty}$[Cu(Pyc)(Tfa)] (**12**).

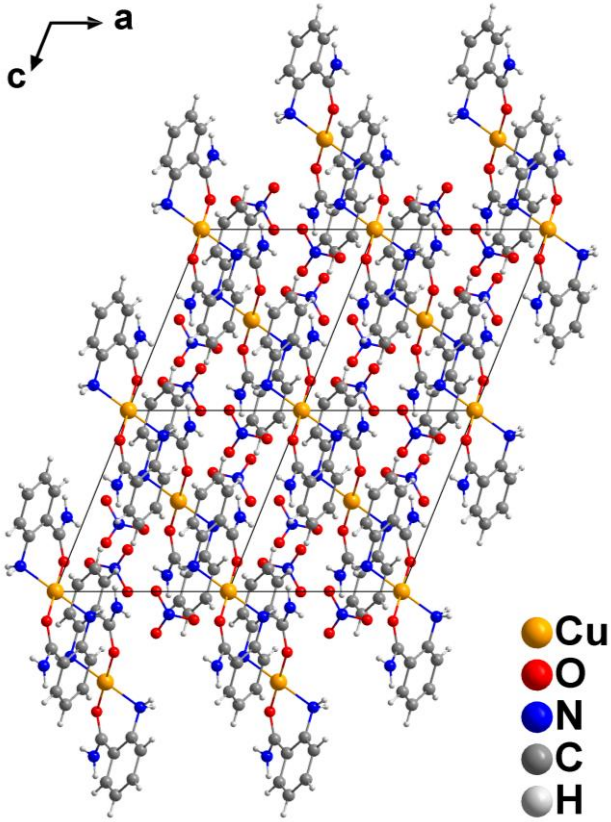

Figure S26. Crystal structure of [Cu(2-Aba)$_2$(NO$_3$)$_2$] (**13**) viewed along the *b* axis.

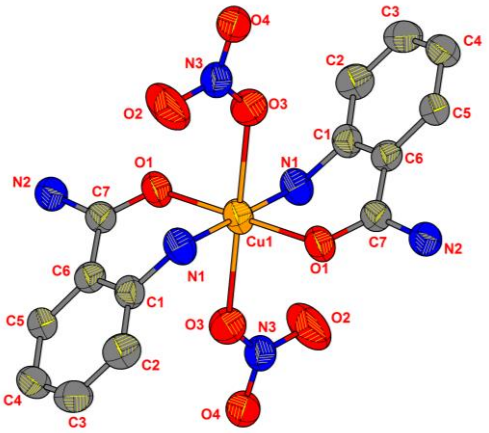

Figure S27. Molecular structure of [Cu(2-Aba)$_2$(NO$_3$)$_2$] (**13**) at 50% probability level (with numbering); protons were omitted for clarity.

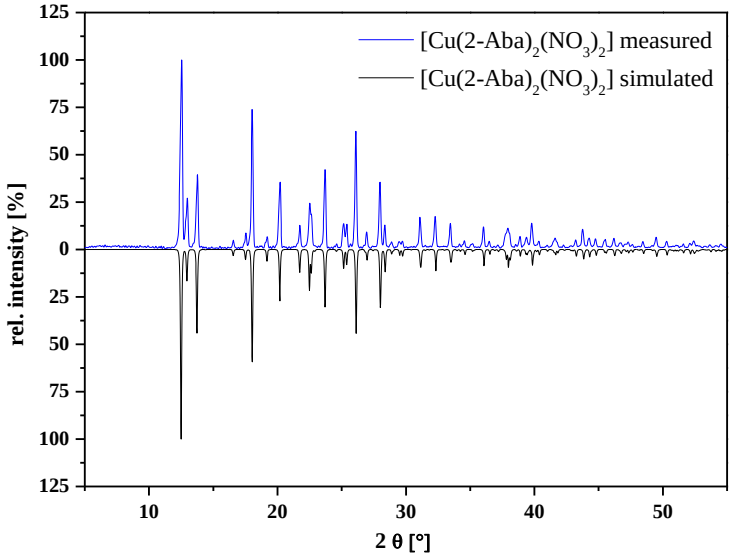

Figure S28. Powder XRD of [Cu(2-Aba)$_2$(NO$_3$)$_2$] (**13**).

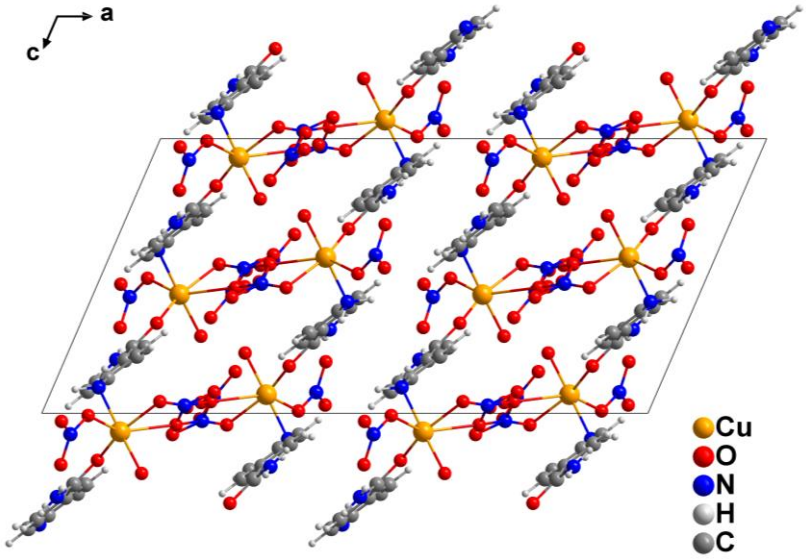

Figure S29. Crystal structure of $^{1}_{\infty}$[Cu$_2$(4-Aba)$_2$(H$_2$O)$_3$(NO$_3$)$_3$](NO$_3$) (**14**) viewed along the *b* axis.

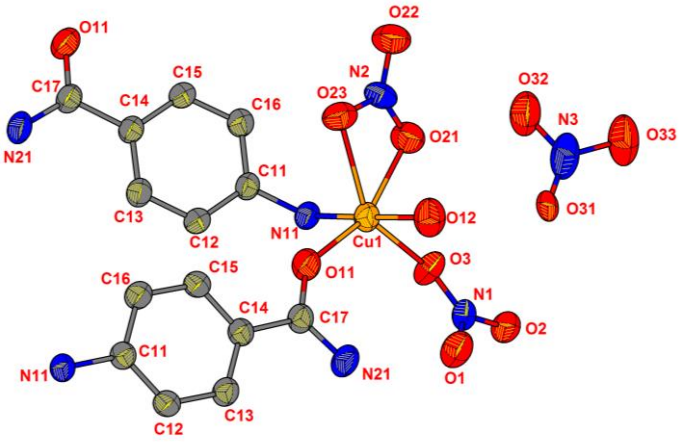

Figure S30. Molecular entity in the structure of $^{1}_{\infty}$[Cu$_2$(4-Aba)$_2$(H$_2$O)$_3$(NO$_3$)$_3$](NO$_3$) (**14**) at 50% probability level; protons were omitted for clarity.

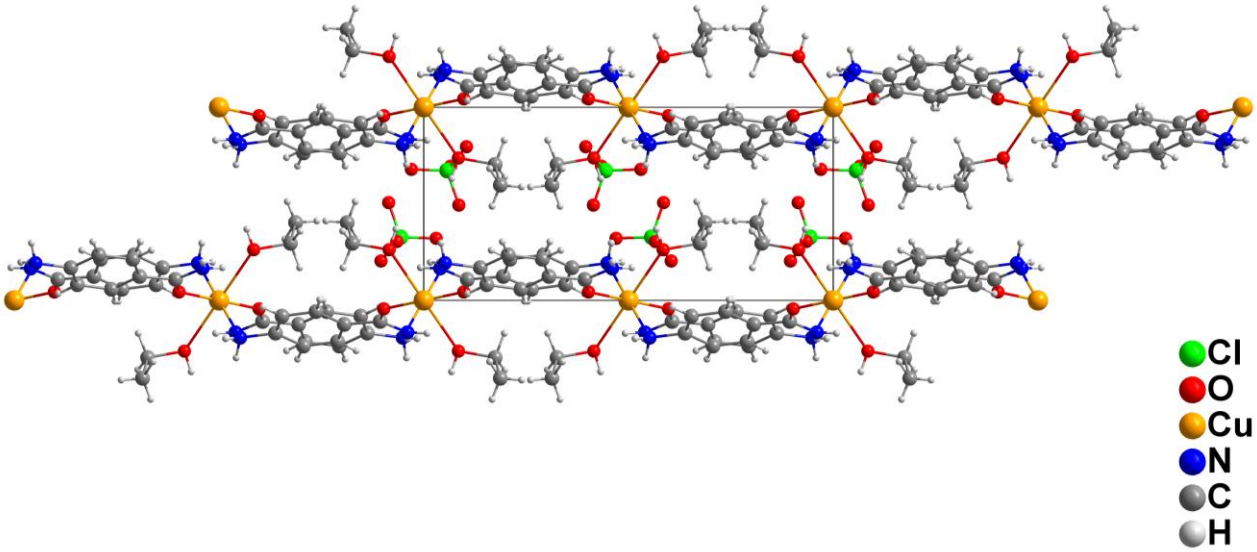

Figure S31. Crystal structure of $^{2}_{\infty}$[Cu(4-Aba)$_2$(EtOH)$_2$](ClO$_4$)$_2$ (**15**) viewed left along the *c* axis.

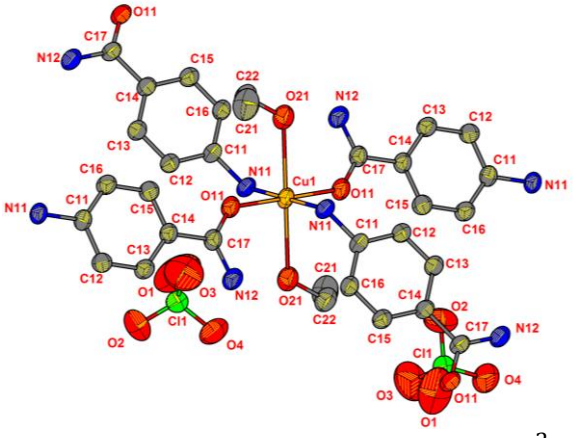

Figure S32. Molecular entity in the structure of $^{2}_{\infty}$[Cu(4-Aba)$_2$(EtOH)$_2$](ClO$_4$)$_2$ (**15**) at 50% probability level; protons were omitted for clarity.

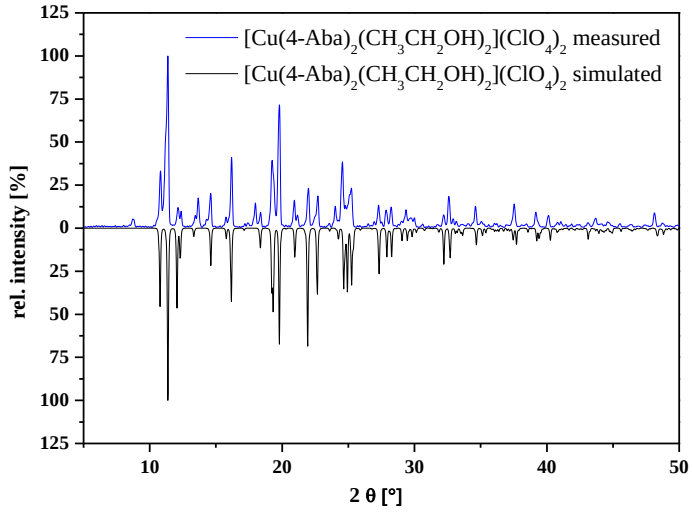

Figure S33. Powder XRD of $^{2}_{\infty}$[Cu(4-Aba)$_2$(CH$_3$CH$_2$OH)$_2$](ClO$_4$)$_2$ (**15**).

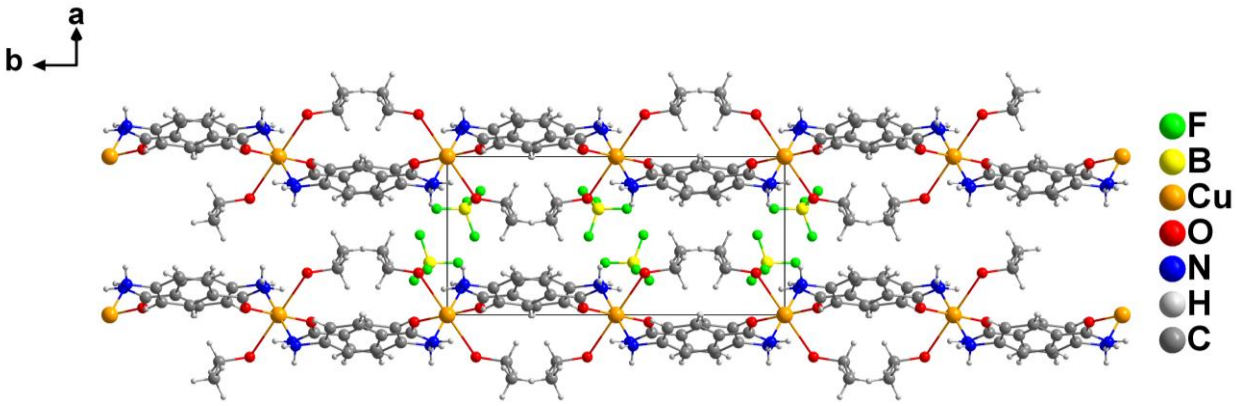

Figure S34. Crystal structure of $^{2}_{\infty}$[Cu(4-Aba)$_2$(EtOH)$_2$](BF$_4$)$_2$ (**16**) viewed along the *c* axis.

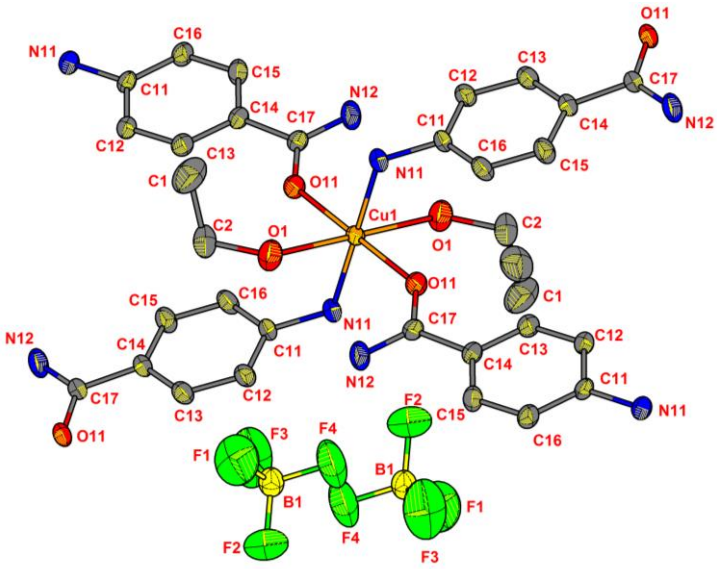

Figure S35. Molecular entities within $^{2}_{\infty}$[Cu(4-Aba)$_2$(EtOH)$_2$](BF$_4$)$_2$ (**16**) at 50% probability level; protons were omitted for clarity.

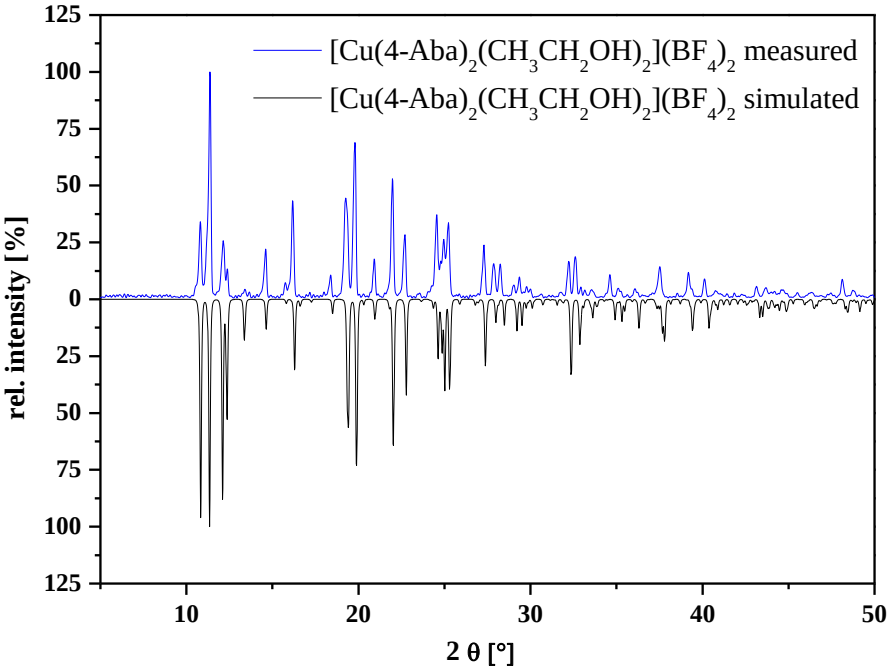

Figure S36. Powder XRD of $^{2}_{\infty}$[Cu(4-Aba)$_2$(EtOH)$_2$](BF$_4$)$_2$ (**16**).

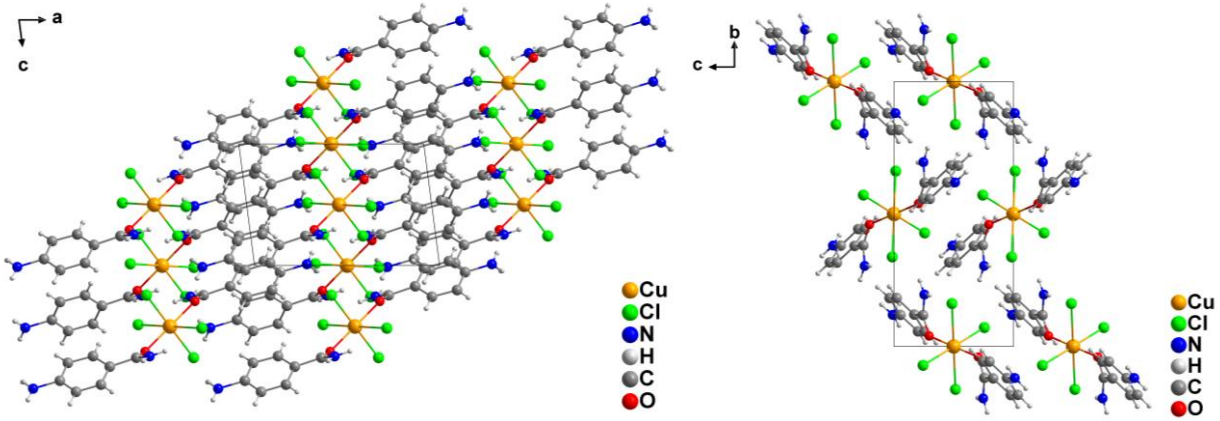

Figure S37. Crystal structure of [Cu(4-AbaH)$_2$Cl$_4$] (**17**) viewed along the *b* axis (left) and *a* axis (right).

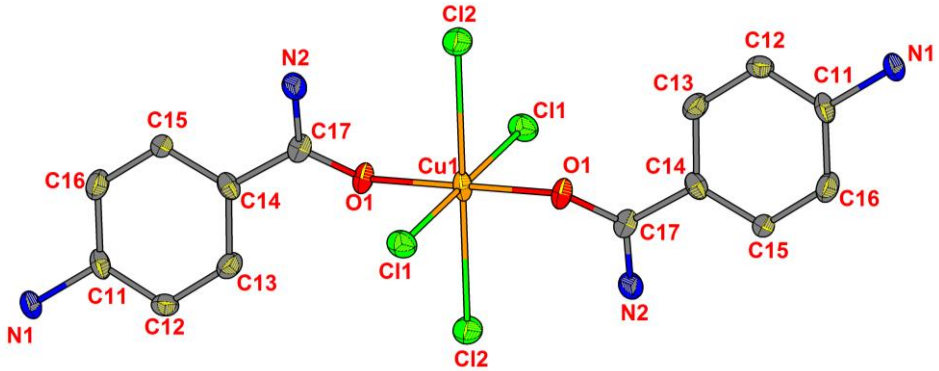

Figure S38. Molecular structure of [Cu(4-AbaH)$_2$Cl$_4$] (**17**) at 50% probability level; protons were omitted for clarity.

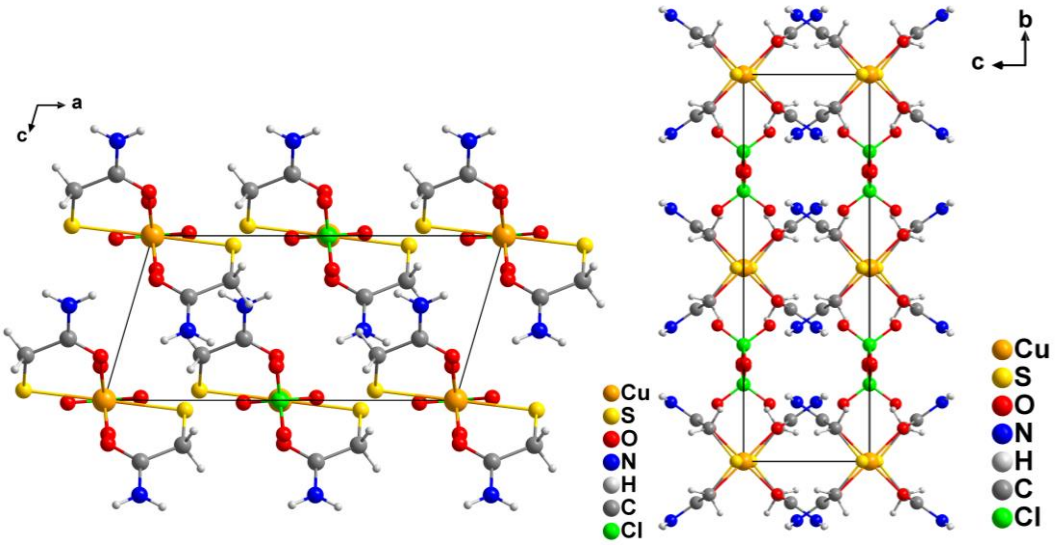

Figure S39. Crystal structure of $[Cu(Tba)_2](ClO_4)_2$ (**18**) viewed along the *b* axis (left) and *a* axis (right).

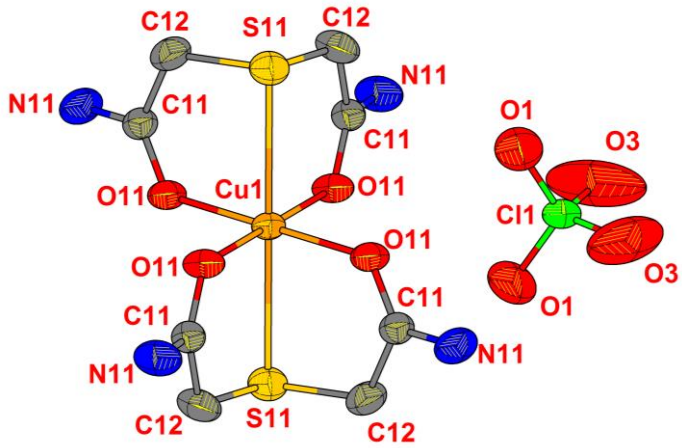

Figure S40. Molecular structure of $[Cu(Tba)_2](ClO_4)_2$ (**18**) at 50% probability level; protons were omitted for clarity.

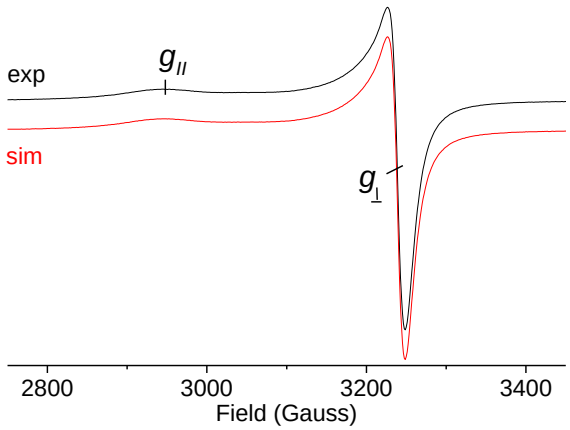

Figure S41. X-Band EPR spectra of a solid sample of $[Cu(Ina)_2(H_2O)_2(NO_3)_2]$ (**3**) at 298 K, frequency = 9.453122 GHz; simulation in red with parameters in Table 3.

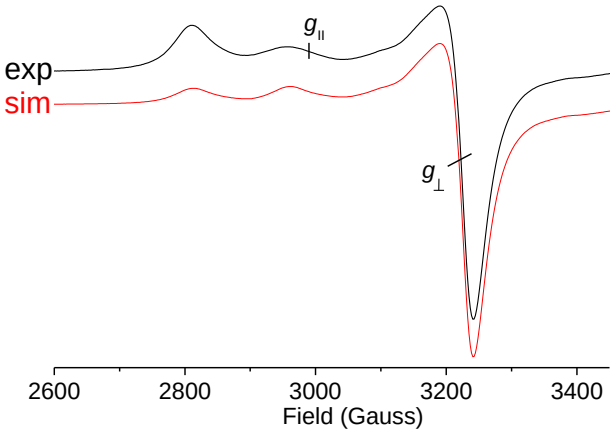

Figure S42. X-Band EPR spectrum of solid samples of $[Cu(Tba)_2](ClO_4)_2$ (**18**) (frequency = 9.455336 GHz) at 298 K, simulation in red with parameters in Table 3.

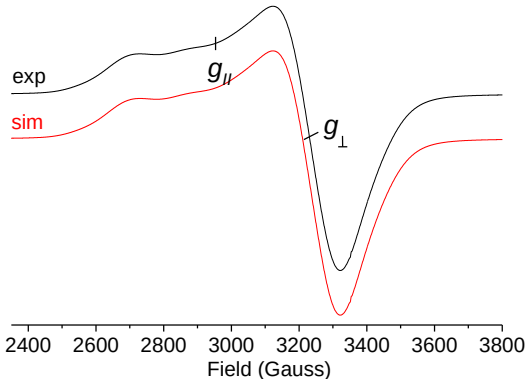

Figure S43. X-Band EPR spectrum of a solid $[Cu(Pya)_2(H_2O)(NO_3)](NO_3)$ (**10**) at 298 K, frequency = 9.464210 GHz; simulation in red with parameters in Table 3.

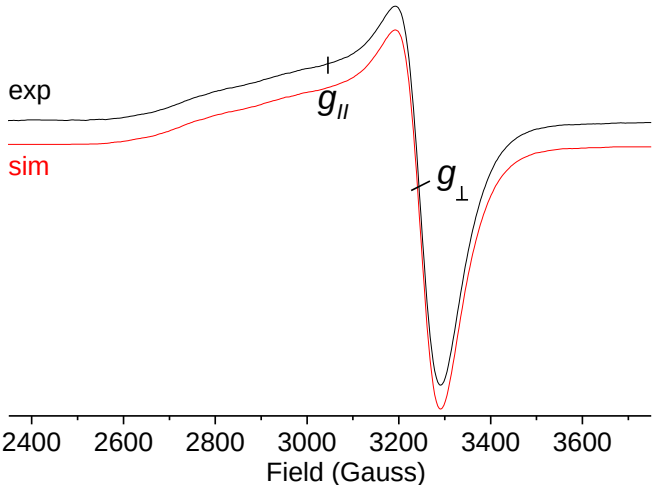

Figure S44. X-Band EPR spectrum of a solid sample of $[Cu(Ina)_2(H_2O)_3(SiF_6)]\cdot H_2O$ (**4**) at 295 K; frequency = 9.449110 GHz; simulation in red with parameters in Table 3.

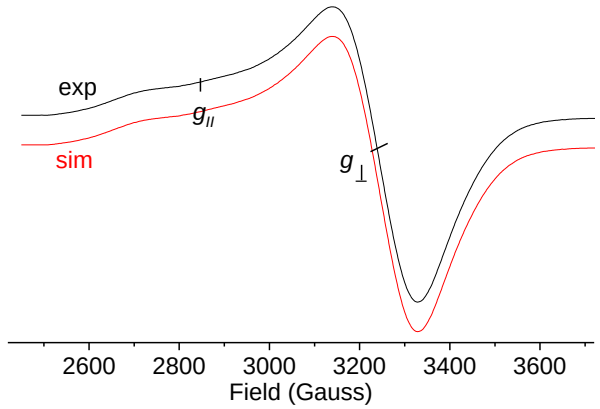

Figure S45. X-Band EPR spectrum of a solid sample of [Cu(Pya)(NO_3)$_2$] (**11**) at 298 K; frequency = 9.449076 GHz; simulation in red with parameters in Table 3.

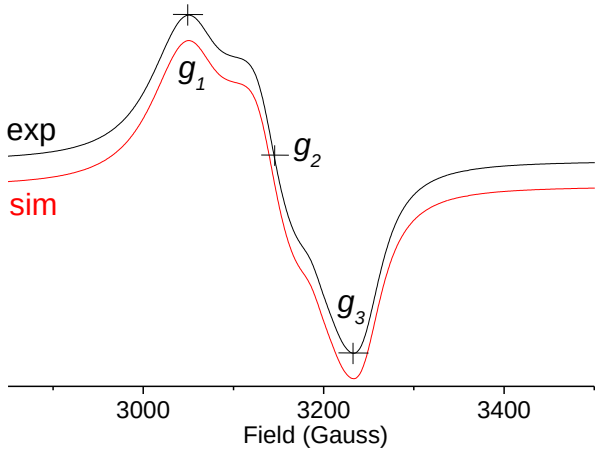

Figure S46. X-Band EPR spectrum of a solid sample of [Cu(Pia)$_2$](BF_4)$_2$ (**8**) at 298 K; frequency = 9.459716 GHz; simulation in red with parameters in Table 3.

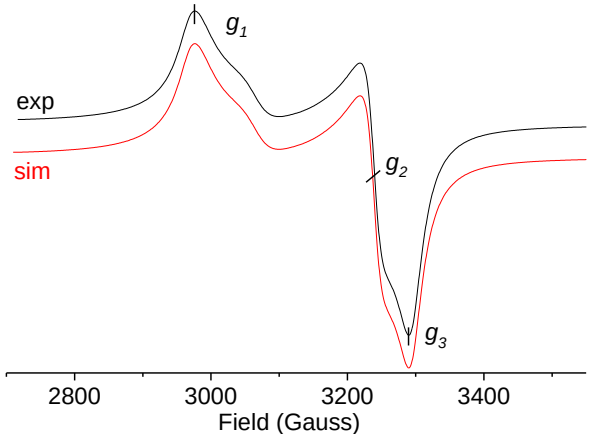

Figure S47. X-Band EPR spectrum of a solid sample of (HIna)$_2$[$CuCl_4$]·2H_2O (**6**) at 298 K; frequency = 9.441647 GHz; simulation in red with parameters in Table 3.

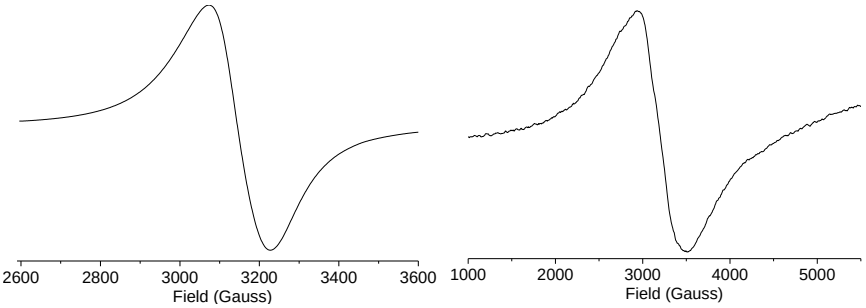

Figure S48. X-Band EPR spectrum of solid samples of [Cu(Pyc)(Tfa)] (**12**) (left) (frequency = 9.455336 GHz) and $^{1}_{\infty}$[Cu(Ina)$_2$Br$_2$] (right) (frequency = 9.453117 GHz) at 298 K.

Supplementary Tables (Tables S1–S39)

Table S1. Crystal structure and refinement data of [Cu(Pia)$_2$(BF$_4$)$_2$] (**8**), $^{1}_{\infty}$[Cu(Ina)$_2$(NO$_3$)$_2$] (**2**), and [Cu(Ina)$_4$(H$_2$O)$_2$](BF$_4$)$_2$ (**1**).

	[Cu(Pia)$_2$(BF$_4$)$_2$] (**8**)	[Cu(Ina)$_2$(NO$_3$)$_2$] (**2**)	[Cu(Ina)$_4$(H$_2$O)$_2$](BF$_4$)$_2$ (**1**)
formula	$C_{12}H_{12}B_2CuF_8N_4O_2$	$C_{12}H_{12}CuN_6O_8$	$C_{24}H_{28}B_2CuF_8N_8O_6$
f. w. /g mol^{-1}	481.42	431.82	761.70
crystal shape	plate-like	rhombohedral	rhombohedral
colour	light blue	blue	blue
crystal system	triclinic	orthorhombic	monoclinic
space group	$P\bar{1}$ (No. 2)	$P2_12_12_1$ (No. 19)	$C2/c$ (No. 15)
a /Å	5.9090(6)	14.8942(15)	18.707(4)
b /Å	8.9092(8)	13.5399(19)	9.4634(19)
c /Å	9.0708(8)	7.8743(7)	18.262(4)
α/°	93.055(7)	90	90
β/°	100.843(7)	90	92.27(3)
γ/°	107.447(8)	90	90
volume /Å^3, Z	444.35(8), 1	1588(3), 4	3230.3(11), 4
F(000)	239	876	1548
density / g cm^{-1}	1.799	1.806	1.566
abs. coeff / mm^{-1}	1.326	1.471	0.774
refl. coll.	6230	15370	16775
data / restr. / param.	2376 / 0 / 134	3681/ 0 / 247	3636 / 0 / 252
h, k, l,	–7 < h < 8	–19 < h < 19	–23 < h < 23
	–12 < k < 12	–17< k < 17	–12 < k < 12
	–12 < l < 12	–9 < l < 9	–23 < l < 23
Goof on F^2	1.000	0.779	1.099
R_{int}	0.052	0.1043	0.0486
final R indices	R1 = 0.0526	R1 = 0.0379	R1 = 0.0741
[I>2σ(I)]	wR2 = 0.1343	wR2 = 0.0557	wR2 = 0.2400
R indices (all data)	R1 = 0.0933	R1 = 0.0935	R1 = 0.0842
	wR2 = 0.1576	wR2 = 0.0657	wR2 = 0.2541
CCDC	1058949	1058950	1058951
largest diff. p. a. h. /e Å^{-3}	0.75 and –0.45	0.43 and –0.41	2.47 and –0.82

Table S2. Crystal structure and refinement data of $[Cu(Ina)_2(H_2O)_3(SiF_6)]\cdot H_2O$ (**4**), $(HIna)_2[CuCl_4]\cdot 2H_2O$ (**6**), $(HIna)[Cu(H_2O)Cl_3]$ (**7**), and $[Cu(Ina)_2Br_2]$ (**5**).

	$[Cu(Ina)_2(H_2O)_3(SiF_6)]\cdot H_2O$ (**4**)	$(HIna)_2[CuCl_4]\cdot 2H_2O$ (**6**)	$(HIna)[Cu(H_2O)Cl_3]$ (**7**)	$[Cu(Ina)_2Br_2]$ (**5**)
formula	$C_{12}H_{20}CuF_6N_4O_6Si$	$C_{12}H_{18}Cl_4CuN_4O_4$	$C_6H_9Cl_3CuN_2O_2$	$C_{12}H_{12}Br_2CuN_4O_2$
f. w. /g mol^{-1}	519.93	487.65	311.04	467.62
crystal shape	needle	plate	plate	needle
colour	light blue	blue	light blue	green
crystal system	triclinic	triclinic	triclinic	monoclinic
space group	$P\bar{1}$ (No. 2)	$P\bar{1}$ (No. 2)	$P\bar{1}$ (No. 2)	$P2_1$ (No. 4)
a /Å	6.575(1)	7.0935(17)	8.1250(13)	16.008(4)
b /Å	7.922(1)	8.5388(19)	8.6601(12)	23.780(10)
c /Å	18.691(3)	8.924(2)	8.7265(12)	3.9293(10)
α/°	83.46(2)	81.224(17)	116.698(15)	90
β/°	82.99(2)	74.088(18)	97.964(18)	97.00(3)
γ/°	89.84(2)	65.908(17)	96.994(18)	90
volume /Å^3, Z	960(2), 2	474.0(2), 1	531.39(13), 2	1484.7(8), 4
F(000)	530	243	310	908
density / g cm^{-1}	1.806	1.694	1.944	2.092
abs. coeff / mm^{-1}	1.296	1.740	2.782	6.862
refl. coll.	11597	4502	6395	15424
data / restr. / param.	4297 / 0 / 306	2596 /0 /122	2363 / 0 / 142	6516 / 7 / 296
h, k, l,	$-8 \le h \le 8$	$-9 \le h \le 9$	$-10 \le h \le 10$	$-21 \le h \le 21$
	$-9 \le k \le 9$	$-11 \le k \le 11$	$-11 \le k \le 11$	$-31 \le k \le 31$
	$-24 \le l \le 24$	$-12 \le l \le 12$	$-11 \le l \le 11$	$-4 \le l \le 4$
Goof on F^2	1.060	0.884	1.043	1.856
R_{int}	0.064	0.0349	0.0741	0.1492
final R indices	R1 = 0.0353	R1 = 0.0387	R1 = 0.0542	R1 = 0.1584
[I>2σ(I)]	wR2 = 0.0982	wR2 = 0.0922	wR2 = 0.1371	wR2 = 0.4240
R indices (all data)	R1 = 0.0447	R1 = 0.0651	R1 = 0.0625	R1 = 0.3552
	wR2 = 0.1028	wR2 = 0.0987	wR2 = 0.1426	wR2 = 0.5598
CCDC	2025467	2025470	1058953	/[a]
largest diff.	0.61 and –0.51	0.52 and -0.47	0.82 and –1.12	7.954 and –6.627

[a] No deposit at CCDC

Table S3. Crystal structure and refinement data of $[Cu(Pya)_2](BF_4)_2$ (**9**), $[Cu(Pya)_2(H_2O)(NO_3)](NO_3)$ (**10**), $[Cu(Pya)(NO_3)_2]$ (**11**), and [Cu(Pyc)(Tfa)] (**12**).

	$[Cu(Pya)_2](BF_4)_2$ (**9**)	$[Cu(Pya)_2(H_2O)(NO_3)](NO_3)$ (**10**)	$[Cu(Pya)(NO_3)_2]$ (**11**)	[Cu(Pyc)(Tfa)] (**12**)
formula	$C_{10}H_{10}B_2CuF_8N_6O_2$	$C_{10}H_{12}CuN_8O_9$	$C_5H_5CuN_5O_7$	$C_7H_3CuF_3N_2O_4$
f. w. /g mol^{-1}	483.40	451.82	310.68	299.65
crystal shape	rhombohedral	plate	rhombohedral	rectangle
colour	blue	blue	blue	turquoise
crystal system	monoclinic	triclinic	monoclinic	orthorhombic
space group	$P2_1/c$ (No. 14)	$P\bar{1}$ (No. 2)	$C2/c$ (No. 15)	$P2_12_12_1$ (No. 19)
a /Å	8.6767(16)	8.0341(17)	22.938(3)	7.5449(10)
b /Å	9.8423(11)	9.518(2)	6.7704(6)	10.6925(13)
c /Å	10.3590(17)	12.029(2)	13.3514(18)	12.072(2)
α/°	90	112.17(2)	90	90
β/°	109.972(19)	102.03(2)	101.901(16)	90
γ/°	90	94.54(3)	90	90
volume /Å^3, Z	831.4(2), 2	820.4(3), 2	2028.9(4), 8	973.9(2), 4
F(000)	478	458	1240	588
density / g cm^{-1}	1.931	1.829	2.034	2.044

abs. coeff / mm^{-1}	1.421	1.402	2.195	2.294
refl. coll.	6430	7421	9362	6889
data / restr. / param.	1811 / 0 / 136	2728 / 2 / 264	2321 / 0 / 170	1674 / 0 / 156
h, k, l,	–11 ≤ h ≤ 11 –12 ≤ k ≤ 12 –13 ≤ l ≤ 13	–9 ≤ h ≤ 9 –11 ≤ k ≤ 11 –14 ≤ l ≤ 14	–28 ≤ h ≤ 30 –8 ≤ k ≤ 8 –17 ≤ l ≤ 17	–8 ≤ h ≤ 8 –12 ≤ k ≤ 11 –14 ≤ l ≤ 14
Goof on F^2	0.818	0.760	1.016	0.876
R_{int}	0.0902	0.0727	0.0551	0.0970
final R indices [I>2σ(I)]	R1 = 0.0432 wR2 = 0.0884	R1 = 0.0386 wR2 = 0.0610	R1 = 0.0336 wR2 = 0.0749	R1 = 0.0402 wR2 = 0.0800
R indices (all data)	R1 = 0.0911 wR2 = 0.0977	R1 = 0.0875 wR2 = 0.0681	R1 = 0.0513 wR2 = 0.0798	R1 = 0.0647 wR2 = 0.0851
CCDC	1058954	1058955	1058956	1058957
largest diff. p. a. h. /e $Å^{-3}$	0.42 and –0.35	0.34 and –0.26	0.58 and –0.40	0.50 and –0.32

Table S4. Crystal structure and refinement data of $[Cu(2\text{-}Aba)_2(NO_3)_2]$ (**13**), $[Cu_2(4\text{-}Aba)_2(H_2O)_3(NO_3)_3](NO_3)$ (**14**), and $[Cu(4\text{-}Aba)_2(EtOH)_2](ClO_4)_2$ (**15**).

	$[Cu(2\text{-}Aba)_2(NO_3)_2]$ (**13**)	$[Cu_2(4\text{-}Aba)_2(H_2O)_3(NO_3)_3](NO_3)$ (**14**)	$[Cu(4\text{-}Aba)_2(EtOH)_2](ClO_4)_2$ (**15**)
formula	$C_{14}H_{16}CuN_6O_8$	$C_{14}H_{24}Cu_2N_8O_{17}$	$C_{18}H_{28}Cl_2CuN_4O_{12}$
f. w. /g mol^{-1}	459.87	703.49	626.67
crystal shape	plate	needle	rhombohedral
colour	green	green	green
crystal system	monoclinic	monoclinic	monoclinic
space group	$P2_1/n$ (No. 14)	$C2/c$ (No. 15)	$P2_1/c$ (No. 14)
a /Å	7.8005(13)	22.755(3)	8.463(3)
b /Å	14.155(3)	10.9608(18)	15.557(4)
c /Å	8.8095(13)	11.2299(14)	11.149(4)
α/°	90	90	90
β/°	111.965(11)	113.368(9)	119.93(2)
γ/°	90	90	90
volume /$Å^3$, Z	902.1 (3), 2	2571.2(6), 4	1272.1(8), 2
F(000)	470	1432	646
density / g cm^{-1}	1.693	1.817	1.636
abs. coeff / mm^{-1}	1.270	1.749	1.137
refl. coll.	2538	9118	9319
data / restr. / param.	2538 / 0 / 149	2262 / 0 / 221	2823 / 0 / 226
h, k, l,	–10 ≤ h ≤ 10 –19 ≤ k ≤ 19 –12 ≤ l ≤ 11	–28 ≤ h ≤ 29 –14 ≤ k ≤ 14 –12 ≤ l ≤ 14	–10 ≤ h ≤ 10 –19 ≤ k ≤ 19 –14 ≤ l ≤ 14
Goof on F^2	1.027	1.098	1.061
R_{int}	0.0999	0.0415	0.0447
final R indices [I>2σ(I)]	R1 = 0.0645 wR2 = 0.1577	R1 = 0.0585 wR2 = 0.1757	R1 = 0.0493 wR2 = 0.1341
R indices (all data)	R1 = 0.1255 wR2 = 0.2040	R1 = 0.0843 wR2 = 0.1884	R1 = 0.0612 wR2 = 0.1471
CCDC	2025469	1058960	1058961
largest diff. p. a. h. /e $Å^{-3}$	0.76 and –0.62	1.10 and –0.61	0.74 and –0.46

Table S5. Crystal structure and refinement data of $[Cu(4\text{-}Aba)_2(EtOH)_2](BF_4)_2$ (**16**), $[Cu(4\text{-}AbaH)_2Cl_4]$ (**17**), and $[Cu(Tba)_2](ClO_4)_2$ (**18**)

	$[Cu(4\text{-}Aba)_2(EtOH)_2](BF_4)_2$ (**16**)	$[Cu(4\text{-}AbaH)_2Cl_4]$ (**17**)	$[Cu(Tba)_2](ClO_4)_2$ (**18**)
formula	$C_{18}H_{28}B_2CuF_8N_4O_4$	$C_{14}H_{18}Cl_4CuN_4O_2$	$C_8H_{16}Cl_2Cu_1N_4O_{12}S_2$
f. w. /g mol^{-1}	601.61	479.66	558.80
crystal shape	rhombohedral	plate	plate
colour	green	green	turquoise
crystal system	monoclinic	monoclinic	monoclinic
space group	$P2_1/c$ (No. 14)	$P2_1/c$ (No. 14)	$C2/m$ (No. 12)
a /Å	8.4237(13)	9.8364(12)	11.354(2)
b /Å	15.593(14)	14.278(2)	16.265(3)
c /Å	11.055(2)	6.5068(8)	5.5218(8)
α/°	90	90	90
β/°	119.863(13)	82.571(14)	106.402(16)
γ/°	90	90	90
volume /Å^3, Z	1259.3(12), 2	906.2(2), 2	978.2(3)
F(000)	614	486	566.0
density / g cm^{-1}	1.587	1.758	1.897
abs. coeff / mm^{-1}	0.959	1.811	1.670
refl. coll.	9627	5313	4650
data / restr. / param.	2995 / 0 / 174	1576 / 4 / 128	1128/0/72
h, k, l,	$-11 \le h \le 11$	$-11 \le h \le 11$	$15 \le h \le 14$
	$-18 \le k \le 20$	$-16 \le k \le 16$	$-21 \le k \le 21$
	$-14 \le l \le 13$	$-7 \le l \le 7$	$-6 \le l \le 6$
Goof on F^2	0.927	1.216	1.000
R_{int}	0.0375	0.0755	0.0349
final R indices	R1 = 0.0430	R1 = 0.0705	R1 = 0.0399
[I>2σ(I)]	wR2 = 0.1084	wR2 = 0.2017	wR2 = 0.1045
R indices (all data)	R1 = 0.0733	R1 = 0.0928	R1 = 0.0536
	wR2 = 0.1177	wR2 = 0.2076	wR2 = 0.1102
CCDC	1058962	1058963	2025471
largest diff. p. a. h. /e Å^{-3}	0.55 and –0.42	1.98 and –0.63	0.83 and -0.42

Table S6. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for $[Cu(Pia)_2(BF_4)_2]$ (**8**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Cu1	5000	5000	0	55.5(3)
O1	3159(5)	5006(4)	1552(3)	63.9(7)
N1	5788(5)	3271(4)	1000(3)	52.5(7)
N2	2437(7)	4012(5)	3679(4)	67.7(9)
C1	7090(7)	2400(5)	595(5)	60.8(9)
C2	7487(9)	1214(6)	1418(6)	71.9(11)
C3	6516(9)	930(6)	2680(6)	77.7(13)
C4	5177(8)	1835(5)	3098(5)	67.9(10)
C5	4834(7)	2988(5)	2232(4)	52.4(8)
C6	3417(7)	4064(5)	2497(4)	55.3(8)
F1	508(8)	3979(4)	-3577(4)	112.4(12)

F2	1944(8)	2045(4)	-3934(4)	112.8(13)
F3	-1782(8)	1558(6)	-3446(5)	156(2)
F4	1412(6)	2725(5)	-1625(3)	105.3(11)
B1	479(9)	2509(6)	-3135(5)	58.3(10)

Table S7. Anisotropic Displacement Parameters ($Å^2×10^3$) for $[Cu(Pia)_2(BF_4)_2]$ (**8**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu1	68.4(5)	66.9(5)	47.3(4)	23.8(3)	28.7(3)	32.1(3)
O1	79.1(18)	76.7(18)	58.0(14)	26.7(13)	35.4(13)	41.2(15)
N1	57.3(17)	58.7(17)	46.6(14)	13.9(13)	16.7(12)	21.2(14)
N2	81(2)	84(2)	52.4(16)	23.4(16)	32.6(15)	33.0(19)
C1	64(2)	65(2)	58(2)	14.5(18)	18.5(17)	24.0(19)
C2	76(3)	63(2)	85(3)	14(2)	21(2)	32(2)
C3	89(3)	64(3)	88(3)	32(2)	23(2)	29(2)
C4	78(3)	70(3)	62(2)	28.1(19)	23.1(19)	23(2)
C5	55.3(19)	55(2)	45.8(16)	13.8(15)	13.7(14)	13.7(16)
C6	60(2)	62(2)	43.6(16)	12.7(15)	18.5(15)	13.7(17)
F1	171(3)	104(2)	115(3)	50(2)	79(2)	87(3)
F2	187(4)	124(3)	97(2)	57(2)	87(2)	109(3)
F3	115(3)	171(4)	115(3)	7(3)	23(3)	-48(3)
F4	99(2)	156(3)	57.7(14)	19.3(17)	17.2(14)	36(2)
B1	68(3)	62(3)	51(2)	12.2(19)	22.5(19)	23(2)

Table S8. Fractional Atomic Coordinates ($×10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2×10^3$) for $^1_\infty[Cu(Ina)_2(NO_3)_2]$ (**2**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cu01	9162.0(5)	6176.7(5)	8850.2(10)	29.76(19)
O21	7872(3)	10037(3)	3581(7)	39.4(12)
O11	10152(3)	2370(3)	14494(6)	38.4(12)
O42	7492(3)	5452(3)	8851(8)	50.3(12)
O41	8128(3)	6636(3)	10275(6)	37.4(11)
N41	7444(4)	6061(4)	10023(8)	36.5(13)
O31	9954(3)	5498(3)	7189(7)	55.2(15)
O33	10895(5)	6717(4)	7410(7)	74.3(16)
C13	9422(4)	3366(4)	12448(8)	25.7(15)
N22	7935(3)	8864(4)	1590(6)	38.1(14)
O32	10943(4)	5785(3)	5248(7)	61.9(15)
N11	9333(3)	5016(3)	10391(7)	28.8(13)
C23	8255(4)	8431(4)	4499(8)	24.0(15)
N31	10606(3)	5998(4)	6601(8)	36.1(14)
C26	8002(4)	9172(4)	3157(8)	24.3(14)
C14	9136(5)	3295(4)	10807(8)	33.8(15)
N12	8801(3)	1860(3)	13553(8)	46.2(17)
N21	8805(3)	7126(3)	7036(7)	29.1(13)
C16	9489(4)	2481(4)	13600(8)	26.4(14)

O43	6787(3)	6142(5)	10938(7)	67.2(14)
C24	8169(4)	7419(4)	4298(8)	33.8(16)
C22	8597(3)	8758(4)	5997(8)	31.0(13)
C12	9681(4)	4283(4)	13059(9)	32.4(17)
C15	9115(5)	4125(4)	9795(8)	37.3(16)
C11	9600(4)	5083(5)	11992(9)	31.8(17)
C25	8452(4)	6803(4)	5602(9)	35.4(18)
C21	8873(4)	8109(4)	7229(9)	34.5(16)

Table S9. Anisotropic Displacement Parameters ($Å^2×10^3$) for $^1_\infty$[Cu(Ina)$_2$(NO$_3$)$_2$] (**2**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Cu01	37.3(4)	25.9(3)	26.0(4)	5.1(4)	-2.3(4)	4.1(4)
O21	57(3)	23(2)	37(3)	3(2)	-1(3)	3(2)
O11	43(3)	33(2)	40(3)	12(2)	-16(2)	2(2)
O42	45(3)	52(3)	54(4)	-16(3)	-6(3)	-3(2)
O41	39(3)	34(2)	39(3)	1(2)	-4(2)	-5(2)
N41	35(3)	42(3)	32(4)	7(3)	2(3)	9(3)
O31	56(3)	34(3)	76(5)	19(2)	24(3)	2(2)
O33	76(4)	91(4)	55(4)	-29(3)	-12(4)	-18(4)
C13	28(4)	25(3)	25(4)	7(3)	-2(3)	3(2)
N22	66(4)	30(3)	19(4)	1(3)	-3(2)	9(3)
O32	71(4)	69(3)	45(4)	-15(2)	25(3)	-4(3)
N11	37(3)	31(3)	19(3)	-3(2)	-3(2)	-1(2)
C23	30(3)	21(3)	21(4)	3(2)	1(3)	-1(3)
N31	34(3)	42(3)	33(4)	1(3)	-2(2)	11(3)
C26	30(3)	20(3)	23(4)	2(2)	4(3)	0(2)
C14	43(3)	25(3)	33(5)	-7(2)	-7(4)	1(3)
N12	46(3)	33(3)	60(5)	18(3)	-6(3)	-15(2)
N21	42(3)	23(3)	22(4)	-6(2)	-3(2)	-1(2)
C16	36(3)	17(3)	26(4)	0(3)	2(3)	1(2)
O43	46(3)	105(4)	51(4)	14(4)	17(3)	-1(3)
C24	51(4)	24(3)	26(5)	1(3)	-15(3)	-8(3)
C22	52(3)	17(3)	24(4)	-2(3)	-11(3)	3(3)
C12	45(4)	27(3)	25(5)	5(3)	-10(3)	-11(3)
C15	61(4)	29(3)	22(4)	-3(2)	-18(4)	4(4)
C11	42(4)	16(3)	37(5)	-3(3)	-8(3)	-3(3)
C25	59(5)	19(3)	28(5)	1(3)	-9(3)	-7(3)
C21	48(4)	28(3)	27(5)	-9(3)	-11(3)	4(3)

Table S10. Fractional Atomic Coordinates ($×10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2×10^3$) for [Cu(Ina)$_4$(H$_2$O)$_2$](BF$_4$)$_2$ (**1**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Cu1	0	2771.1(8)	7500	28.7(3)
N21	1059.9(18)	2951(3)	7749.6(18)	29.0(7)
C22	2128(2)	2222(4)	8403(2)	28.6(8)

N11	-231.0(19)	2641(4)	8583.0(18)	29.4(7)
C21	1402(2)	2119(4)	8241(2)	28.4(8)
C13	-515(2)	2248(4)	10055(2)	28.5(8)
C11	-719(2)	1712(5)	8788(2)	36.6(9)
C15	122(2)	3387(4)	9110(2)	30.0(8)
C23	2527(2)	3202(4)	8027.3(19)	27.1(7)
C14	-2(2)	3202(4)	9848(2)	30.6(8)
C24	2172(2)	4062(5)	7519(3)	40.5(10)
C12	-884(2)	1479(5)	9512(2)	36.6(9)
C25	1441(2)	3926(5)	7399(3)	40.8(10)
O1	0	243(5)	7500	41.4(10)
C16	-655(2)	2088(4)	10859(2)	32.4(8)
C26	3328(2)	3353(4)	8117(2)	31.2(8)
O11	-188(2)	2465(5)	11314.8(18)	48.6(9)
O21	3654.8(17)	3962(4)	7635.5(17)	44.5(8)
N12	-1271(2)	1523(5)	11038(2)	43.1(9)
N22	3646(2)	2815(6)	8706(3)	55.8(13)
O2	0	5566(5)	7500	49.0(12)
F1	3406(4)	-399(6)	10605(3)	123(2)
B1	2987(5)	21(9)	10038(4)	69(2)
F4	3207(9)	-324(13)	9379(5)	259(8)
F2	2317(4)	321(13)	10067(7)	112(4)
F3	3210(4)	1545(7)	10021(4)	60.6(17)

Table S11. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $[Cu(Ina)_4(H_2O)_2](BF_4)_2$ (**1**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Cu1	16.7(4)	51.0(5)	18.4(4)	0	1.3(2)	0
N21	20.4(16)	40.2(17)	26.3(16)	5.9(12)	0.6(12)	-3.4(12)
C22	26(2)	35.4(18)	24.7(17)	4.0(14)	0.7(14)	2.8(14)
N11	24.8(17)	41.7(17)	22.0(15)	-4.5(12)	3.1(12)	-6.4(13)
C21	26(2)	33.0(18)	26.6(17)	4.3(13)	3.0(14)	-4.0(13)
C13	27(2)	37.9(18)	20.8(17)	-0.8(13)	1.5(14)	-2.5(14)
C11	32(2)	54(2)	24.3(18)	-9.7(17)	2.3(15)	-17.7(18)
C15	25.8(19)	37.8(19)	26.4(17)	-3.3(14)	2.7(14)	-8.5(14)
C23	19.6(18)	37.4(17)	24.3(16)	-0.9(14)	-0.2(13)	-3.4(13)
C14	32(2)	37.4(18)	22.7(17)	-4.3(14)	-0.9(14)	-5.0(15)
C24	26(2)	50(2)	46(2)	19.5(19)	1.2(17)	-8.9(17)
C12	33(2)	49(2)	27.6(19)	-6.0(16)	5.4(15)	-18.4(17)
C25	24(2)	57(2)	42(2)	25(2)	-2.0(16)	-3.1(17)
O1	28(2)	37(2)	60(3)	0	12(2)	0
C16	31(2)	45(2)	21.8(17)	0.1(14)	2.3(14)	1.8(15)
C26	19.9(19)	44(2)	29.6(18)	-3.1(15)	-0.8(14)	-5.1(14)
O11	36.2(19)	86(2)	23.6(15)	-2.5(14)	-2.2(13)	-7.8(17)
O21	25.5(16)	74(2)	33.9(15)	5.5(15)	3.1(12)	-13.4(14)
N12	42(2)	64(2)	23.9(16)	4.5(16)	4.9(14)	-11.1(18)
N22	24(2)	93(4)	49(3)	24(2)	-9.2(18)	-11(2)

O2	60(3)	41(2)	44(3)	0	-7(2)	0
F1	152(6)	104(4)	109(4)	21(3)	-61(4)	15(4)
B1	74(5)	75(4)	57(4)	-1(3)	-15(3)	23(4)
F4	450(20)	216(10)	105(6)	-52(6)	-46(8)	161(12)
F2	18(4)	156(9)	163(10)	64(8)	-4(4)	-18(4)
F3	79(5)	53(3)	51(3)	13(3)	1(3)	-10(3)

Table S12. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for $[Cu(Ina)_2(H_2O)_3(SiF_6)]\cdot H_2O$ (**4**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Cu01	5744.7(4)	5142.7(4)	2299.1(2)	25.24(10)
F1	3387(2)	7428(2)	2088.5(9)	38.9(4)
F5	2697(3)	9840(2)	1279.7(8)	46.0(4)
F2	5016(2)	10087(2)	2143.4(10)	43.3(4)
F4	107(2)	8774(2)	2221.6(10)	41.5(4)
F3	1735(2)	11412(2)	2271.1(11)	45.8(4)
O2	7356(3)	6430(2)	2892.6(10)	30.5(4)
O1	4228(3)	3890(2)	1677.7(10)	26.9(3)
O21	13577(3)	7007(3)	-485.9(10)	38.5(4)
F6	2425(3)	9017(3)	3078.1(8)	55.8(5)
N12	388(4)	1599(4)	5647.6(11)	42.7(6)
O11	-2174(3)	2578(4)	5025.1(12)	63.8(7)
C23	10290(4)	7135(3)	177.1(11)	24.1(4)
N22	11388(4)	8879(3)	-960.0(11)	36.6(5)
C21	6947(4)	7018(3)	851.5(13)	29.7(5)
C14	509(4)	4065(4)	3868.4(13)	34.5(6)
C22	8240(4)	7585(3)	226.2(12)	29.6(5)
C11	4518(4)	3194(4)	3734.2(13)	36.2(6)
C24	10966(4)	6103(3)	751.0(12)	27.4(5)
N21	7608(3)	6033(3)	1410.3(10)	26.0(4)
C12	3228(4)	2532(4)	4348.4(13)	38.8(6)
C26	11874(4)	7676(3)	-458.9(12)	26.9(5)
C25	9588(4)	5586(3)	1353.6(12)	29.0(5)
C13	1188(4)	2978(3)	4419.5(12)	30.6(5)
N11	3858(3)	4254(3)	3201.9(10)	26.2(4)
C16	-337(4)	2357(4)	5063.1(14)	37.2(6)
C15	1884(4)	4673(3)	3270.8(13)	31.4(5)
Si1	2574.0(9)	9403.4(8)	2172.8(3)	22.56(14)
O3	5402(3)	8220(4)	3922.7(12)	50.6(6)
O4	7712(3)	2462(3)	2555.4(12)	40.6(5)

Table S13. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $[Cu(Ina)_2(H_2O)_3(SiF_6)]\cdot H_2O$ (**4**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Cu01	21.37(15)	32.22(18)	20.33(14)	0.99(10)	1.10(10)	-7.13(11)
F1	36.2(9)	26.3(9)	50.4(9)	2.6(6)	3.6(7)	3.9(6)

F5	46.1(10)	59.7(12)	27.4(7)	10.6(7)	-0.5(7)	10.5(8)
F2	20.4(7)	46.5(11)	62.7(11)	-9.1(8)	-1.3(7)	-4.9(6)
F4	22.9(7)	37.7(10)	61.4(10)	0.7(7)	-0.6(7)	-8.5(6)
F3	27.4(8)	28.5(10)	78.5(12)	-11.5(8)	10.2(8)	-1.0(6)
O2	27.8(9)	34.9(11)	27.8(9)	-1.9(7)	-1.2(7)	-8.2(7)
O1	23.7(8)	28.4(10)	27.8(8)	-2.8(7)	-0.2(7)	-2.3(7)
O21	29.0(9)	51.8(13)	30.6(9)	2.2(8)	5.9(7)	5.0(8)
F6	48.9(11)	91.6(16)	23.7(8)	0.1(8)	1.8(7)	8.4(10)
N12	27.9(11)	70.4(18)	24.5(10)	8.9(10)	5.0(8)	-2.2(11)
O11	22.4(10)	119(2)	40.3(12)	23.3(12)	4.6(8)	0.1(11)
C23	26.7(11)	24.5(12)	20.8(10)	-3.2(8)	-1.9(8)	-2.4(8)
N22	37.5(12)	41.2(14)	26.3(10)	6.5(8)	5.2(9)	1.8(10)
C21	22.4(11)	36.2(15)	28.5(11)	2.7(9)	-1.1(9)	0.3(9)
C14	21.6(11)	47.0(17)	31.3(12)	5.4(10)	1.5(9)	3.8(10)
C22	26.8(12)	35.3(14)	25.5(11)	3.0(9)	-4.3(9)	1.5(9)
C11	24.2(12)	55.3(18)	25.6(11)	6.2(10)	1.3(9)	5.0(11)
C24	22.6(11)	36.9(14)	21.8(10)	-0.3(9)	-2.2(8)	-0.3(9)
N21	24.0(9)	31.1(12)	20.9(9)	1.2(7)	1.5(7)	-6.4(8)
C12	26.1(13)	61.5(19)	24.0(11)	11.0(11)	0.8(9)	5.8(12)
C26	27.6(12)	30.4(13)	22.3(10)	-3.8(8)	0.0(9)	-1.6(9)
C25	24.3(12)	37.5(15)	23.5(10)	3.9(9)	-3.0(9)	-3.2(9)
C13	25.6(12)	41.6(16)	22.8(11)	-0.5(9)	0.7(9)	-2.5(10)
N11	20.3(9)	33.0(12)	23.0(9)	1.9(7)	2.2(7)	-5.7(8)
C16	26.0(12)	54.2(18)	27.7(12)	3.5(10)	3.7(10)	-1.5(11)
C15	21.0(11)	38.6(15)	30.6(12)	8.5(9)	0.9(9)	-1.2(9)
Si1	17.8(3)	24.4(4)	23.5(3)	1.7(2)	1.3(2)	-1.8(2)
O3	30.0(11)	87.2(19)	31.9(10)	-2.1(11)	2.2(9)	3.7(11)
O4	29.0(10)	41.0(13)	52.3(12)	-12.9(9)	0.6(9)	1.9(9)

Table S14. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for $(HIna)_2[CuCl_4]\cdot 2H_2O$ (**6**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Cu01	10000	0	0	36.00(18)
Cl02	10413.0(14)	2529.7(9)	-198.3(10)	51.2(2)
Cl01	7698.6(14)	1152.2(10)	-1571.1(11)	54.6(2)
O2	11013(4)	2982(3)	-3943(3)	59.1(6)
N1	3674(4)	1843(3)	1985(3)	44.6(6)
N6	6754(5)	5378(4)	3504(4)	63.5(9)
O1	8815(5)	2747(4)	4136(4)	84.4(10)
C2	6316(5)	1372(4)	3283(4)	43.4(7)
C3	6010(4)	3081(4)	3035(3)	38.1(6)
C6	7328(5)	3749(5)	3613(4)	48.6(8)
C1	5115(5)	773(4)	2734(4)	45.2(7)
C4	4499(5)	4160(4)	2247(4)	46.6(7)
C5	3341(5)	3503(4)	1720(4)	49.0(8)

Table S15. Anisotropic Displacement Parameters ($Å^2×10^3$) for $(HIna)_2[CuCl_4]·2H_2O$ (**6**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu01	38.0(3)	32.1(3)	39.0(3)	-0.2(2)	-10.8(2)	-14.0(2)
Cl02	71.5(5)	38.4(4)	59.7(5)	8.1(3)	-34.9(4)	-28.1(4)
Cl01	60.4(5)	39.3(4)	79.1(6)	11.2(4)	-40.8(5)	-23.2(4)
O2	69.8(16)	64.1(15)	57.5(15)	5.9(12)	-23.0(13)	-37.6(14)
N1	39.2(13)	47.2(14)	52.9(16)	-10.2(12)	-11.0(12)	-19.4(12)
N006	48.3(16)	60.3(18)	98(3)	-31.8(17)	-10.7(16)	-31.5(15)
O1	59.2(16)	107(2)	93(2)	-38.3(18)	-38.1(16)	-13.5(16)
C2	41.1(16)	41.3(15)	44.5(17)	0.4(13)	-14.4(13)	-10.5(13)
C3	34.2(14)	43.3(15)	39.5(15)	-8.9(12)	-8.4(12)	-15.3(13)
C6	35.3(16)	61(2)	54.1(19)	-18.9(15)	-9.9(14)	-18.1(15)
C1	46.3(17)	35.5(15)	53.0(18)	-1.7(13)	-12.5(14)	-14.6(14)
C4	49.2(17)	34.6(15)	59.0(19)	-3.6(13)	-17.1(15)	-15.9(14)
C5	45.7(17)	40.9(16)	62(2)	-2.2(14)	-22.1(16)	-11.9(14)

Table S16. Fractional Atomic Coordinates ($×10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2×10^3$) for $(HIna)[Cu(H_2O)Cl_3]$ (**7**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cu1	-818.9(6)	8590.0(5)	2521.8(5)	32.1(2)
Cl2	-2241.6(13)	9429.1(12)	4705.8(12)	38.0(3)
Cl3	-1138.8(13)	10955.9(13)	2093.7(12)	38.8(3)
Cl1	-1226.8(14)	5751.3(12)	2023.7(14)	42.4(3)
O1	706(5)	7960(4)	846(4)	51.6(8)
N2	4912(5)	2049(4)	74(4)	40.3(8)
O2	4286(5)	986(4)	1867(4)	49.7(8)
C3	3780(4)	3804(5)	2480(5)	33.5(8)
C2	4180(5)	5288(6)	2292(5)	40.4(9)
C1	3645(5)	6800(5)	3318(6)	41.4(9)
C4	2876(5)	3843(5)	3737(5)	35.6(8)
N1	2777(4)	6790(4)	4509(4)	37.4(7)
C5	2369(5)	5381(6)	4730(6)	40.9(9)
C6	4363(5)	2139(5)	1397(5)	35.2(8)

Table S17. Anisotropic Displacement Parameters ($Å^2×10^3$) for $(HIna)[Cu(H_2O)Cl_3]$ (**7**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu1	44.2(3)	25.5(3)	27.8(3)	11.0(2)	14.87(19)	10.02(18)
Cl2	50.6(5)	31.0(5)	38.5(5)	16.4(4)	23.4(4)	14.4(4)
Cl3	52.2(5)	36.2(5)	36.8(5)	21.0(4)	17.8(4)	15.6(4)
Cl1	58.9(6)	26.2(4)	44.1(5)	14.3(4)	24.0(4)	11.0(4)
O1	85(2)	34.4(15)	46.6(17)	18.2(14)	41.0(17)	24.3(15)
N2	63(2)	21.5(14)	34.5(16)	6.8(13)	25.5(15)	10.5(13)
O2	73(2)	34.7(15)	39.8(16)	13.1(13)	18.0(15)	17.9(14)
C3	30.4(16)	28.1(16)	31.1(17)	6.8(14)	2.1(13)	2.5(13)
C2	49(2)	35.3(19)	35.1(19)	13.6(17)	16.3(16)	6.7(16)

C1	47(2)	31.9(19)	46(2)	17.1(17)	14.8(17)	10.4(16)
C4	36.4(17)	29.7(17)	36.3(18)	12.3(15)	7.7(14)	5.3(14)
N1	37.6(16)	31.8(16)	37.0(16)	10.1(14)	9.6(13)	10.6(13)
C5	37.3(18)	43(2)	44(2)	19.7(18)	14.0(16)	10.7(16)
C6	39.1(18)	26.1(16)	30.0(17)	5.5(15)	6.5(14)	3.6(14)

Table S18. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for [Cu(Ina)₂Br₂] (**5**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Br(01)	4687(3)	2640(2)	2369(13)	40(1)
Br(02)	7797(3)	1610(2)	3903(14)	42(1)
Cu(1)	3768(3)	2140(2)	-3139(18)	40(2)
Br(04)	9684(5)	2631(4)	1890(20)	40(2)
Br(4)	2802(5)	1619(4)	-540(18)	27(2)
Br(2)	9692(5)	2653(4)	-2081(17)	25(2)
Cu(2)	8761(7)	2143(5)	1270(30)	35(2)
C(22)	5947(13)	1114(9)	-2020(60)	0(4)
N(22)	6130(14)	-366(9)	-2050(70)	15(6)
C(16)	1230(20)	4143(14)	-4320(90)	20(7)
O(31)	12047(17)	233(9)	1140(90)	44(9)
C(14)	2587(19)	3734(13)	-3600(80)	15(6)
O(11)	450(20)	4067(19)	-4840(190)	160(30)
N(21)	4570(13)	1469(9)	-2780(70)	21(7)
C(13)	1840(20)	3654(13)	-3920(90)	20(7)
N(11)	2920(30)	2784(15)	-3470(90)	44(10)
C(21)	5348(16)	1536(11)	-2330(70)	16(7)
C(15)	3165(19)	3299(13)	-3390(80)	18(7)
C(35)	9300(20)	955(16)	-220(120)	40(10)
N(12)	1480(20)	4661(13)	-4490(140)	69(17)
C(34)	9880(20)	516(13)	60(140)	50(15)
C(23)	5750(20)	575(13)	-2170(130)	55(16)
C(36)	11330(30)	100(20)	700(400)	200(70)
O(21)	6880(20)	19(12)	2600(200)	800(40)
C(11)	2130(40)	2690(50)	-3690(130)	200(60)
C(24)	4830(40)	510(20)	-2800(300)	310(100)
C(26)	6410(40)	150(20)	-2100(300)	140(50)
C(25)	4270(40)	1000(30)	-2900(200)	420(150)
Br(5)	2806(5)	1603(4)	-6590(20)	38(2)
N(32)	11136(19)	-332(12)	-100(300)	680(100)
N(31)	9560(30)	1479(18)	1620(120)	57(10)
C(31)	10370(30)	1580(20)	3460(150)	62(13)
C(32)	10930(40)	1140(20)	3950(160)	70(15)
C(33)	10730(30)	560(20)	1730(150)	61(14)
C(12)	1640(40)	3100(30)	-3850(140)	85(19)
Cu(2)	8755(7)	2124(5)	7400(30)	35(2)

Table S19. Anisotropic Displacement Parameters (Å²×10³) for $^{1}_{\infty}$[Cu(Ina)₂Br₂] (**5**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Br(1)	27(2)	22(2)	71(3)	5(2)	3(2)	-3(2)
Br(2)	26(2)	24(2)	75(4)	4(2)	5(2)	-4(2)

Cu(1)	21(2)	18(2)	81(5)	-3(2)	3(2)	6(1)
Br(3)	39(5)	36(4)	41(6)	-7(4)	-7(4)	-6(4)
Br(4)	45(4)	39(4)	0(4)	-1(3)	15(3)	-7(3)
Br(2)	40(4)	39(4)	0(4)	-1(3)	15(3)	-1(3)
Cu(2)	33(4)	28(4)	48(7)	15(4)	26(4)	8(3)
C(22)	0(9)	0(10)	0(14)	0(8)	-3(8)	-6(7)
N(22)	0(10)	0(10)	47(18)	6(10)	12(10)	-1(7)
C(16)	30(20)	12(16)	20(20)	-1(12)	1(14)	0(13)
O(31)	29(17)	0(11)	100(30)	-9(13)	-6(16)	4(10)
C(14)	19(16)	20(16)	8(17)	2(11)	13(12)	2(11)
O(11)	30(20)	110(30)	340(90)	100(40)	110(40)	50(20)
N(21)	1(10)	0(10)	60(20)	1(10)	2(10)	18(8)
C(13)	18(16)	10(14)	30(20)	0(12)	0(13)	14(11)
N(11)	70(30)	40(20)	30(20)	7(14)	-14(17)	6(16)
C(21)	3(13)	0(12)	50(20)	-1(12)	5(13)	-2(9)
C(15)	14(15)	19(16)	20(20)	-3(12)	2(12)	0(11)
C(35)	18(17)	20(20)	80(30)	-10(18)	1(16)	13(14)
N(12)	10(15)	10(15)	180(50)	20(20)	-10(20)	-5(11)
C(34)	9(16)	0(14)	130(50)	-5(18)	-29(19)	5(11)
C(23)	17(18)	4(16)	140(50)	20(20)	0(20)	-23(13)
C(36)	0(20)	20(30)	600(200)	50(60)	-50(50)	-3(19)
O(21)	400(20)	230(20)	2000(110)	140(60)	1020(50)	0(20)
C(11)	10(30)	170(110)	430(190)	-30(110)	10(50)	20(40)
C(24)	30(30)	0(20)	900(300)	-70(70)	50(80)	10(20)
C(26)	60(40)	20(30)	350(160)	-10(50)	-10(60)	30(30)
C(25)	30(40)	20(30)	1100(400)	90(90)	-150(100)	-10(30)
Br(5)	37(4)	35(4)	38(6)	-5(4)	-7(3)	-1(3)
N(32)	48(17)	50(17)	2000(300)	380(60)	330(60)	-57(10)

Table S20. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for $^2_\infty$[Cu(Pya)$_2$](BF$_4$)$_2$ (**9**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Cu01	5000	0	5000	28.4(2)
O11	7352(3)	-310(3)	5434(2)	29.9(7)
F4	8192(4)	609(3)	2555(3)	76.1(9)
F2	9649(4)	-991(3)	2045(3)	82.1(10)
F3	7430(4)	-257(4)	392(3)	94.1(11)
N12	4853(3)	-1208(3)	3429(3)	24.1(7)
N11	5097(4)	-3034(3)	1472(3)	32.5(8)
N13	9155(4)	-1703(4)	5022(3)	41.0(9)
C15	7689(5)	-1218(4)	4739(4)	28.0(9)
C14	6314(4)	-1760(4)	3517(4)	24.8(8)
C13	6415(5)	-2671(4)	2558(4)	31.6(9)
F1	9608(5)	1114(4)	1208(4)	107.4(13)
C11	3700(5)	-2441(4)	1391(4)	34.1(9)
C12	3531(5)	-1551(4)	2349(4)	31.5(9)
B11	8681(6)	122(6)	1511(5)	44.0(12)

Table S21. Anisotropic Displacement Parameters (Å^2×10^3) for $^2_\infty$[Cu(Pya)$_2$](BF$_4$)$_2$ (**9**). The Anisotropic displacement

factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu01	28.1(3)	33.9(4)	25.0(3)	-9.3(4)	11.6(2)	1.3(4)
O11	26.6(13)	36.6(18)	26.8(13)	-7.1(12)	9.5(10)	3.1(11)
F4	84(2)	82(2)	75(2)	-16.4(17)	43.7(17)	-0.7(17)
F2	85(2)	71(2)	80(2)	-1.5(19)	16.4(18)	19.0(18)
F3	85(2)	110(3)	59.8(18)	-13.3(19)	-10.6(16)	-17(2)
N12	23.5(16)	24.8(17)	25.3(17)	0.7(14)	9.8(13)	3.3(13)
N11	32(2)	34.4(19)	29.8(19)	-7.4(15)	9.2(15)	-0.8(15)
N13	30(2)	50(2)	38(2)	-13.2(18)	5.2(16)	10.4(16)
C15	33(2)	28(2)	24(2)	3.4(17)	10.7(17)	-0.8(17)
C14	29(2)	25(2)	22.0(19)	3.2(16)	10.8(16)	-0.4(16)
C13	34(2)	31(2)	33(2)	-6.0(19)	15.5(18)	1.7(18)
F1	128(3)	102(3)	104(3)	15(2)	55(2)	-60(2)
C11	32(2)	33(2)	35(2)	-2.3(19)	8.7(19)	-4.5(18)
C12	30(2)	34(2)	30(2)	-5.1(18)	8.5(18)	3.5(18)
B11	46(3)	49(3)	36(2)	0(3)	12(2)	-10(3)

Table S22. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2\times 10^3$) for $[Cu(Pya)_2(H_2O)(NO_3)](NO_3)$ (**10**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cu01	1242.8(8)	3408.3(8)	2567.2(6)	32.50(19)
O11	1165(4)	3641(4)	4224(3)	37.2(9)
O43	-1705(4)	4808(4)	2371(3)	47.2(10)
O21	1104(4)	3376(3)	929(3)	36.8(9)
O05	3274(4)	1923(4)	2455(4)	58.2(11)
N21	2967(4)	5299(4)	3096(3)	26.6(9)
O42	-4050(4)	3406(4)	1021(3)	50.8(10)
O31	1890(4)	-465(4)	3814(3)	53.8(10)
O41	-3527(4)	3553(4)	2895(3)	52.5(10)
O33	379(4)	-2564(4)	2380(3)	51.3(10)
N23	2119(5)	4594(4)	-111(3)	39.8(11)
N22	5498(5)	7676(5)	3431(4)	44.2(12)
O32	1907(5)	-1037(4)	1904(3)	60.0(11)
N41	-3109(5)	3928(4)	2090(4)	34.6(10)
N11	-647(4)	1637(4)	2069(3)	25.3(9)
N12	-3153(5)	-722(5)	1757(4)	45.9(13)
N31	1397(5)	-1349(5)	2711(4)	38.3(10)
N13	14(5)	2562(4)	5310(3)	40.7(11)
C14	-950(5)	1420(5)	3059(4)	24.5(12)
C25	2104(5)	4454(5)	914(4)	29.0(12)
C22	3261(5)	5563(5)	2118(4)	24.7(12)
C12	-2852(6)	-458(6)	803(5)	40.7(14)
C24	3921(6)	6221(5)	4219(4)	33.7(12)
C11	-2200(6)	220(5)	2871(5)	37.0(13)
C15	133(5)	2591(5)	4251(4)	29.3(12)
C13	-1582(6)	715(5)	955(4)	30.7(12)

C23	5169(6)	7398(6)	4371(5)	40.8(14)
C21	4528(6)	6749(5)	2313(4)	34.0(13)

Table S23. Anisotropic Displacement Parameters ($Å^2×10^3$) for $[Cu(Pya)_2(H_2O)(NO_3)](NO_3)$ (**10**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu01	36.8(3)	34.8(3)	22.5(3)	13.1(3)	5.2(2)	-14.7(2)
O11	42(2)	41.3(19)	26(2)	15.2(16)	7.5(15)	-13.4(16)
O43	51(2)	45(2)	39(2)	17.1(18)	9.0(16)	-21.6(17)
O21	43.7(19)	41.1(19)	22.3(19)	15.6(16)	4.7(14)	-14.2(15)
O05	40(2)	48(2)	94(3)	38(2)	20(2)	-2.9(17)
N21	26(2)	31(2)	23(2)	13(2)	6.0(17)	-2.7(17)
O42	50(2)	57(2)	31(2)	17.2(19)	-5.9(18)	-15.3(18)
O31	67(2)	43(2)	28(2)	-1.2(19)	3.3(19)	-13.9(18)
O41	52(2)	70(2)	47(3)	36(2)	17.8(19)	-7.0(18)
O33	61(2)	45(2)	34(2)	14.7(18)	0.9(16)	-25.7(17)
N23	49(2)	46(3)	21(2)	17(2)	2.9(19)	-11(2)
N22	48(3)	43(3)	38(3)	18(2)	8(2)	-11(2)
O32	85(3)	60(2)	45(2)	32(2)	24(2)	-6(2)
N41	38(2)	34(2)	32(3)	15(2)	8.8(19)	-4.4(18)
N11	27(2)	27(2)	19(2)	8.7(19)	5.9(17)	-6.1(17)
N12	48(3)	42(3)	36(3)	12(2)	5(2)	-19(2)
N31	41(2)	40(3)	38(3)	21(2)	10(2)	0(2)
N13	47(2)	48(2)	23(2)	13(2)	9.7(19)	-14(2)
C14	26(3)	28(3)	20(3)	12(2)	6(2)	3(2)
C25	32(3)	29(3)	33(3)	17(2)	14(2)	4(2)
C22	26(3)	29(3)	25(3)	17(2)	8(2)	6(2)
C12	43(3)	38(3)	27(3)	6(3)	1(2)	-14(2)
C24	36(3)	38(3)	23(3)	13(3)	3(2)	-4(2)
C11	41(3)	38(3)	29(3)	15(3)	5(2)	-10(2)
C15	31(3)	30(3)	29(3)	15(2)	9(2)	0(2)
C13	38(3)	31(3)	16(3)	6(2)	4(2)	-5(2)
C23	40(3)	43(3)	32(3)	17(3)	-2(2)	-13(2)
C21	38(3)	38(3)	27(3)	18(3)	5(2)	-9(2)

Table S24. Fractional Atomic Coordinates ($×10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2×10^3$) for $^1_\infty[Cu(Pya)(NO_3)_2]$ (**11**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cu1	1145.5(2)	-5601.5(5)	1381.7(2)	19.21(11)
O11	1356.0(10)	-2826(3)	1271.9(14)	29.5(5)
O21	2006.1(8)	-7268(3)	1631.8(16)	31.4(5)
O22	2821.4(11)	-7811(5)	1115(2)	56.0(8)
O23	2538.3(12)	-4818(4)	1258(2)	52.7(7)
O31	808.5(9)	-8291(3)	1394.4(16)	30.5(5)
O32	-57.8(17)	-9592(6)	1318(3)	97.2(14)
O33	33.2(12)	-6438(6)	1174(3)	69.3(9)

N11	1109.0(9)	-5508(4)	-130.3(15)	19.0(5)
N12	1130.7(10)	-4830(4)	-2143.1(16)	19.4(5)
N13	1787.0(12)	-776(4)	320.2(19)	32.6(6)
N21	2467.7(10)	-6617(4)	1346.2(19)	28.9(6)
N31	238.3(13)	-8133(5)	1288(2)	42.4(8)
C11	900.6(12)	-6850(5)	-829(2)	22.5(6)
C12	906.9(12)	-6502(5)	-1856(2)	23.7(6)
C13	1348.1(12)	-3482(4)	-1434.7(19)	21.6(6)
C14	1333.8(11)	-3818(4)	-416.8(19)	19.4(6)
C15	1508.3(12)	-2383(4)	449(2)	22.2(6)

Table S25. Anisotropic Displacement Parameters ($Å^2×10^3$) for $^1_\infty$[Cu(Pya)(NO_3)$_2$] (**11**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Cu1	25.17(17)	21.5(2)	12.62(16)	-0.82(14)	7.80(11)	-3.58(15)
O11	48.2(12)	25.6(14)	17.8(10)	-3.3(8)	13.8(9)	-7.3(10)
O21	23.9(10)	36.5(14)	36.3(12)	2.2(10)	12.3(9)	-0.9(9)
O22	33.0(13)	58(2)	83(2)	0.1(15)	25.6(13)	15.0(12)
O23	61.0(17)	35.1(18)	71.4(19)	-9.1(13)	35.6(15)	-15.5(13)
O31	32.8(11)	25.9(13)	34.7(12)	-2.9(9)	11.3(9)	-6.1(9)
O32	92(2)	111(3)	93(3)	-20(2)	30(2)	-85(2)
O33	33.5(14)	92(3)	81(2)	10.3(19)	6.9(14)	14.2(16)
N11	21.0(10)	22.3(14)	15.0(10)	0.3(9)	6.4(8)	-1.8(9)
N12	21.4(10)	24.3(14)	14.0(10)	0.9(8)	7.0(8)	1.9(9)
N13	48.3(15)	25.5(16)	27.1(13)	-5.5(11)	14.6(11)	-13.2(12)
N21	21.9(12)	39.8(19)	25.1(13)	-1.6(11)	5.0(9)	-2.3(11)
N31	38.4(16)	57(2)	33.5(15)	-8.6(14)	11.7(12)	-24.7(16)
C11	26.8(14)	22.4(17)	19.0(13)	-1.0(11)	6.2(10)	-6.0(11)
C12	24.1(13)	27.0(17)	21.0(14)	-3.7(11)	7.1(11)	-5.0(12)
C13	25.3(13)	23.5(17)	17.6(13)	1.0(11)	7.8(10)	-0.6(11)
C14	20.9(12)	20.1(16)	18.2(13)	2.7(10)	6.4(10)	-0.5(10)
C15	30.8(14)	19.3(16)	17.6(13)	-0.1(10)	7.8(10)	-1.7(11)

Table S26. Fractional Atomic Coordinates ($×10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2×10^3$) for $^2_\infty$[Cu(Pyc)(Tfa)] (**12**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Cu01	2486.5(19)	2123.8(9)	8606.6(7)	26.1(3)
O12	6234(8)	3982(6)	10314(4)	30.5(15)
N12	5726(10)	5641(8)	7148(6)	31.7(19)
O1	882(8)	1893(7)	7365(4)	35.6(18)
O11	4095(10)	2619(8)	9786(5)	56(2)
N11	3646(9)	3681(8)	7899(5)	29.1(19)
F2	-1631(15)	1081(10)	5886(7)	129(4)
C13	5967(11)	5127(9)	8164(6)	28(2)
F1	-761(12)	2770(10)	5392(5)	115(4)
C14	4923(9)	4169(8)	8532(7)	21.2(18)

C15	5125(11)	3550(9)	9645(7)	26(2)
C11	3363(12)	4203(10)	6893(7)	36(3)
C12	4390(12)	5172(10)	6556(8)	41(3)
O2	-1202(14)	3162(12)	7922(6)	110(5)
C1	-520(14)	2412(13)	7280(8)	50(4)
F3	-3129(10)	2606(15)	6247(10)	166(6)
C2	-1507(13)	2216(16)	6187(8)	51(3)

Table S27. Anisotropic Displacement Parameters ($Å^2×10^3$) for $^2_\infty$[Cu(Pyc)(Tfa)] (**12**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Cu01	29.5(4)	32.9(5)	16.0(4)	2.0(5)	0.6(7)	-2.6(8)
O12	40(4)	31(4)	21(3)	5(3)	-15(3)	-5(3)
N12	44(4)	28(5)	23(4)	13(3)	4(4)	-11(4)
O1	25(3)	53(6)	29(3)	-7(3)	-4(3)	6(3)
O11	68(5)	66(7)	34(4)	4(4)	-10(3)	-17(5)
N11	33(4)	35(6)	20(4)	-3(3)	4(3)	-7(4)
F2	219(12)	87(9)	81(5)	-10(5)	-61(6)	-41(7)
C13	27(5)	35(7)	21(4)	-2(4)	-5(4)	-4(4)
F1	147(8)	170(10)	30(4)	29(5)	-22(4)	-59(8)
C14	22(4)	21(5)	20(4)	4(4)	7(4)	0(3)
C15	26(5)	27(6)	24(4)	-3(4)	5(4)	-4(4)
C11	38(5)	42(7)	27(5)	10(4)	-9(4)	-22(5)
C12	45(6)	57(8)	20(5)	18(5)	-12(4)	-12(5)
O2	134(8)	163(13)	32(4)	4(5)	2(5)	106(9)
C1	43(6)	79(12)	30(5)	8(6)	12(5)	4(6)
F3	55(4)	290(17)	152(9)	-53(12)	-52(5)	50(7)
C2	27(6)	94(11)	31(6)	0(7)	-12(4)	10(6)

Table S28. Fractional Atomic Coordinates ($×10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2×10^3$) for $[Cu(2\text{-}Aba)_2(NO_3)_2]$ (**13**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Cu1	10000	0	10000	47.3(3)
O3	11333(5)	1050(3)	8430(5)	60.4(9)
O1	10195(5)	988(2)	11642(4)	51.2(8)
O4	13205(6)	1888(3)	7694(4)	62.7(10)
N3	12902(6)	1382(3)	8735(5)	50.1(9)
C6	12155(6)	65(3)	13932(5)	42.9(9)
N2	11071(6)	1642(3)	14111(5)	49.4(9)
N1	12601(6)	-372(4)	11399(5)	50.1(9)
C7	11114(6)	928(3)	13166(5)	43.0(9)
C5	12390(7)	-172(3)	15537(5)	46.0(10)
O2	14181(7)	1212(5)	10022(6)	105(2)
C4	13234(7)	-999(4)	16255(6)	55.0(12)
C1	12817(6)	-574(3)	13062(5)	43.9(10)
C3	13859(7)	-1623(4)	15380(7)	55.9(12)

C2	13638(7)	-1409(4)	13774(7)	53.8(11)

Table S29. Anisotropic Displacement Parameters ($Å^2×10^3$) for $[Cu(_2\text{-Aba})_2(NO_3)_2]$ (**13**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu1	50.4(5)	52.2(5)	36.7(4)	-2.1(3)	13.4(3)	5.2(4)
O3	55(2)	66(2)	60(2)	1.7(17)	20.6(17)	-12.7(17)
O1	62(2)	51.7(17)	35.5(15)	-1.6(13)	12.8(14)	8.3(15)
O4	77(3)	68(2)	48.4(19)	-3.6(17)	28.4(19)	-23.8(19)
N3	53(2)	53(2)	43.6(19)	-4.8(16)	17.6(18)	-3.7(18)
C6	43(2)	43(2)	43(2)	-1.2(18)	16.6(17)	-7.7(19)
N2	58(2)	46(2)	44(2)	-1.7(16)	18.6(19)	3.5(18)
N1	51(2)	61(2)	40.6(19)	-1.2(18)	20.8(18)	4(2)
C7	46(2)	45(2)	39(2)	-0.4(16)	16.6(18)	-4.0(18)
C5	53(2)	46(3)	36.6(19)	-0.7(16)	13.9(18)	-5.3(18)
O2	71(3)	149(5)	65(3)	38(3)	-9(2)	-23(3)
C4	55(3)	58(3)	45(2)	11(2)	10(2)	-6(2)
C1	40(2)	50(2)	39(2)	-1.3(17)	11.7(18)	-4.6(17)
C3	51(3)	49(3)	64(3)	11(2)	18(2)	-1(2)
C2	49(3)	50(2)	64(3)	1(2)	23(2)	5(2)

Table S30. Fractional Atomic Coordinates ($×10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2×10^3$) for $^1_\infty[Cu_2(4\text{-Aba})_2(H_2O)_3(NO_3)_3](NO_3)$ (**14**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cu01	8573.5(3)	6536.1(5)	9323.7(6)	39.4(3)
O02	9616(2)	3144(4)	9702(4)	50.2(10)
O001	7924(2)	5727(4)	7806(4)	57.2(11)
O01	9318(2)	4448(4)	8123(4)	57.9(12)
O11	8746(2)	7788(3)	8281(4)	50.7(10)
O21	8135(2)	5810(4)	10425(4)	51.2(10)
N11	9247(2)	7255(4)	10943(4)	37.0(10)
O03	9218(2)	4879(4)	9917(4)	49.1(10)
N21	9153(3)	6924(4)	6948(5)	53.0(14)
N02	7699(4)	6594(9)	10281(9)	42(2)
C15	8767(3)	10096(5)	7396(5)	37.9(12)
N01	9378(2)	4159(4)	9235(4)	37.4(10)
C12	9400(3)	9444(5)	10794(5)	38.6(12)
C14	9009(2)	9128(4)	6933(5)	34.3(11)
O31	7895(4)	3272(8)	8485(10)	56(2)
C16	8840(3)	8712(5)	12076(5)	39.9(12)
C11	9168(2)	8482(4)	11287(5)	33.4(10)
C17	8964(3)	7883(5)	7405(5)	36.9(11)
C13	9321(3)	10635(5)	11117(5)	38.3(11)
N03	7722(5)	2909(10)	9422(13)	67(4)
O32	7650(8)	3676(11)	10212(14)	77(4)
O22	7308(5)	6523(9)	10776(10)	60(2)

O23	7703(4)	7497(9)	9578(9)	53(2)
O33	7552(9)	1781(11)	9610(13)	82(4)

Table S31. Anisotropic Displacement Parameters ($Å^2×10^3$) for $^1_\infty$[Cu_2(4-Aba)$_2$(H_2O)$_3$(NO_3)$_3$](NO_3) (**14**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Cu01	54.8(5)	30.1(4)	38.8(4)	-0.6(3)	24.3(3)	-3.9(3)
O02	63(3)	31.4(19)	66(3)	7.0(18)	36(2)	9.5(18)
O001	71(3)	49(2)	46(2)	-0.9(19)	18(2)	-7(2)
O01	89(3)	42(2)	49(3)	2.2(18)	34(2)	7(2)
O11	81(3)	35(2)	51(2)	3.0(17)	41(2)	-2.7(19)
O21	51(2)	53(2)	54(3)	5.4(19)	25(2)	2(2)
N11	46(3)	28(2)	41(2)	-1.3(17)	22(2)	0.9(17)
O03	62(3)	38(2)	46(2)	-3.5(17)	21(2)	13.3(18)
N21	87(4)	27(2)	62(3)	5(2)	48(3)	6(2)
N02	43(5)	52(5)	36(5)	7(4)	22(4)	-3(4)
C15	45(3)	33(3)	42(3)	3(2)	25(2)	0(2)
N01	43(2)	26(2)	41(2)	0.2(17)	15(2)	-0.4(17)
C12	47(3)	33(3)	44(3)	-4(2)	27(3)	-1(2)
C14	39(3)	30(2)	35(3)	3.4(19)	16(2)	0.2(19)
O31	64(5)	45(5)	72(6)	-38(4)	42(5)	-37(4)
C16	50(3)	33(3)	43(3)	-1(2)	25(3)	-3(2)
C11	39(3)	29(2)	33(2)	-5.2(19)	15(2)	-3(2)
C17	49(3)	30(2)	34(3)	2.2(19)	19(2)	-1(2)
C13	50(3)	30(2)	39(3)	-2(2)	22(2)	-2(2)
N03	49(6)	46(6)	77(9)	-18(6)	-5(6)	-6(5)
O32	116(11)	45(7)	74(8)	-4(6)	44(8)	-13(6)
O22	63(6)	68(6)	62(6)	7(5)	39(5)	5(5)
O23	61(5)	57(5)	54(5)	-3(4)	35(4)	4(4)
O33	130(12)	46(7)	61(7)	4(5)	30(7)	-18(7)

Table S32. Fractional Atomic Coordinates ($×10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2×10^3$) for $^2_\infty$[Cu(4-Aba)$_2$($EtOH$)$_2$](ClO_4)$_2$ (**15**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Cl1	-3276.5(11)	-568.2(5)	-6815.8(8)	48.5(3)
O1	-3050(10)	-657(3)	-7969(6)	149(2)
O2	-2042(6)	-1044(3)	-5684(4)	124.3(18)
O3	-5064(6)	-857(3)	-7267(6)	123.5(16)
O4	-3215(7)	303(2)	-6461(4)	106.6(15)
Cu1	0	-5000	-5000	34.5(2)
O11	438(3)	-4022.5(12)	-3776(2)	41.0(5)
O21	2626(4)	-5845.9(15)	-3129(3)	50.8(6)
N11	1929(4)	-515.7(15)	-429(3)	36.7(5)
N12	1657(4)	-4599.2(18)	-1652(3)	47.8(7)
C11	1694(4)	-1380.2(17)	-946(3)	33.8(6)
C12	2363(4)	-2062.1(19)	-15(3)	39.7(6)

C13	2133(4)	-2893.6(19)	-505(3)	40.0(6)
C14	1242(4)	-3057.8(17)	-1932(3)	34.6(6)
C15	578(4)	-2369.9(18)	-2842(3)	38.5(6)
C16	815(4)	-1538.6(18)	-2354(3)	37.5(6)
C17	1087(4)	-3936.3(17)	-2489(3)	35.2(6)
C21	4031(8)	-6869(3)	-3961(7)	71.7(12)
C22	2958(5)	-6743(2)	-3235(4)	51.4(8)

Table S33. Anisotropic Displacement Parameters ($Å^2×10^3$) for $^2_\infty$[Cu(4-Aba)$_2$(EtOH)$_2$](ClO$_4$)$_2$ (**15**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Cl1	52.3(5)	42.9(4)	44.2(4)	-0.6(3)	19.5(3)	-1.2(3)
O1	268(7)	120(4)	134(4)	-33(3)	156(5)	-55(4)
O2	109(3)	91(3)	92(3)	17(2)	-10(2)	24(2)
O3	65(2)	141(4)	147(4)	-14(3)	40(2)	-22(2)
O4	172(4)	49.3(18)	67(2)	-12.0(17)	35(2)	-2(2)
Cu1	52.1(4)	23.2(3)	32.7(3)	-3.75(16)	24.5(2)	-5.60(18)
O11	59.5(13)	27.6(10)	37.9(10)	-4.8(8)	25.9(10)	-3.4(8)
O21	54.3(15)	37.1(12)	58.1(14)	-3.2(10)	25.9(12)	0.0(10)
N11	46.4(14)	25.9(11)	39.2(12)	-4.5(9)	22.5(12)	-2.0(9)
N12	72(2)	28.8(13)	40.3(15)	-2.4(11)	25.9(14)	1.4(12)
C11	39.5(14)	26.9(13)	38.6(13)	-4.4(10)	22.3(11)	0.2(10)
C12	50.6(17)	32.2(14)	32.4(13)	-2.7(10)	17.8(12)	4.1(11)
C13	55.7(18)	29.7(13)	33.7(13)	0.3(11)	21.6(13)	2.4(12)
C14	41.0(14)	28.3(13)	35.6(13)	-3.5(10)	19.9(11)	-1.6(10)
C15	49.3(16)	33.0(14)	33.3(13)	-2.7(11)	20.7(13)	2.3(11)
C16	47.7(16)	30.0(14)	35.5(13)	-0.2(11)	21.3(12)	5.1(11)
C17	45.6(15)	28.8(13)	35.3(13)	-5.3(10)	23.3(12)	-2.7(10)
C21	67(3)	59(3)	101(4)	-8(2)	51(3)	2(2)
C22	55(2)	36.1(16)	63(2)	2.6(14)	29.5(17)	3.3(14)

Table S34. Fractional Atomic Coordinates ($×10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2×10^3$) for $^2_\infty$[Cu(4-Aba)$_2$(EtOH)$_2$](BF$_4$)$_2$ (**16**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
F1	-5047(4)	-810(2)	-7375(4)	96.8(10)
F2	-2862(7)	-591(2)	-7848(5)	129.8(16)
F3	-2178(5)	-984.0(19)	-5708(3)	110.3(13)
F4	-3299(4)	319.7(16)	-6464(3)	87.6(10)
B1	-3303(5)	-522(2)	-6834(4)	35.6(8)
Cu1	0	0	0	23.02(14)
O1	-2653(3)	-851.0(13)	-1893(2)	39.0(5)
O11	-448(3)	975.9(12)	-1235(2)	29.5(4)
N11	1929(3)	-505.0(14)	-429(2)	26.1(5)
N12	-1701(4)	404.2(15)	-3385(3)	37.2(6)
C1	-4004(5)	-1907(3)	-1046(5)	59.6(11)
C2	-2951(4)	-1756.2(19)	-1781(4)	40.4(7)

C11	1719(3)	-1372.3(16)	-933(3)	22.3(5)
C12	816(4)	-1533.3(17)	-2366(3)	26.4(6)
C13	591(4)	-2370.9(17)	-2841(3)	26.7(6)
C14	1271(3)	-3055.0(16)	-1912(3)	23.3(5)
C15	2171(4)	-2884.2(17)	-483(3)	29.0(6)
C16	2390(4)	-2050.8(17)	0(3)	28.1(6)
C17	-1111(4)	1060.7(16)	-2529(3)	24.1(5)

Table S35. Anisotropic Displacement Parameters ($Å^2×10^3$) for $^2_\infty$[Cu(4-Aba)$_2$(EtOH)$_2$](BF$_4$)$_2$ (**16**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
F1	52.0(15)	108(2)	111(3)	-21.1(19)	26.0(16)	-20.1(14)
F2	224(5)	100(3)	153(4)	-18(2)	161(4)	-30(3)
F3	111(3)	77(2)	76(2)	20.5(16)	-4.4(18)	19.3(17)
F4	136(3)	41.9(13)	59.0(16)	-13.0(12)	29.0(17)	-3.0(15)
B1	38.3(18)	31.6(18)	31.0(17)	-1.2(14)	12.7(15)	-2.4(13)
Cu1	39.7(3)	12.9(2)	21.9(2)	3.7(2)	19.48(18)	5.40(19)
O1	44.8(12)	27.3(11)	42.8(13)	1.9(9)	20.1(10)	-2.4(9)
O11	48.8(12)	17.4(9)	25.1(10)	5.9(8)	20.5(9)	4.3(8)
N11	36.1(13)	16.6(11)	28.8(12)	-4.7(9)	18.7(10)	-2.4(8)
N12	63.3(18)	16.5(12)	28.6(13)	1.7(10)	20.5(13)	-0.6(11)
C1	51(2)	53(2)	86(3)	14(2)	43(2)	0.5(17)
C2	41.3(17)	26.5(15)	50(2)	-5.1(14)	20.4(15)	-4.9(12)
C11	27.9(13)	15.7(12)	27.2(13)	-4.5(10)	16.7(11)	-0.2(9)
C12	38.2(14)	19.0(13)	24.5(13)	0.4(10)	17.6(11)	4.4(10)
C13	36.4(15)	22.2(13)	21.6(12)	-2.6(10)	14.6(12)	1.1(10)
C14	30.5(13)	17.6(12)	23.3(13)	-4.3(10)	14.7(11)	-1.3(9)
C15	42.3(16)	18.7(13)	22.6(13)	0.9(10)	13.6(12)	5.6(11)
C16	40.2(15)	21.9(14)	19.9(12)	-3.1(10)	13.2(12)	3.6(10)
C17	32.8(14)	17.9(12)	26.7(13)	4.6(10)	18.7(11)	2.7(9)

Table S36. Fractional Atomic Coordinates ($×10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2×10^3$) for [Cu(4-HAba)$_2$Cl$_4$] (**17**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Cu1	-5000	0	5000	19.7(5)
Cl1	-3945(2)	-713.7(14)	7566(4)	25.7(6)
Cl2	-13293(2)	1620.3(15)	15147(4)	27.6(7)
N1	-12834(7)	1192(5)	10114(13)	23.7(18)
C15	-9140(9)	1834(6)	9781(16)	26(2)
C13	-9368(9)	570(6)	7439(14)	22(2)
O1	-6519(6)	396(4)	7061(10)	22.3(14)
C12	-10772(9)	570(6)	7991(13)	20.6(19)
C11	-11333(8)	1192(5)	9459(14)	20(2)
C14	-8536(8)	1204(6)	8302(15)	19.0(19)
C16	-10538(10)	1827(6)	10372(16)	26(2)
C17	-7040(9)	1182(5)	7566(13)	16.7(18)

N2	-6314(7)	1959(5)	7459(13)	25.1(19)

Table S37. Anisotropic Displacement Parameters ($Å^2×10^3$) for $[Cu(4\text{-}HAba)_2Cl_4]$ (**17**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu1	16.1(8)	25.3(8)	16.6(9)	1.7(6)	1.9(6)	7.8(6)
Cl1	25.9(12)	24.1(11)	28.6(14)	2.9(9)	-9.2(9)	-0.2(8)
Cl2	25.3(12)	22.8(11)	33.7(15)	-1.9(9)	-0.5(10)	-4.7(8)
N1	13(4)	24(4)	33(5)	-3(3)	0(3)	2(3)
C15	16(4)	25(5)	37(6)	-15(4)	-4(4)	2(3)
C13	25(5)	22(4)	20(5)	-6(4)	0(4)	1(3)
O1	23(3)	22(3)	21(4)	-3(3)	4(3)	7(2)
C12	21(4)	22(4)	20(5)	-2(3)	-7(4)	-2(3)
C11	12(4)	19(4)	27(6)	6(3)	3(4)	2(3)
C14	15(4)	21(4)	22(5)	5(3)	-4(4)	3(3)
C16	24(5)	23(5)	28(6)	-6(4)	4(4)	4(4)
C17	24(5)	15(4)	10(5)	5(3)	1(3)	3(3)
N2	17(4)	19(4)	39(5)	-2(3)	-2(3)	-1(3)

Table S38. Fractional Atomic Coordinates ($×10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2×10^3$) for $[Cu(Tba)_2](ClO_4)_2$ (**18**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cu1	0	0	0	26.7(2)
S11	2377.7(9)	0	606(2)	37.4(3)
O11	469.8(17)	852.5(14)	2649(4)	34.8(5)
N11	1794(3)	1530.4(18)	5761(6)	46.4(7)
C11	1542(2)	1070.0(19)	3744(6)	31.9(7)
C12	2606(3)	858(2)	2730(8)	45.2(9)
Cl1	0	3010.7(7)	0	36.7(3)
O1	1016(3)	2535(2)	-156(8)	77.3(10)
O3	392(4)	3513(4)	2075(11)	150(3)

Table S39. Anisotropic Displacement Parameters ($Å^2×10^3$) for $[Cu(Tba)_2](ClO_4)_2$ (**18**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu1	21.1(3)	32.8(4)	24.1(4)	0	3.0(3)	0
S11	31.4(5)	44.5(6)	39.5(8)	0	15.5(5)	0
O11	23.2(9)	46.5(12)	33.1(13)	-8.4(10)	5.2(8)	0.3(8)
N11	36.3(15)	59.3(18)	39.3(19)	-15.4(14)	3.6(12)	-6.3(13)
C11	28.2(13)	33.1(15)	32.4(19)	2.2(12)	5.3(12)	-0.8(11)
C12	30.4(15)	49.9(19)	57(3)	-11.2(17)	15.9(15)	-10.0(13)
Cl1	23.7(5)	42.4(6)	41.9(7)	0	5.9(4)	0
O1	48.7(15)	61.7(19)	136(3)	2.4(18)	49.4(19)	7.6(13)
O3	62(2)	226(6)	155(5)	-139(4)	21(2)	-26(3)