Table S1. Crystal data and structure refinement for 1.

Identification code	1	
Chemical formula (moiety)	$C_{10}H_{10}Cu_2O_{12}\cdot 2H_2O$	
Chemical formula (total)	$C_{10}H_{14}Cu_2O_{14}$	
Formula weight	485.29	
Temperature	240(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 6.5120(10) Å	α = 95.448(10)°
	b = 6.9010(10) Å	β = 108.706(8)°
	c = 9.328(2) Å	γ = 108.090(8)°
Cell volume	368.51(11) Å^3	
Z	1	
Calculated density	2.187 g/cm^3	
Absorption coefficient μ	2.968 mm^{-1}	
F(000)	244	
Crystal colour and size	blue, 0.520 × 0.280 × 0.040 mm^3	
Reflections for cell refinement	32 (θ range 10.0 to 12.5°)	
Data collection method	Stoe-Siemens four-circle diffractometer ω/θ scans with on-line profile fitting	
θ range for data collection	2.4 to 25.0°	
Index ranges	h −7 to 7, k −8 to 8, l −11 to 11	
Completeness to θ = 25.0°	100.0 %	
Reflections collected	2592	
Independent reflections	1296 (R_{int} = 0.0262)	
Reflections with $F^2>2\sigma$	1249	
Absorption correction	multi-scan	
Min. and max. transmission	0.588 and 0.944	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0399, 0.4199	
Data / restraints / parameters	1296 / 9 / 137	
Final R indices [$F^2>2\sigma$]	R1 = 0.0260, wR2 = 0.0688	
R indices (all data)	R1 = 0.0270, wR2 = 0.0700	
Goodness-of-fit on F^2	1.092	
Extinction coefficient	0.016(4)	
Largest and mean shift/su	0.000 and 0.000	
Largest diff. peak and hole	0.46 and −0.70 e Å^{-3}	

Table S2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for 1. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cu	0.00502(5)	0.26574(4)	0.13393(3)	0.01161(17)
C1	0.3626(4)	0.8823(4)	0.3489(3)	0.0104(5)
C2	0.5903(4)	1.0185(4)	0.3827(3)	0.0100(5)
C3	0.7242(4)	1.1352(4)	0.5326(3)	0.0117(5)
C4	0.1982(4)	0.7654(4)	0.1868(3)	0.0114(5)
C5	0.7089(4)	1.0327(4)	0.2664(3)	0.0117(5)
O1	0.0371(3)	0.5999(3)	0.16939(19)	0.0146(4)
O2	0.2297(3)	0.8515(3)	0.0761(2)	0.0165(4)
O3	0.7477(3)	0.8788(3)	0.2199(2)	0.0198(4)
O4	0.7741(3)	1.2106(3)	0.2321(2)	0.0148(4)
O5	0.2489(3)	0.3179(3)	0.3382(2)	0.0181(4)
O6	0.2657(4)	0.2776(4)	0.0646(2)	0.0295(5)
O7	0.6921(3)	0.5450(3)	0.3652(2)	0.0180(4)

Table S3. Bond lengths [Å] and angles [°] for 1.

Cu–O1	2.2319(17)	Cu–O2a	1.9592(18)
Cu–O4b	1.9589(18)	Cu–O5	1.9636(18)
Cu–O6	1.984(2)	C1–C2	1.400(3)
C1–C3c	1.393(3)	C1–C4	1.509(3)
C2–C3	1.390(3)	C2–C5	1.514(3)
C3–C1c	1.393(3)	C3–H3	0.940
C4–O1	1.242(3)	C4–O2	1.280(3)
C5–O3	1.238(3)	C5–O4	1.276(3)
O2–Cua	1.9592(18)	O4–Cud	1.9590(18)
O5–H5A	0.837(10)	O5–H5B	0.836(10)
O6–H6A	0.827(10)	O6–H6B	0.835(10)
O7–H7A	0.829(10)	O7–H7B	0.833(10)

O1–Cu–O2a	102.39(7)	O1–Cu–O4b	88.40(7)
O1–Cu–O5	91.22(7)	O1–Cu–O6	101.58(9)
O2a–Cu–O4b	93.62(8)	O2a–Cu–O5	166.19(8)
O2a–Cu–O6	93.15(8)	O4b–Cu–O5	89.02(8)
O4b–Cu–O6	166.45(9)	O5–Cu–O6	81.70(8)
C2–C1–C3c	119.0(2)	C2–C1–C4	123.1(2)
C3c–C1–C4	117.7(2)	C1–C2–C3	119.7(2)
C1–C2–C5	123.0(2)	C3–C2–C5	117.1(2)
C1c–C3–C2	121.3(2)	C1c–C3–H3	119.3
C2–C3–H3	119.3	C1–C4–O1	119.0(2)
C1–C4–O2	116.5(2)	O1–C4–O2	124.4(2)
C2–C5–O3	118.7(2)	C2–C5–O4	116.0(2)
O3–C5–O4	125.2(2)	Cu–O1–C4	132.93(16)
Cua–O2–C4	119.01(16)	Cud–O4–C5	117.99(16)
Cu–O5–H5A	125(2)	Cu–O5–H5B	113(2)
H5A–O5–H5B	106.7(16)	Cu–O6–H6A	116(3)
Cu–O6–H6B	115(3)	H6A–O6–H6B	108.9(17)
H7A–O7–H7B	108.6(17)		

Symmetry operations for equivalent atoms
a –x,–y+1,–z b x–1,y–1,z c –x+1,–y+2,–z+1
d x+1,y+1,z

Table S4. Torsion angles [°] for 1.

C3c–C1–C2–C3	–0.8(4)	C3c–C1–C2–C5	173.7(2)
C4–C1–C2–C3	174.1(2)	C4–C1–C2–C5	–11.4(4)
C1–C2–C3–C1c	0.8(4)	C5–C2–C3–C1c	–174.0(2)
C2–C1–C4–O1	155.1(2)	C2–C1–C4–O2	–28.2(3)
C3c–C1–C4–O1	–29.9(3)	C3c–C1–C4–O2	146.8(2)
C1–C2–C5–O3	–64.6(3)	C1–C2–C5–O4	119.8(3)
C3–C2–C5–O3	110.1(3)	C3–C2–C5–O4	–65.6(3)
C1–C4–O1–Cu	–92.2(2)	O2–C4–O1–Cu	91.3(3)
C1–C4–O2–Cua	–170.09(16)	O1–C4–O2–Cua	6.4(3)
C2–C5–O4–Cud	162.22(16)	O3–C5–O4–Cud	–13.1(3)

Symmetry operations for equivalent atoms
a –x,–y+1,–z c –x+1,–y+2,–z+1 d x+1,y+1,z

Table S5. Anisotropic displacement parameters ($Å^2$) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu	0.0105(2)	0.0152(2)	0.0064(2)	0.00091(13)	0.00357(14)	0.00098(14)
C1	0.0106(12)	0.0110(11)	0.0089(11)	0.0017(9)	0.0038(9)	0.0030(9)
C2	0.0116(12)	0.0111(11)	0.0084(11)	0.0030(9)	0.0048(9)	0.0039(9)
C3	0.0087(11)	0.0128(11)	0.0117(12)	0.0020(9)	0.0040(10)	0.0013(9)
C4	0.0114(12)	0.0134(11)	0.0093(12)	–0.0006(9)	0.0039(10)	0.0053(10)
C5	0.0085(11)	0.0160(12)	0.0068(11)	0.0010(9)	0.0015(9)	0.0012(9)
O1	0.0148(9)	0.0116(8)	0.0127(9)	0.0001(7)	0.0041(7)	0.0001(7)
O2	0.0151(9)	0.0207(9)	0.0082(8)	0.0021(7)	0.0041(7)	–0.0006(7)
O3	0.0270(11)	0.0205(9)	0.0193(10)	0.0044(7)	0.0164(8)	0.0102(8)
O4	0.0169(10)	0.0148(8)	0.0137(9)	0.0036(7)	0.0096(7)	0.0029(7)
O5	0.0135(9)	0.0269(10)	0.0098(9)	0.0008(7)	0.0040(7)	0.0032(8)
O6	0.0194(11)	0.0592(15)	0.0105(9)	0.0041(9)	0.0063(8)	0.0153(10)
O7	0.0200(10)	0.0198(9)	0.0150(9)	0.0028(7)	0.0092(8)	0.0057(8)

Table S6. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for 1.

	x	y	z	U
H3	0.8762	1.2278	0.5544	0.014
H5A	0.243(5)	0.361(5)	0.423(2)	0.027
H5B	0.382(3)	0.385(4)	0.342(3)	0.027
H6A	0.243(7)	0.287(6)	–0.0265(19)	0.044
H6B	0.320(7)	0.184(5)	0.083(4)	0.044
H7A	0.723(6)	0.451(3)	0.324(3)	0.027
H7B	0.711(6)	0.643(3)	0.319(3)	0.027

Table S7. Hydrogen bonds for 1 [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
O5–H5A...O7e	0.837(10)	1.884(14)	2.701(3)	165(3)
O5–H5B...O7	0.836(10)	1.904(11)	2.739(3)	176(3)
O6–H6A...O1a	0.827(10)	2.29(3)	2.827(3)	123(3)
O6–H6A...O3f	0.827(10)	2.07(3)	2.732(3)	137(3)
O6–H6B...O2g	0.835(10)	2.17(3)	2.891(3)	144(4)
O7–H7A...O4g	0.829(10)	1.966(10)	2.793(3)	175(3)
O7–H7B...O3	0.833(10)	1.937(10)	2.768(3)	176(3)

Symmetry operations for equivalent atoms

a –x,–y+1,–z e –x+1,–y+1,–z+1 f –x+1,–y+1,–z

g x,y–1,z

Table S8. Crystal data and structure refinement for 2.

Identification code	2	
Chemical formula (moiety)	$C_{10}H_{14}Cu_2O_{14}\cdot 4H_2O$	
Chemical formula (total)	$C_{10}H_{22}Cu_2O_{18}$	
Formula weight	557.35	
Temperature	160(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, C2/c	
Unit cell parameters	a = 12.1518(8) Å	α = 90°
	b = 18.1413(11) Å	β = 113.503(2)°
	c = 9.5816(6) Å	γ = 90°
Cell volume	1937.0(2) Å^3	
Z	4	
Calculated density	1.911 g/cm^3	
Absorption coefficient μ	2.287 mm^{-1}	
F(000)	1136	
Crystal colour and size	Blue, 0.210 × 0.200 × 0.200 mm^3	
Reflections for cell refinement	6591 (θ range 2.3 to 28.1°)	
Data collection method	Bruker SMART 1K CCD diffractometer narrow-frame ω scans	
θ range for data collection	2.1 to 28.2°	
Index ranges	h −15 to 16, k −23 to 23, l −12 to 12	
Completeness to θ = 25.2°	100.0 %	
Reflections collected	7999	
Independent reflections	2253 (R_{int} = 0.0258)	
Reflections with $F^2>2\sigma$	2063	
Absorption correction	multi-scan	
Min. and max. transmission	0.640 and 0.660	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0285, 2.8396	
Data / restraints / parameters	2253 / 15 / 166	
Final R indices [$F^2>2\sigma$]	R1 = 0.0235, wR2 = 0.0593	
R indices (all data)	R1 = 0.0266, wR2 = 0.0608	
Goodness-of-fit on F^2	1.084	
Largest and mean shift/su	0.002 and 0.000	
Largest diff. peak and hole	0.52 and −0.43 e Å^{-3}	

Table S9. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for 2. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cu	0.22001(2)	0.55931(2)	0.33081(2)	0.01032(8)
C1	0.44016(15)	0.71960(9)	0.24300(19)	0.0112(3)
C2	0.38191(15)	0.78628(9)	0.23552(19)	0.0113(3)
C3	0.43980(14)	0.85345(9)	0.24163(18)	0.0098(3)
C4	0.37234(15)	0.64845(9)	0.2286(2)	0.0131(3)
C5	0.36641(15)	0.92225(9)	0.22504(19)	0.0097(3)
O1	0.37017(13)	0.60314(7)	0.13036(17)	0.0231(3)
O2	0.32068(12)	0.64135(7)	0.32001(15)	0.0164(3)
O3	0.29707(11)	0.92515(7)	0.29231(15)	0.0145(3)
O4	0.37426(11)	0.97418(6)	0.13968(14)	0.0114(2)
O5	0.34838(12)	0.53638(7)	0.52782(16)	0.0179(3)
O6	0.10433(12)	0.57889(8)	0.12393(15)	0.0181(3)
O7	0.11551(12)	0.63051(7)	0.42583(14)	0.0145(3)
O8	0.55669(13)	0.61173(9)	0.61276(18)	0.0244(3)
O9	0.12325(18)	0.77701(9)	0.4006(2)	0.0422(5)

Table S10. Bond lengths [Å] and angles [°] for 2.

Cu–O2	1.9553(12)	Cu–O4a	2.0090(12)
Cu–O5	1.9548(13)	Cu–O6	1.9517(13)
Cu–O7	2.2432(13)	C1–C1b	1.406(3)
C1–C2	1.389(2)	C1–C4	1.508(2)
C2–H2	0.950	C2–C3	1.397(2)
C3–C3b	1.407(3)	C3–C5	1.505(2)
C4–O1	1.242(2)	C4–O2	1.271(2)
C5–O3	1.250(2)	C5–O4	1.276(2)
O4–Cuc	2.0090(12)	O5–H5A	0.828(9)
O5–H5B	0.827(9)	O6–H6A	0.828(9)
O6–H6B	0.829(9)	O7–H7A	0.832(9)
O7–H7B	0.843(9)	O8–H8A	0.832(10)
O8–H8B	0.832(9)	O9–H9A	0.843(10)
O9–H9B	0.838(10)		

O2–Cu–O4a	175.22(5)	O2–Cu–O5	86.44(6)
O2–Cu–O6	91.15(6)	O2–Cu–O7	92.90(5)
O4a–Cu–O5	88.90(5)	O4a–Cu–O6	93.60(6)
O4a–Cu–O7	86.48(5)	O5–Cu–O6	173.57(6)
O5–Cu–O7	95.36(5)	O6–Cu–O7	90.71(5)
C1b–C1–C2	119.43(10)	C1b–C1–C4	121.03(9)
C2–C1–C4	119.48(15)	C1–C2–H2	119.3
C1–C2–C3	121.33(15)	H2–C2–C3	119.3
C2–C3–C3b	119.23(10)	C2–C3–C5	116.86(14)
C3b–C3–C5	123.88(9)	C1–C4–O1	118.78(16)
C1–C4–O2	115.20(15)	O1–C4–O2	126.01(16)
C3–C5–O3	118.26(15)	C3–C5–O4	119.16(15)
O3–C5–O4	122.54(15)	Cu–O2–C4	127.22(12)
Cuc–O4–C5	106.55(10)	Cu–O5–H5A	119.3(15)
Cu–O5–H5B	123.0(16)	H5A–O5–H5B	110.1(15)
Cu–O6–H6A	124.0(16)	Cu–O6–H6B	121.2(16)
H6A–O6–H6B	109.2(15)	Cu–O7–H7A	100.8(16)
Cu–O7–H7B	120.2(16)	H7A–O7–H7B	107.1(14)
H8A–O8–H8B	108.6(15)	H9A–O9–H9B	106.7(16)

Symmetry operations for equivalent atoms
a –x+1/2,y–1/2,–z+1/2 b –x+1,y,–z+1/2 c –x+1/2,y+1/2,–z+1/2

Table S11. Torsion angles [°] for 2.

C1b–C1–C2–C3	0.0(3)	C4–C1–C2–C3	–177.16(16)
C1–C2–C3–C3b	–1.1(3)	C1–C2–C3–C5	177.16(15)
C1b–C1–C4–O1	–51.5(3)	C1b–C1–C4–O2	129.3(2)
C2–C1–C4–O1	125.59(19)	C2–C1–C4–O2	–53.6(2)
C2–C3–C5–O3	41.6(2)	C2–C3–C5–O4	–136.21(17)
C3b–C3–C5–O3	–140.2(2)	C3b–C3–C5–O4	42.0(3)
C1–C4–O2–Cu	177.49(11)	O1–C4–O2–Cu	–1.6(3)
C3–C5–O4–Cuc	–173.10(12)	O3–C5–O4–Cuc	9.19(19)

Symmetry operations for equivalent atoms
b –x+1,y,–z+1/2 c –x+1/2,y+1/2,–z+1/2

Table S12. Anisotropic displacement parameters (Å^2) for 2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu	0.01063(12)	0.00805(12)	0.01335(12)	0.00044(7)	0.00590(9)	–0.00194(7)
C1	0.0127(8)	0.0100(8)	0.0126(8)	–0.0004(6)	0.0067(7)	–0.0015(6)
C2	0.0101(7)	0.0103(8)	0.0149(8)	–0.0009(6)	0.0065(7)	–0.0008(6)
C3	0.0107(8)	0.0088(8)	0.0106(8)	–0.0004(6)	0.0051(6)	0.0013(6)
C4	0.0104(8)	0.0095(8)	0.0198(9)	0.0012(6)	0.0065(7)	0.0009(6)
C5	0.0088(8)	0.0081(7)	0.0103(8)	–0.0020(6)	0.0017(6)	–0.0002(6)
O1	0.0292(8)	0.0135(7)	0.0350(8)	–0.0101(6)	0.0215(7)	–0.0076(6)
O2	0.0183(6)	0.0115(6)	0.0230(7)	–0.0007(5)	0.0119(6)	–0.0052(5)
O3	0.0144(6)	0.0123(6)	0.0201(7)	0.0008(5)	0.0104(5)	0.0028(5)
O4	0.0134(6)	0.0081(6)	0.0132(6)	0.0014(4)	0.0059(5)	0.0022(4)
O5	0.0140(6)	0.0131(6)	0.0228(7)	0.0053(5)	0.0032(5)	–0.0021(5)
O6	0.0164(6)	0.0248(7)	0.0143(6)	0.0013(5)	0.0073(5)	0.0057(5)
O7	0.0172(6)	0.0127(6)	0.0144(6)	–0.0003(5)	0.0072(5)	0.0007(5)
O8	0.0158(7)	0.0296(8)	0.0277(8)	–0.0005(6)	0.0085(6)	–0.0002(6)
O9	0.0559(12)	0.0180(8)	0.0326(9)	–0.0024(7)	–0.0035(8)	0.0061(8)

Table S13. Hydrogen coordinates and isotropic displacement parameters (Å^2) for 2.

	x	y	z	U
H2	0.3011	0.7862	0.2261	0.014
H5A	0.3523(19)	0.4945(7)	0.564(3)	0.027
H5B	0.4162(12)	0.5547(11)	0.557(3)	0.027
H6A	0.1067(19)	0.5594(12)	0.0470(19)	0.027
H6B	0.0341(11)	0.5906(14)	0.107(2)	0.027
H7A	0.1516(19)	0.6223(11)	0.5185(12)	0.022
H7B	0.114(2)	0.6766(6)	0.414(2)	0.022
H8A	0.6191(15)	0.5988(15)	0.6851(18)	0.037
H8B	0.571(2)	0.6158(16)	0.5353(17)	0.037
H9A	0.156(2)	0.7936(17)	0.4900(16)	0.063
H9B	0.0594(18)	0.8007(17)	0.358(3)	0.063

Table S14. Hydrogen bonds for 2 [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
O5–H5A...O1d	0.828(9)	1.866(10)	2.6897(19)	173(2)
O5–H5B...O8	0.827(9)	1.883(9)	2.701(2)	170(2)
O6–H6A...O4e	0.828(9)	1.989(10)	2.8103(18)	172(2)
O6–H6B...O7f	0.829(9)	1.865(10)	2.6880(19)	172(3)
O7–H7A...O3g	0.832(9)	1.874(10)	2.6746(18)	161(2)
O7–H7B...O9	0.843(9)	1.833(10)	2.674(2)	175(2)
O8–H8A...O3h	0.832(10)	2.037(14)	2.816(2)	156(2)
O8–H8B...O1b	0.832(9)	1.995(12)	2.809(2)	166(3)
O9–H9A...O2g	0.843(10)	2.093(15)	2.893(2)	158(3)
O9–H9B...O8g	0.838(10)	2.22(2)	2.941(2)	145(2)

Symmetry operations for equivalent atoms

b –x+1,y,–z+1/2 d x,–y+1,z+1/2 e –x+1/2,–y+3/2,–z

f –x,y,–z+1/2 g –x+1/2,–y+3/2,–z+1 h x+1/2,–y+3/2,z+1/2

Table S15. Crystal data and structure refinement for 3.

Identification code	3	
Chemical formula (moiety)	$C_{10}H_{10}CuO_{11}\cdot 3H_2O$	
Chemical formula (total)	$C_{10}H_{16}CuO_{14}$	
Formula weight	423.77	
Temperature	160(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, Pn	
Unit cell parameters	a = 6.7846(4) Å	α = 90°
	b = 10.9535(6) Å	β = 91.810(2)°
	c = 10.6835(6) Å	γ = 90°
Cell volume	793.55(8) Å^3	
Z	2	
Calculated density	1.774 g/cm^3	
Absorption coefficient μ	1.452 mm^{-1}	
F(000)	434	
Crystal colour and size	Blue, 0.420 × 0.300 × 0.200 mm^3	
Reflections for cell refinement	6245 (θ range 2.7 to 28.1°)	
Data collection method	Bruker SMART 1K CCD diffractometer narrow-frame ω scans	
θ range for data collection	1.9 to 28.3°	
Index ranges	h −8 to 9, k −14 to 14, l −13 to 13	
Completeness to θ = 25.2°	99.9 %	
Reflections collected	6540	
Independent reflections	3467 (R_{int} = 0.0173)	
Reflections with $F^2>2\sigma$	3379	
Absorption correction	multi-scan	
Min. and max. transmission	0.580 and 0.760	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0260,	
Data / restraints / parameters	3467 / 20 / 269	
Final R indices [$F^2>2\sigma$]	R1 = 0.0191, wR2 = 0.0484	
R indices (all data)	R1 = 0.0199, wR2 = 0.0488	
Goodness-of-fit on F^2	1.058	
Absolute structure parameter	0.257(10)	
Largest and mean shift/su	0.000 and 0.000	
Largest diff. peak and hole	0.41 and −0.31 e Å^{-3}	

Table S16. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for 3. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cu	0.76183(5)	0.48926(2)	0.30815(4)	0.01561(8)
C1	0.7077(3)	0.8636(2)	0.2370(2)	0.0134(4)
C2	0.8577(3)	0.9305(2)	0.1811(2)	0.0132(4)
C3	0.8430(3)	1.0573(2)	0.1714(2)	0.0146(4)
C4	0.6813(3)	1.1185(2)	0.2182(2)	0.0140(5)
C5	0.5331(3)	1.0519(2)	0.2758(2)	0.0135(4)
C6	0.5469(3)	0.9250(2)	0.2849(2)	0.0145(4)
C7	0.7007(3)	0.7255(2)	0.2335(2)	0.0144(5)
C8	1.0337(3)	0.8664(2)	0.1317(2)	0.0157(4)
C9	0.6762(3)	1.2560(2)	0.2060(2)	0.0152(5)
C10	0.3608(3)	1.1166(2)	0.3287(2)	0.0157(4)
O1	0.6303(3)	0.67768(16)	0.13688(19)	0.0248(4)
O2	0.7600(3)	0.66650(14)	0.33000(17)	0.0181(4)
O3	1.0644(3)	0.75791(17)	0.1466(2)	0.0274(4)
O4	1.1519(3)	0.93993(16)	0.07205(18)	0.0221(4)
O5	0.5948(3)	1.30471(17)	0.11443(18)	0.0239(4)
O6	0.7698(3)	1.31239(14)	0.2955(2)	0.0186(4)
O7	0.3445(3)	1.22747(16)	0.3277(2)	0.0289(4)
O8	0.2284(3)	1.04273(17)	0.37434(19)	0.0221(4)
O9	0.9171(5)	0.48837(18)	0.4943(3)	0.0393(6)
O10	0.9907(4)	0.50110(16)	0.1973(3)	0.0265(5)
O11	0.4933(3)	0.4750(2)	0.3754(3)	0.0300(6)
O12	1.1268(3)	0.29584(18)	0.08627(18)	0.0260(4)
O13	0.2803(3)	0.68048(18)	0.37682(19)	0.0280(4)
O14	1.4483(3)	0.82649(15)	–0.02735(17)	0.0169(3)

Table S17. Bond lengths [Å] and angles [°] for 3.

Cu–O2	1.9555(16)	Cu–O6a	1.9430(15)
Cu–O9	2.220(3)	Cu–O10	1.986(2)
Cu–O11	1.985(2)	C1–C2	1.403(3)
C1–C6	1.393(3)	C1–C7	1.513(3)
C2–C3	1.396(3)	C2–C8	1.495(3)
C3–H3	0.950	C3–C4	1.392(3)
C4–C5	1.401(3)	C4–C9	1.512(3)
C5–C6	1.396(3)	C5–C10	1.493(3)
C6–H6	0.950	C7–O1	1.240(3)
C7–O2	1.271(3)	C8–O3	1.216(3)
C8–O4	1.315(3)	C9–O5	1.230(3)
C9–O6	1.288(3)	C10–O7	1.219(3)
C10–O8	1.315(3)	O4–H4	0.77(4)
O6–Cub	1.9430(15)	O8–H8	0.73(4)
O9–H9A	0.842(14)	O9–H9B	0.839(14)
O10–H10A	0.845(14)	O10–H10B	0.833(14)
O11–H11A	0.839(14)	O11–H11B	0.834(14)
O12–H12A	0.837(13)	O12–H12B	0.835(13)
O13–H13A	0.837(13)	O13–H13B	0.838(13)
O14–H14A	0.823(13)	O14–H14B	0.821(13)

O2–Cu–O6a	176.91(11)	O2–Cu–O9	84.38(8)
O2–Cu–O10	90.82(8)	O2–Cu–O11	91.46(9)
O6a–Cu–O9	92.55(9)	O6a–Cu–O10	89.98(8)
O6a–Cu–O11	88.55(10)	O9–Cu–O10	100.16(12)
O9–Cu–O11	95.19(12)	O10–Cu–O11	164.64(10)
C2–C1–C6	119.4(2)	C2–C1–C7	122.3(2)
C6–C1–C7	117.87(19)	C1–C2–C3	120.0(2)
C1–C2–C8	120.2(2)	C3–C2–C8	119.8(2)
C2–C3–H3	119.7	C2–C3–C4	120.6(2)
H3–C3–C4	119.7	C3–C4–C5	119.4(2)
C3–C4–C9	117.7(2)	C5–C4–C9	122.8(2)
C4–C5–C6	120.1(2)	C4–C5–C10	120.0(2)
C6–C5–C10	119.9(2)	C1–C6–C5	120.5(2)
C1–C6–H6	119.8	C5–C6–H6	119.8
C1–C7–O1	117.0(2)	C1–C7–O2	118.6(2)
O1–C7–O2	124.4(2)	C2–C8–O3	123.2(2)
C2–C8–O4	112.9(2)	O3–C8–O4	123.9(2)
C4–C9–O5	120.6(2)	C4–C9–O6	113.9(2)
O5–C9–O6	125.5(2)	C5–C10–O7	122.8(2)
C5–C10–O8	113.6(2)	O7–C10–O8	123.6(2)
Cu–O2–C7	114.26(16)	C8–O4–H4	114(3)
Cub–O6–C9	121.02(17)	C10–O8–H8	113(3)
Cu–O9–H9A	120(2)	Cu–O9–H9B	132(2)
H9A–O9–H9B	106(2)	Cu–O10–H10A	119(2)
Cu–O10–H10B	120(2)	H10A–O10–H10B	106(2)
Cu–O11–H11A	127(3)	Cu–O11–H11B	114(3)
H11A–O11–H11B	106(2)	H12A–O12–H12B	107(2)
H13A–O13–H13B	107(2)	H14A–O14–H14B	112(2)

Symmetry operations for equivalent atoms

a x,y−1,z b x,y+1,z

Table S18. Torsion angles [°] for 3.

C6–C1–C2–C3	−1.4(3)	C6–C1–C2–C8	178.6(2)
C7–C1–C2–C3	171.0(2)	C7–C1–C2–C8	−9.0(3)
C1–C2–C3–C4	0.8(3)	C8–C2–C3–C4	−179.3(2)
C2–C3–C4–C5	0.3(3)	C2–C3–C4–C9	179.21(19)
C3–C4–C5–C6	−0.7(3)	C3–C4–C5–C10	178.8(2)
C9–C4–C5–C6	−179.5(2)	C9–C4–C5–C10	−0.1(3)
C2–C1–C6–C5	1.0(3)	C7–C1–C6–C5	−171.7(2)
C4–C5–C6–C1	0.0(3)	C10–C5–C6–C1	−179.5(2)
C2–C1–C7–O1	−81.5(3)	C2–C1–C7–O2	100.8(3)
C6–C1–C7–O1	90.9(3)	C6–C1–C7–O2	−86.7(3)
C1–C2–C8–O3	−6.6(4)	C1–C2–C8–O4	174.1(2)
C3–C2–C8–O3	173.4(2)	C3–C2–C8–O4	−5.9(3)
C3–C4–C9–O5	92.0(3)	C3–C4–C9–O6	−85.3(3)
C5–C4–C9–O5	−89.2(3)	C5–C4–C9–O6	93.6(3)
C4–C5–C10–O7	−2.4(4)	C4–C5–C10–O8	176.8(2)
C6–C5–C10–O7	177.1(2)	C6–C5–C10–O8	−3.7(3)
C1–C7–O2–Cu	−175.52(15)	O1–C7–O2–Cu	7.0(3)
C4–C9–O6–Cub	−174.01(15)	O5–C9–O6–Cub	8.9(3)

Symmetry operations for equivalent atoms
b x,y+1,z

Table S19. Anisotropic displacement parameters (Å^2) for 3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu	0.02122(14)	0.00539(12)	0.02019(14)	–0.00022(16)	–0.00009(9)	0.00070(16)
C1	0.0173(11)	0.0078(10)	0.0151(10)	0.0005(8)	–0.0005(9)	–0.0005(8)
C2	0.0138(11)	0.0106(10)	0.0152(11)	–0.0012(8)	–0.0005(8)	0.0008(8)
C3	0.0165(11)	0.0096(10)	0.0176(11)	0.0007(8)	–0.0006(8)	0.0002(8)
C4	0.0164(11)	0.0092(11)	0.0163(12)	–0.0005(8)	–0.0023(9)	–0.0002(8)
C5	0.0155(11)	0.0098(10)	0.0153(11)	–0.0010(8)	–0.0007(8)	0.0016(8)
C6	0.0149(11)	0.0112(10)	0.0175(11)	0.0018(8)	0.0023(8)	–0.0018(8)
C7	0.0139(12)	0.0101(11)	0.0192(11)	0.0008(9)	0.0024(9)	0.0006(8)
C8	0.0178(11)	0.0131(11)	0.0159(11)	–0.0004(8)	–0.0003(9)	0.0012(8)
C9	0.0165(11)	0.0097(11)	0.0197(11)	0.0016(8)	0.0035(9)	0.0020(8)
C10	0.0160(11)	0.0144(11)	0.0168(11)	–0.0009(8)	0.0010(8)	0.0015(8)
O1	0.0370(11)	0.0106(8)	0.0261(9)	–0.0033(7)	–0.0102(8)	0.0000(7)
O2	0.0262(8)	0.0095(7)	0.0186(11)	0.0014(7)	0.0004(8)	0.0032(8)
O3	0.0277(10)	0.0123(8)	0.0431(11)	0.0042(8)	0.0135(8)	0.0058(7)
O4	0.0206(9)	0.0161(9)	0.0302(10)	0.0015(7)	0.0103(7)	0.0036(7)
O5	0.0327(10)	0.0136(8)	0.0250(10)	0.0045(7)	–0.0045(8)	0.0037(7)
O6	0.0240(8)	0.0088(6)	0.0228(11)	–0.0002(8)	–0.0010(7)	0.0002(9)
O7	0.0259(9)	0.0116(8)	0.0501(12)	–0.0006(8)	0.0148(9)	0.0027(7)
O8	0.0199(9)	0.0148(8)	0.0322(10)	0.0016(8)	0.0102(8)	0.0026(7)
O9	0.0640(17)	0.0122(9)	0.0399(13)	–0.0010(8)	–0.0262(11)	0.0016(9)
O10	0.0317(12)	0.0101(10)	0.0384(15)	0.0012(8)	0.0122(11)	0.0002(7)
O11	0.0287(12)	0.0120(9)	0.0501(16)	–0.0063(9)	0.0121(11)	–0.0029(8)
O12	0.0310(10)	0.0231(9)	0.0241(10)	0.0011(8)	0.0041(8)	–0.0010(8)
O13	0.0281(10)	0.0262(10)	0.0297(11)	–0.0007(8)	0.0016(8)	0.0015(8)
O14	0.0188(8)	0.0133(8)	0.0188(8)	–0.0002(7)	0.0008(6)	–0.0005(6)

Table S20. Hydrogen coordinates and isotropic displacement parameters (Å^2) for 3.

	x	y	z	U
H3	0.9441	1.1021	0.1326	0.018
H6	0.4460	0.8803	0.3241	0.017
H4	1.245(5)	0.909(3)	0.048(3)	0.033
H8	0.144(6)	1.075(4)	0.400(3)	0.033
H9A	0.952(7)	0.5544(16)	0.528(4)	0.059
H9B	0.971(6)	0.4326(19)	0.537(3)	0.059
H10A	1.022(6)	0.4396(16)	0.155(3)	0.040
H10B	1.001(6)	0.5609(16)	0.150(2)	0.040
H11A	0.406(4)	0.529(2)	0.375(4)	0.045
H11B	0.436(5)	0.4098(17)	0.357(4)	0.045
H12A	1.163(4)	0.293(3)	0.0122(13)	0.039
H12B	1.228(3)	0.291(3)	0.132(2)	0.039
H13A	0.192(4)	0.687(3)	0.320(2)	0.042
H13B	0.227(4)	0.693(3)	0.4453(16)	0.042
H14A	1.503(4)	0.779(2)	0.022(2)	0.025
H14B	1.401(4)	0.791(2)	–0.0887(19)	0.025

Table S21. Hydrogen bonds for 3 [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
O4–H4...O14	0.77(4)	1.86(4)	2.618(2)	173(4)
O8–H8...O14c	0.73(4)	1.90(4)	2.625(3)	173(4)
O9–H9A...O5d	0.842(14)	2.025(17)	2.853(3)	168(4)
O9–H9B...O1e	0.839(14)	1.922(16)	2.754(3)	171(4)
O10–H10A...O12	0.845(14)	1.883(15)	2.718(3)	169(4)
O10–H10B...O3	0.833(14)	2.201(19)	2.911(3)	143(3)
O11–H11A...O13	0.839(14)	1.864(15)	2.675(3)	162(3)
O11–H11B...O7a	0.834(14)	2.112(14)	2.932(3)	168(3)
O12–H12A...O2f	0.837(13)	2.120(16)	2.939(3)	166(4)
O12–H12B...O5g	0.835(13)	2.50(2)	3.181(3)	139(3)
O12–H12B...O7g	0.835(13)	2.32(2)	3.026(3)	143(3)
O13–H13A...O3h	0.837(13)	2.169(19)	2.948(3)	155(3)
O13–H13B...O5i	0.838(13)	2.043(15)	2.873(3)	171(4)
O14–H14A...O1j	0.823(13)	1.846(13)	2.669(3)	178(3)
O14–H14B...O6k	0.821(13)	1.878(16)	2.687(3)	168(3)

Symmetry operations for equivalent atoms

a x,y−1,z c x−3/2,−y+2,z+1/2 d x+1/2,−y+2,z+1/2
e x+1/2,−y+1,z+1/2 f x+1/2,−y+1,z−1/2 g x+1,y−1,z
h x−1,y,z i x−1/2,−y+2,z+1/2 j x+1,y,z
k x+1/2,−y+2,z−1/2

Table S22. Crystal data and structure refinement for 4.

Identification code	4	
Chemical formula (moiety)	$C_{10}H_2O_8CuK_2 \cdot 4H_2O$	
Chemical formula (total)	$C_{10}H_{10}CuK_2O_{12}$	
Formula weight	463.92	
Temperature	295(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 7.7391(15) Å	α = 112.867(10)°
	b = 10.6004(19) Å	β = 90.411(13)°
	c = 10.6159(19) Å	γ = 104.192(10)°
Cell volume	772.8(3) $Å^3$	
Z	2	
Calculated density	1.994 g/cm^3	
Absorption coefficient μ	2.016 mm^{-1}	
F(000)	466	
Crystal colour and size	blue, 0.600 × 0.350 × 0.040 mm^3	
Reflections for cell refinement	32 (θ range 10.0 to 12.5°)	
Data collection method	Stoe-Siemens four-circle diffractometer ω/θ scans with on-line profile fitting	
θ range for data collection	2.1 to 25.0°	
Index ranges	h −9 to 9, k −12 to 12, l −12 to 12	
Completeness to θ = 25.0°	100.0 %	
Reflections collected	5452	
Independent reflections	2726 (R_{int} = 0.0265)	
Reflections with $F^2>2\sigma$	2383	
Absorption correction	multi-scan	
Min. and max. transmission	0.62 and 0.95	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0457, 0.7234	
Data / restraints / parameters	2726 / 9 / 253	
Final R indices [$F^2>2\sigma$]	R1 = 0.0285, wR2 = 0.0789	
R indices (all data)	R1 = 0.0360, wR2 = 0.0837	
Goodness-of-fit on F^2	1.062	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	0.72 and −0.55 e $Å^{-3}$	

Table S23. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for 4. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cu	0.50268(4)	0.23363(3)	0.76455(3)	0.01668(12)
K1	0.82029(10)	0.19096(7)	0.49184(7)	0.03570(18)
K2	0.80028(11)	0.51691(8)	0.14863(7)	0.0412(2)
C1	0.3343(3)	0.2414(3)	0.3963(2)	0.0170(5)
C2	0.3886(3)	0.1380(3)	0.2879(3)	0.0168(5)
C3	0.4133(4)	0.1544(3)	0.1651(3)	0.0203(5)
C4	0.3826(4)	0.2701(3)	0.1475(3)	0.0182(5)
C5	0.3275(4)	0.3735(3)	0.2553(3)	0.0177(5)
C6	0.3035(4)	0.3577(3)	0.3789(3)	0.0187(5)
C7	0.3227(4)	0.2355(3)	0.5358(3)	0.0200(5)
C8	0.4038(4)	0.0008(3)	0.2930(2)	0.0190(5)
C9	0.3981(4)	0.2730(3)	0.0071(3)	0.0191(5)
C10	0.3091(4)	0.5083(3)	0.2463(3)	0.0216(6)
O1	0.2030(3)	0.2735(2)	0.6053(2)	0.0303(5)
O2	0.4480(3)	0.1924(2)	0.57214(18)	0.0271(4)
O3	0.2667(3)	–0.0833(2)	0.3040(2)	0.0299(5)
O4	0.5536(3)	–0.02732(19)	0.27529(19)	0.0222(4)
O5	0.5481(3)	0.2678(2)	–0.03986(18)	0.0238(4)
O6	0.2663(3)	0.2726(2)	–0.0597(2)	0.0318(5)
O7	0.4337(3)	0.5628(2)	0.1894(2)	0.0284(5)
O8	0.1861(3)	0.5593(2)	0.2976(2)	0.0316(5)
O9	0.8641(4)	0.3601(4)	0.3236(4)	0.0687(9)
O10	0.9477(4)	–0.0132(4)	0.3075(4)	0.0856(12)
O11	0.9407(5)	0.3187(4)	–0.0308(5)	0.0994(15)
O12	0.8887(10)	0.0893(8)	0.1143(7)	0.186(3)

Table S24. Bond lengths [Å] and angles [°] for 4.

Cu–O2	1.9354(18)	Cu–O4a	1.9907(18)
Cu–O5b	1.9771(18)	Cu–O7c	1.9476(19)
K1–O1d	2.975(2)	K1–O2	3.013(2)
K1–O3a	2.832(2)	K1–O4	2.890(2)
K1–O8c	2.734(2)	K1–O9	2.952(3)
K1–O10	2.696(3)	K2–O1c	2.698(2)
K2–O5	2.846(2)	K2–O6e	2.885(2)
K2–O7	3.001(2)	K2–O8d	3.216(2)
K2–O9	3.041(4)	K2–O11	2.695(4)
K2–O11f	2.939(5)	C1–C2	1.398(3)
C1–C6	1.390(4)	C1–C7	1.509(3)
C2–C3	1.389(4)	C2–C8	1.510(3)
C3–H3	0.930	C3–C4	1.384(4)
C4–C5	1.398(4)	C4–C9	1.509(3)
C5–C6	1.395(4)	C5–C10	1.509(3)
C6–H6	0.930	C7–O1	1.235(3)
C7–O2	1.283(3)	C8–O3	1.246(3)
C8–O4	1.264(3)	C9–O5	1.271(3)
C9–O6	1.237(3)	C10–O7	1.279(3)
C10–O8	1.235(3)	O1–K1g	2.975(2)
O1–K2c	2.698(2)	O3–K1a	2.832(2)
O4–Cua	1.9906(18)	O5–Cuh	1.9771(18)
O6–K2e	2.885(2)	O7–Cuc	1.9477(19)
O8–K1c	2.734(2)	O8–K2g	3.216(2)
O9–H9A	0.842(10)	O9–H9B	0.837(10)
O10–H10A	0.847(10)	O10–H10B	0.845(10)
O11–K2f	2.939(5)	O11–H11A	0.850(10)
O11–H11B	0.863(10)		

O2–Cu–O4a	91.27(8)	O2–Cu–O5b	177.13(8)
O2–Cu–O7c	91.03(8)	O4a–Cu–O5b	86.56(8)
O4a–Cu–O7c	177.28(8)	O5b–Cu–O7c	91.19(8)
O1d–K1–O2	143.23(6)	O1d–K1–O3a	87.65(6)
O1d–K1–O4	142.84(6)	O1d–K1–O8c	83.62(7)
O1d–K1–O9	97.52(8)	O1d–K1–O10	77.46(9)
O2–K1–O3a	66.66(6)	O2–K1–O4	69.36(6)
O2–K1–O8c	67.78(6)	O2–K1–O9	101.86(8)
O2–K1–O10	131.60(8)	O3a–K1–O4	96.74(6)
O3a–K1–O8c	82.19(6)	O3a–K1–O9	164.83(8)
O3a–K1–O10	101.99(11)	O4–K1–O8c	133.54(6)
O4–K1–O9	87.77(8)	O4–K1–O10	65.51(8)
O8c–K1–O9	84.21(9)	O8c–K1–O10	160.37(9)
O9–K1–O10	93.07(12)	O1c–K2–O5	136.33(7)
O1c–K2–O6e	79.96(6)	O1c–K2–O7	68.11(6)
O1c–K2–O8d	79.68(6)	O1c–K2–O9	83.39(8)
O1c–K2–O11	153.73(10)	O1c–K2–O11f	99.12(9)
O5–K2–O6e	100.66(6)	O5–K2–O7	72.49(6)
O5–K2–O8d	130.92(6)	O5–K2–O9	90.79(8)
O5–K2–O11	64.20(9)	O5–K2–O11f	117.00(9)
O6e–K2–O7	65.89(6)	O6e–K2–O8d	121.05(6)
O6e–K2–O9	163.33(8)	O6e–K2–O11	116.16(12)
O6e–K2–O11f	54.77(8)	O7–K2–O8d	145.61(6)
O7–K2–O9	106.92(7)	O7–K2–O11	136.34(9)
O7–K2–O11f	120.65(8)	O8d–K2–O9	55.92(7)

O8d–K2–O11	74.21(9)	O8d–K2–O11f	75.01(9)
O9–K2–O11	79.69(13)	O9–K2–O11f	129.74(10)
O11–K2–O11f	77.06(14)	C2–C1–C6	119.5(2)
C2–C1–C7	121.3(2)	C6–C1–C7	119.0(2)
C1–C2–C3	119.4(2)	C1–C2–C8	122.5(2)
C3–C2–C8	117.8(2)	C2–C3–H3	119.4
C2–C3–C4	121.1(2)	H3–C3–C4	119.4
C3–C4–C5	119.8(2)	C3–C4–C9	117.5(2)
C5–C4–C9	122.6(2)	C4–C5–C6	119.2(2)
C4–C5–C10	121.9(2)	C6–C5–C10	118.7(2)
C1–C6–C5	120.9(2)	C1–C6–H6	119.5
C5–C6–H6	119.5	C1–C7–O1	120.3(2)
C1–C7–O2	113.8(2)	O1–C7–O2	125.9(2)
C2–C8–O3	119.0(2)	C2–C8–O4	117.5(2)
O3–C8–O4	123.3(2)	C4–C9–O5	116.6(2)
C4–C9–O6	120.2(2)	O5–C9–O6	123.0(2)
C5–C10–O7	114.0(2)	C5–C10–O8	119.8(2)
O7–C10–O8	126.1(2)	K1g–O1–K2c	100.21(7)
K1g–O1–C7	123.81(17)	K2c–O1–C7	134.21(19)
Cu–O2–K1	97.07(8)	Cu–O2–C7	119.53(16)
K1–O2–C7	133.23(16)	K1a–O3–C8	132.00(18)
Cua–O4–K1	124.16(8)	Cua–O4–C8	104.03(16)
K1–O4–C8	108.90(15)	Cuh–O5–K2	121.61(8)
Cuh–O5–C9	104.89(16)	K2–O5–C9	105.08(15)
K2e–O6–C9	131.14(18)	Cuc–O7–K2	98.46(8)
Cuc–O7–C10	119.92(17)	K2–O7–C10	129.24(17)
K1c–O8–K2g	93.78(6)	K1c–O8–C10	133.05(19)
K2g–O8–C10	128.21(18)	K1–O9–K2	164.59(12)
K1–O9–H9A	115(4)	K1–O9–H9B	97(4)
K2–O9–H9A	79(4)	K2–O9–H9B	84(4)
H9A–O9–H9B	107.0(17)	K1–O10–H10A	92(5)
K1–O10–H10B	132(5)	H10A–O10–H10B	105.6(17)
K2–O11–K2f	102.94(14)	K2–O11–H11A	134(5)
K2f–O11–H11A	59(4)	K2–O11–H11B	86(5)
K2f–O11–H11B	161(5)	H11A–O11–H11B	103.2(16)

Symmetry operations for equivalent atoms

a	–x+1,–y,–z+1	b	x,y,z+1	c	–x+1,–y+1,–z+1
d	x+1,y,z	e	–x+1,–y+1,–z	f	–x+2,–y+1,–z
g	x–1,y,z	h	x,y,z–1		

Table S25. Torsion angles [°] for 4.

C6–C1–C2–C3	0.9(4)	C6–C1–C2–C8	–172.7(3)
C7–C1–C2–C3	–174.1(3)	C7–C1–C2–C8	12.3(4)
C1–C2–C3–C4	–1.0(4)	C8–C2–C3–C4	173.0(3)
C2–C3–C4–C5	0.7(4)	C2–C3–C4–C9	–175.1(3)
C3–C4–C5–C6	–0.3(4)	C3–C4–C5–C10	174.1(3)
C9–C4–C5–C6	175.2(2)	C9–C4–C5–C10	–10.4(4)
C2–C1–C6–C5	–0.6(4)	C7–C1–C6–C5	174.5(2)
C4–C5–C6–C1	0.3(4)	C10–C5–C6–C1	–174.3(2)
C2–C1–C7–O1	–144.2(3)	C2–C1–C7–O2	37.5(3)
C6–C1–C7–O1	40.8(4)	C6–C1–C7–O2	–137.5(3)
C1–C2–C8–O3	61.7(4)	C1–C2–C8–O4	–123.5(3)
C3–C2–C8–O3	–112.0(3)	C3–C2–C8–O4	62.7(3)
C3–C4–C9–O5	–58.3(3)	C3–C4–C9–O6	117.9(3)
C5–C4–C9–O5	126.1(3)	C5–C4–C9–O6	–57.7(4)
C4–C5–C10–O7	–40.1(4)	C4–C5–C10–O8	143.2(3)
C6–C5–C10–O7	134.3(3)	C6–C5–C10–O8	–42.4(4)
C1–C7–O1–K1g	44.8(3)	C1–C7–O1–K2c	–116.8(2)
O2–C7–O1–K1g	–137.1(2)	O2–C7–O1–K2c	61.3(4)
C1–C7–O2–Cu	160.45(17)	C1–C7–O2–K1	23.9(3)
O1–C7–O2–Cu	–17.8(4)	O1–C7–O2–K1	–154.4(2)
C2–C8–O3–K1a	–119.2(2)	O4–C8–O3–K1a	66.4(3)
C2–C8–O4–Cua	–164.06(18)	C2–C8–O4–K1	61.7(2)
O3–C8–O4–Cua	10.5(3)	O3–C8–O4–K1	–123.7(2)
C4–C9–O5–Cuh	168.62(17)	C4–C9–O5–K2	–62.1(2)
O6–C9–O5–Cuh	–7.4(3)	O6–C9–O5–K2	121.9(2)
C4–C9–O6–K2e	115.3(2)	O5–C9–O6–K2e	–68.7(3)
C5–C10–O7–Cuc	–153.55(18)	C5–C10–O7–K2	–20.0(3)
O8–C10–O7–Cuc	23.0(4)	O8–C10–O7–K2	156.5(2)
C5–C10–O8–K1c	116.0(2)	C5–C10–O8–K2g	–95.7(3)
O7–C10–O8–K1c	–60.3(4)	O7–C10–O8–K2g	88.0(3)

Symmetry operations for equivalent atoms

a –x+1,–y,–z+1 c –x+1,–y+1,–z+1 e –x+1,–y+1,–z

g x–1,y,z h x,y,z–1

Table S26. Anisotropic displacement parameters (Å^2) for 4. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu	0.0281(2)	0.01386(18)	0.01396(18)	0.00929(13)	0.00588(13)	0.00962(13)
K1	0.0399(4)	0.0332(4)	0.0327(4)	0.0104(3)	0.0093(3)	0.0121(3)
K2	0.0486(4)	0.0375(4)	0.0374(4)	0.0102(3)	0.0096(3)	0.0192(3)
C1	0.0231(13)	0.0164(12)	0.0141(12)	0.0089(10)	0.0022(10)	0.0053(10)
C2	0.0222(13)	0.0140(12)	0.0185(12)	0.0098(10)	0.0044(10)	0.0067(10)
C3	0.0320(14)	0.0163(12)	0.0173(12)	0.0087(10)	0.0070(11)	0.0113(11)
C4	0.0264(13)	0.0158(12)	0.0154(12)	0.0092(10)	0.0043(10)	0.0059(10)
C5	0.0247(13)	0.0142(12)	0.0172(12)	0.0091(10)	0.0032(10)	0.0058(10)
C6	0.0265(13)	0.0159(12)	0.0164(12)	0.0066(10)	0.0072(10)	0.0100(10)
C7	0.0320(15)	0.0138(12)	0.0172(12)	0.0086(10)	0.0055(11)	0.0076(11)
C8	0.0307(14)	0.0153(12)	0.0133(11)	0.0068(10)	0.0020(10)	0.0085(11)
C9	0.0324(15)	0.0124(12)	0.0165(12)	0.0089(10)	0.0047(11)	0.0077(11)
C10	0.0353(15)	0.0162(12)	0.0159(12)	0.0077(10)	0.0040(11)	0.0095(11)
O1	0.0388(12)	0.0379(12)	0.0224(10)	0.0158(9)	0.0135(9)	0.0182(10)
O2	0.0456(12)	0.0306(11)	0.0159(9)	0.0130(8)	0.0059(8)	0.0227(10)
O3	0.0304(11)	0.0217(10)	0.0461(12)	0.0226(9)	0.0083(9)	0.0067(9)
O4	0.0297(10)	0.0173(9)	0.0265(10)	0.0126(8)	0.0077(8)	0.0121(8)
O5	0.0338(11)	0.0275(10)	0.0168(9)	0.0129(8)	0.0086(8)	0.0131(9)
O6	0.0370(12)	0.0428(12)	0.0248(10)	0.0207(10)	0.0024(9)	0.0153(10)
O7	0.0477(13)	0.0160(9)	0.0274(10)	0.0134(8)	0.0170(9)	0.0108(9)
O8	0.0409(12)	0.0265(10)	0.0394(12)	0.0185(9)	0.0140(10)	0.0209(10)
O9	0.0541(18)	0.080(2)	0.084(2)	0.0500(19)	0.0111(17)	0.0111(17)
O10	0.0369(16)	0.057(2)	0.116(3)	–0.0147(19)	0.0014(17)	0.0159(14)
O11	0.0455(18)	0.081(3)	0.121(3)	–0.018(2)	–0.0024(19)	0.0281(18)
O12	0.205(7)	0.147(6)	0.164(6)	0.044(5)	–0.041(5)	0.006(5)

Table S27. Hydrogen coordinates and isotropic displacement parameters (Å^2) for 4.

	x	y	z	U
H3	0.4512	0.0864	0.0934	0.024
H6	0.2663	0.4260	0.4508	0.022
H9A	0.963(4)	0.422(4)	0.341(5)	0.103
H9B	0.866(7)	0.294(4)	0.248(3)	0.103
H10A	0.946(8)	0.021(7)	0.247(6)	0.128
H10B	1.048(4)	–0.032(7)	0.306(6)	0.128
H11A	1.046(4)	0.309(8)	–0.039(7)	0.149
H11B	0.897(9)	0.267(7)	0.014(8)	0.149

Table S28. Hydrogen bonds for 4 [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
O9–H9A...O8d	0.842(10)	2.15(3)	2.938(4)	156(5)
O9–H9B...O12	0.837(10)	2.14(3)	2.921(8)	156(6)
O10–H10A...O12	0.847(10)	1.915(16)	2.750(9)	168(6)
O10–H10B...O3d	0.845(10)	1.899(11)	2.744(4)	177(6)
O11–H11A...O6d	0.850(10)	1.832(13)	2.680(4)	175(7)
O11–H11B...O12	0.863(10)	2.49(3)	3.299(9)	156(6)

Symmetry operations for equivalent atoms
d x+1,y,z

Table S29. Crystal data and structure refinement for 5.

Identification code	5	
Chemical formula (moiety)	$C_{10}H_2CuNa_2O_8 \cdot 4H_2O$	
Chemical formula (total)	$C_{10}H_{10}CuNa_2O_{12}$	
Formula weight	431.70	
Temperature	160(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, C2/c	
Unit cell parameters	a = 6.8940(5) Å	α = 90°
	b = 16.3377(11) Å	β = 99.666(2)°
	c = 12.9381(9) Å	γ = 90°
Cell volume	1436.56(17) Å^3	
Z	4	
Calculated density	1.996 g/cm^3	
Absorption coefficient μ	1.649 mm^{-1}	
F(000)	868	
Crystal colour and size	blue, 0.400 × 0.400 × 0.100 mm^3	
Reflections for cell refinement	6028 (θ range 2.5 to 28.5°)	
Data collection method	Bruker SMART 1K diffractometer	
	narrow-frame ω scans	
θ range for data collection	2.5 to 28.5°	
Index ranges	h −8 to 9, k −21 to 21, l −16 to 17	
Completeness to θ = 25.2°	99.8 %	
Reflections collected	6058	
Independent reflections	1732 (R_{int} = 0.0242)	
Reflections with $F^2>2\sigma$	1710	
Absorption correction	multi-scan	
Min. and max. transmission	0.56 and 0.85	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0258, 1.6844	
Data / restraints / parameters	1732 / 6 / 130	
Final R indices [$F^2>2\sigma$]	R1 = 0.0205, wR2 = 0.0564	
R indices (all data)	R1 = 0.0208, wR2 = 0.0565	
Goodness-of-fit on F^2	1.157	
Largest and mean shift/su	0.000 and 0.000	
Largest diff. peak and hole	0.43 and −0.66 e Å^{-3}	

Table S30. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for 5. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cu	0.5000	0.51222(2)	0.7500	0.00760(8)
Na	0.82351(8)	0.40012(3)	0.63321(4)	0.01423(13)
C1	0.70390(19)	0.67631(8)	0.54458(10)	0.0094(2)
C2	0.72402(18)	0.67889(7)	0.43951(10)	0.0091(2)
C3	0.76957(19)	0.75261(8)	0.39555(10)	0.0105(2)
C4	0.6727(2)	0.59790(8)	0.60006(10)	0.0101(2)
C5	0.69376(19)	0.60605(7)	0.36820(10)	0.0092(2)
O1	0.78567(16)	0.54037(6)	0.59587(9)	0.0176(2)
O2	0.53142(15)	0.59977(6)	0.65290(8)	0.0127(2)
O3	0.82406(15)	0.58551(6)	0.31828(8)	0.0133(2)
O4	0.52703(14)	0.57080(6)	0.36032(8)	0.01179(19)
O5	0.86811(16)	0.39613(7)	0.45692(9)	0.0189(2)
O6	0.77637(18)	0.25673(7)	0.63646(10)	0.0225(2)

Table S31. Bond lengths [Å] and angles [°] for 5.

Cu–O2	1.9397(10)	Cu–O2a	1.9397(10)
Cu–O4b	1.9551(9)	Cu–O4c	1.9551(9)
Na–O1	2.3472(11)	Na–O5	2.3531(13)
Na–O6	2.3665(13)	Na–O3c	2.4053(11)
Na–O3d	2.4166(12)	Na–O4b	2.4780(11)
C1–C2	1.3901(18)	C1–C3e	1.3908(17)
C1–C4	1.5016(17)	C2–C3	1.3903(17)
C2–C5	1.4988(17)	C3–C1e	1.3908(17)
C3–H3	0.950	C4–O1	1.2277(17)
C4–O2	1.2808(17)	C5–O3	1.2375(16)
C5–O4	1.2743(16)	O3–Naf	2.4052(11)
O3–Nad	2.4166(12)	O4–Cub	1.9551(9)
O4–Nab	2.4780(11)	O5–H5A	0.826(9)
O5–H5B	0.825(9)	O6–H6A	0.840(10)
O6–H6B	0.841(10)		

O2–Cu–O2a	84.98(6)	O2–Cu–O4b	92.64(4)
O2a–Cu–O4b	167.72(4)	O2–Cu–O4c	167.72(4)
O2a–Cu–O4c	92.64(4)	O4b–Cu–O4c	92.14(6)
O1–Na–O5	81.70(4)	O1–Na–O6	163.58(5)
O5–Na–O6	91.74(4)	O1–Na–O3c	95.23(4)
O5–Na–O3c	171.51(5)	O6–Na–O3c	93.22(4)
O1–Na–O3d	91.76(4)	O5–Na–O3d	88.00(4)
O6–Na–O3d	103.10(4)	O3c–Na–O3d	84.18(4)
O1–Na–O4b	75.20(4)	O5–Na–O4b	108.96(4)
O6–Na–O4b	92.96(4)	O3c–Na–O4b	77.66(4)
O3d–Na–O4b	156.39(4)	C2–C1–C3e	119.60(12)
C2–C1–C4	122.62(11)	C3e–C1–C4	117.53(12)
C1–C2–C3	119.52(12)	C1–C2–C5	123.47(11)
C3–C2–C5	116.98(11)	C2–C3–C1e	120.87(12)
C2–C3–H3	119.6	C1e–C3–H3	119.6
O1–C4–O2	125.93(12)	O1–C4–C1	119.28(12)
O2–C4–C1	114.69(11)	O3–C5–O4	124.04(12)
O3–C5–C2	119.89(12)	O4–C5–C2	116.01(11)
C4–O1–Na	141.96(9)	C4–O2–Cu	120.38(9)
C5–O3–Naf	127.82(9)	C5–O3–Nad	128.64(9)
Naf–O3–Nad	94.73(4)	C5–O4–Cub	110.24(8)
C5–O4–Nab	141.48(8)	Cub–O4–Nab	100.59(4)
Na–O5–H5A	103.0(16)	Na–O5–H5B	119.4(18)
H5A–O5–H5B	109.7(15)	Na–O6–H6A	123.2(18)
Na–O6–H6B	126.6(18)	H6A–O6–H6B	105.7(15)

Symmetry operations for equivalent atoms

a –x+1,y,–z+3/2 b –x+1,–y+1,–z+1 c x,–y+1,z+1/2

d –x+2,–y+1,–z+1 e –x+3/2,–y+3/2,–z+1 f x,–y+1,z–1/2

Table S32. Torsion angles [°] for 5.

C3e–C1–C2–C3	–0.3(2)	C4–C1–C2–C3	–174.44(12)
C3e–C1–C2–C5	–178.55(12)	C4–C1–C2–C5	7.3(2)
C1–C2–C3–C1e	0.3(2)	C5–C2–C3–C1e	178.67(12)
C2–C1–C4–O1	52.03(19)	C3e–C1–C4–O1	–122.24(14)
C2–C1–C4–O2	–131.38(13)	C3e–C1–C4–O2	54.35(16)
C1–C2–C5–O3	–126.26(14)	C3–C2–C5–O3	55.43(17)
C1–C2–C5–O4	56.47(17)	C3–C2–C5–O4	–121.84(13)
O2–C4–O1–Na	15.6(2)	C1–C4–O1–Na	–168.25(11)
O1–C4–O2–Cu	7.84(19)	C1–C4–O2–Cu	–168.49(8)
O4–C5–O3–Naf	69.48(16)	C2–C5–O3–Naf	–107.56(12)
O4–C5–O3–Nad	–151.57(10)	C2–C5–O3–Nad	31.39(17)
O3–C5–O4–Cub	–5.20(16)	C2–C5–O4–Cub	171.94(8)
O3–C5–O4–Nab	–146.24(11)	C2–C5–O4–Nab	30.90(19)

Symmetry operations for equivalent atoms

b –x+1,–y+1,–z+1 d –x+2,–y+1,–z+1 e –x+3/2,–y+3/2,–z+1

f x,–y+1,z–1/2

Table S33. Anisotropic displacement parameters (Å^2) for 5. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu	0.01122(12)	0.00456(12)	0.00756(12)	0.000	0.00315(8)	0.000
Na	0.0158(3)	0.0127(3)	0.0150(3)	0.0006(2)	0.0051(2)	0.0004(2)
C1	0.0108(6)	0.0069(5)	0.0109(6)	0.0007(4)	0.0030(4)	–0.0008(4)
C2	0.0098(6)	0.0065(5)	0.0109(6)	–0.0012(4)	0.0021(4)	–0.0008(4)
C3	0.0134(6)	0.0086(6)	0.0101(6)	0.0000(4)	0.0040(4)	–0.0012(4)
C4	0.0139(6)	0.0078(5)	0.0087(6)	–0.0003(4)	0.0016(4)	–0.0024(4)
C5	0.0132(6)	0.0058(5)	0.0083(5)	0.0010(4)	0.0011(4)	0.0002(4)
O1	0.0180(5)	0.0094(5)	0.0273(6)	0.0048(4)	0.0098(4)	0.0023(4)
O2	0.0180(5)	0.0087(4)	0.0133(5)	0.0021(3)	0.0076(4)	–0.0002(3)
O3	0.0137(5)	0.0138(4)	0.0132(5)	–0.0032(4)	0.0044(4)	0.0009(3)
O4	0.0139(5)	0.0096(4)	0.0126(4)	–0.0032(3)	0.0043(3)	–0.0039(3)
O5	0.0151(5)	0.0221(5)	0.0196(5)	0.0022(4)	0.0034(4)	0.0003(4)
O6	0.0245(6)	0.0181(5)	0.0252(6)	–0.0027(4)	0.0048(5)	–0.0019(5)

Table S34. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for 5.

	x	y	z	U
H3	0.7827	0.7545	0.3237	0.013
H5A	0.7640(18)	0.4152(13)	0.4253(17)	0.037(6)
H5B	0.962(2)	0.4206(14)	0.4393(19)	0.045(7)
H6A	0.869(3)	0.2232(13)	0.651(2)	0.058(9)
H6B	0.682(3)	0.2302(14)	0.602(2)	0.060(9)

Table S35. Hydrogen bonds for 5 [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
O5–H5A...O2b	0.826(9)	2.130(13)	2.8802(15)	151(2)
O5–H5B...O1d	0.825(9)	1.976(10)	2.7905(15)	169(2)
O6–H6A...O2g	0.840(10)	2.303(14)	3.0963(15)	158(2)
O6–H6B...O5h	0.841(10)	2.21(2)	2.8782(16)	137(2)

Symmetry operations for equivalent atoms

b –x+1,–y+1,–z+1 d –x+2,–y+1,–z+1 g x+1/2,y–1/2,z

h –x+3/2,–y+1/2,–z+1

Table S36. Crystal data and structure refinement for 6.

Identification code	6	
Chemical formula (moiety)	$4C_6H_{16}N^+ \cdot C_{24}H_{16}Cu_2O_{18}^{4-}$	
Chemical formula (total)	$C_{48}H_{80}Cu_2N_4O_{18}$	
Formula weight	1128.24	
Temperature	160(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 11.3114(10) Å	α = 80.130(2)°
	b = 11.5464(10) Å	β = 66.441(2)°
	c = 11.7074(11) Å	γ = 71.052(2)°
Cell volume	1324.1(2) Å^3	
Z	1	
Calculated density	1.415 g/cm^3	
Absorption coefficient μ	0.878 mm^{-1}	
F(000)	598	
Crystal colour and size	blue, 0.400 × 0.100 × 0.100 mm^3	
Reflections for cell refinement	4477 (θ range 2.2 to 28.7°)	
Data collection method	Bruker SMART CCD diffractometer narrow-frame ω scans	
θ range for data collection	1.9 to 25.0°	
Index ranges	h −12 to 13, k −13 to 13, l −13 to 13	
Completeness to θ = 25.0°	98.1 %	
Reflections collected	7999	
Independent reflections	4562 (R_{int} = 0.0493)	
Reflections with $F^2>2\sigma$	3103	
Absorption correction	multi-scan	
Min. and max. transmission	0.720 and 0.920	
Structure solution	Patterson synthesis	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.1174,	
Data / restraints / parameters	4562 / 512 / 362	
Final R indices [$F^2>2\sigma$]	R1 = 0.0735, wR2 = 0.1753	
R indices (all data)	R1 = 0.1086, wR2 = 0.1927	
Goodness-of-fit on F^2	0.984	
Largest and mean shift/su	0.000 and 0.000	
Largest diff. peak and hole	1.30 and −1.32 e Å^{-3}	

Table S37. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for 6. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cu	0.37128(7)	0.78960(6)	0.63060(6)	0.0179(2)
C1	0.6217(5)	0.5632(5)	0.6089(5)	0.0171(11)
C2	0.6571(5)	0.6183(4)	0.4883(5)	0.0159(11)
C3	0.7229(5)	0.5431(5)	0.3864(5)	0.0169(12)
C4	0.7474(5)	0.4164(5)	0.3995(5)	0.0167(11)
C5	0.7096(5)	0.3627(4)	0.5203(5)	0.0164(11)
C6	0.6518(6)	0.4365(5)	0.6214(5)	0.0186(12)
C7	0.5630(5)	0.6307(5)	0.7300(5)	0.0169(11)
C8	0.6402(6)	0.7561(5)	0.4552(5)	0.0185(12)
C9	0.8232(6)	0.3477(5)	0.2792(5)	0.0187(12)
C10	0.7376(6)	0.2256(5)	0.5503(5)	0.0183(12)
O1	0.6094(4)	0.5830(3)	0.8115(4)	0.0310(10)
O2	0.4682(4)	0.7293(3)	0.7430(3)	0.0209(9)
O3	0.7396(4)	0.7851(3)	0.3770(4)	0.0274(10)
O4	0.5272(4)	0.8312(3)	0.5067(4)	0.0236(9)
O5	0.9294(4)	0.3691(4)	0.2089(4)	0.0295(10)
O6	0.7720(4)	0.2758(3)	0.2545(3)	0.0214(9)
O7	0.7729(4)	0.1843(3)	0.6407(4)	0.0294(10)
O8	0.7213(4)	0.1578(3)	0.4862(3)	0.0237(9)
O9	0.2787(4)	0.9777(3)	0.7133(4)	0.0291(10)
C11	0.1579(8)	1.0063(6)	0.8158(7)	0.057(2)
C12	0.0458(14)	1.0157(12)	0.7806(15)	0.077(4)
C12X	0.160(2)	1.0773(19)	0.9052(18)	0.074(6)
N1	0.8030(5)	0.4069(4)	0.8869(4)	0.0237(11)
C13	0.9168(6)	0.3541(6)	0.7713(5)	0.0315(14)
C14	0.9498(7)	0.4517(6)	0.6687(6)	0.0404(17)
C15	0.7495(8)	0.3062(7)	0.9738(6)	0.0477(19)
C16	0.6622(8)	0.2644(7)	0.9383(7)	0.052(2)
C17	0.8451(7)	0.4753(6)	0.9534(6)	0.0344(15)
C18	0.7249(9)	0.5540(8)	1.0526(8)	0.070(3)
N2	0.7130(7)	–0.0383(5)	0.7023(5)	0.0531(16)
C19	0.5626(9)	–0.0078(8)	0.7263(8)	0.070(2)
C20	0.4778(10)	0.0982(9)	0.8061(9)	0.080(3)
C21	0.7779(10)	–0.1251(7)	0.6035(8)	0.074(2)
C22	0.9205(10)	–0.1484(10)	0.5665(9)	0.059(3)
C22X	0.891(3)	–0.241(2)	0.597(3)	0.047(7)
C23	0.7469(10)	–0.0765(7)	0.8165(7)	0.062(2)
C24	0.7067(15)	–0.1911(10)	0.8845(11)	0.061(4)
C24X	0.880(2)	–0.069(2)	0.814(2)	0.069(5)

Table S38. Bond lengths [Å] and angles [°] for 6.

Cu–O2	1.940(4)	Cu–O4	1.927(4)
Cu–O6a	1.926(4)	Cu–O8a	1.945(4)
Cu–O9	2.278(4)	C1–C2	1.402(7)
C1–C6	1.386(7)	C1–C7	1.533(7)
C2–C3	1.399(7)	C2–C8	1.539(7)
C3–H3	0.950	C3–C4	1.391(7)
C4–C5	1.398(7)	C4–C9	1.524(7)
C5–C6	1.386(7)	C5–C10	1.517(7)
C6–H6	0.950	C7–O1	1.233(6)
C7–O2	1.267(6)	C8–O3	1.238(6)
C8–O4	1.262(6)	C9–O5	1.231(6)
C9–O6	1.279(6)	C10–O7	1.244(6)
C10–O8	1.271(6)	O6–Cua	1.926(4)
O8–Cua	1.945(4)	O9–H9	0.836(10)
O9–C11	1.395(8)	C11–H11A	0.990
C11–H11B	0.990	C11–H11C	0.990
C11–H11D	0.990	C11–C12	1.450(14)
C11–C12X	1.448(16)	C12–H12A	0.980
C12–H12B	0.980	C12–H12C	0.980
C12X–H12D	0.980	C12X–H12E	0.980
C12X–H12F	0.980	N1–H1	1.000
N1–C13	1.497(7)	N1–C15	1.520(8)
N1–C17	1.485(7)	C13–H13A	0.990
C13–H13B	0.990	C13–C14	1.518(8)
C14–H14A	0.980	C14–H14B	0.980
C14–H14C	0.980	C15–H15A	0.990
C15–H15B	0.990	C15–C16	1.445(10)
C16–H16A	0.980	C16–H16B	0.980
C16–H16C	0.980	C17–H17A	0.990
C17–H17B	0.990	C17–C18	1.523(9)
C18–H18A	0.980	C18–H18B	0.980
C18–H18C	0.980	N2–H2	1.000
N2–C19	1.537(9)	N2–C21	1.457(8)
N2–C23	1.491(8)	C19–H19A	0.990
C19–H19B	0.990	C19–C20	1.484(11)
C20–H20A	0.980	C20–H20B	0.980
C20–H20C	0.980	C21–H21A	0.990
C21–H21B	0.990	C21–H21C	0.990
C21–H21D	0.990	C21–C22	1.436(11)
C21–C22X	1.512(15)	C22–H22A	0.980
C22–H22B	0.980	C22–H22C	0.980
C22X–H22D	0.980	C22X–H22E	0.980
C22X–H22F	0.980	C23–H23A	0.990
C23–H23B	0.990	C23–H23C	0.990
C23–H23D	0.990	C23–C24	1.527(10)
C23–C24X	1.525(14)	C24–H24A	0.980
C24–H24B	0.980	C24–H24C	0.980
C24X–H24D	0.980	C24X–H24E	0.980
C24X–H24F	0.980		

O2–Cu–O4	89.42(16)	O2–Cu–O6a	89.67(16)
O2–Cu–O8a	177.11(15)	O2–Cu–O9	91.64(15)
O4–Cu–O6a	171.63(15)	O4–Cu–O8a	90.12(17)
O4–Cu–O9	93.89(15)	O6a–Cu–O8a	90.37(16)

O6a–Cu–O9	94.46(15)	O8a–Cu–O9	91.23(15)
C2–C1–C6	118.3(5)	C2–C1–C7	125.2(5)
C6–C1–C7	116.2(5)	C1–C2–C3	118.6(5)
C1–C2–C8	126.1(4)	C3–C2–C8	115.1(5)
C2–C3–H3	118.6	C2–C3–C4	122.7(5)
H3–C3–C4	118.6	C3–C4–C5	118.0(5)
C3–C4–C9	116.1(5)	C5–C4–C9	125.8(5)
C4–C5–C6	119.3(5)	C4–C5–C10	124.3(4)
C6–C5–C10	116.2(5)	C1–C6–C5	122.9(5)
C1–C6–H6	118.5	C5–C6–H6	118.5
C1–C7–O1	117.2(4)	C1–C7–O2	119.2(5)
O1–C7–O2	123.6(5)	C2–C8–O3	116.7(5)
C2–C8–O4	118.8(5)	O3–C8–O4	124.5(5)
C4–C9–O5	116.9(5)	C4–C9–O6	119.3(5)
O5–C9–O6	123.8(5)	C5–C10–O7	117.5(4)
C5–C10–O8	120.1(5)	O7–C10–O8	122.3(5)
Cu–O2–C7	124.1(3)	Cu–O4–C8	125.6(3)
Cua–O6–C9	126.8(4)	Cua–O8–C10	127.2(3)
Cu–O9–H9	124(5)	Cu–O9–C11	122.4(4)
H9–O9–C11	105(5)	O9–C11–H11A	109.6
O9–C11–H11B	109.6	O9–C11–H11C	108.9
O9–C11–H11D	108.9	O9–C11–C12	110.5(8)
O9–C11–C12X	113.3(10)	H11A–C11–H11B	108.1
H11A–C11–C12	109.6	H11B–C11–C12	109.6
H11C–C11–H11D	107.7	H11C–C11–C12X	108.9
H11D–C11–C12X	108.9	C11–C12–H12A	109.5
C11–C12–H12B	109.5	C11–C12–H12C	109.5
H12A–C12–H12B	109.5	H12A–C12–H12C	109.5
H12B–C12–H12C	109.5	C11–C12X–H12D	109.5
C11–C12X–H12E	109.5	C11–C12X–H12F	109.5
H12D–C12X–H12E	109.5	H12D–C12X–H12F	109.5
H12E–C12X–H12F	109.5	H1–N1–C13	108.4
H1–N1–C15	108.4	H1–N1–C17	108.4
C13–N1–C15	110.5(5)	C13–N1–C17	111.4(5)
C15–N1–C17	109.7(5)	N1–C13–H13A	109.2
N1–C13–H13B	109.2	N1–C13–C14	112.2(5)
H13A–C13–H13B	107.9	H13A–C13–C14	109.2
H13B–C13–C14	109.2	C13–C14–H14A	109.5
C13–C14–H14B	109.5	C13–C14–H14C	109.5
H14A–C14–H14B	109.5	H14A–C14–H14C	109.5
H14B–C14–H14C	109.5	N1–C15–H15A	108.7
N1–C15–H15B	108.7	N1–C15–C16	114.2(6)
H15A–C15–H15B	107.6	H15A–C15–C16	108.7
H15B–C15–C16	108.7	C15–C16–H16A	109.5
C15–C16–H16B	109.5	C15–C16–H16C	109.5
H16A–C16–H16B	109.5	H16A–C16–H16C	109.5
H16B–C16–H16C	109.5	N1–C17–H17A	109.2
N1–C17–H17B	109.2	N1–C17–C18	111.9(6)
H17A–C17–H17B	107.9	H17A–C17–C18	109.2
H17B–C17–C18	109.2	C17–C18–H18A	109.5
C17–C18–H18B	109.5	C17–C18–H18C	109.5
H18A–C18–H18B	109.5	H18A–C18–H18C	109.5
H18B–C18–H18C	109.5	H2–N2–C19	107.0
H2–N2–C21	107.0	H2–N2–C23	107.0
C19–N2–C21	103.9(6)	C19–N2–C23	114.5(6)
C21–N2–C23	116.9(6)	N2–C19–H19A	108.8

N2–C19–H19B	108.8	N2–C19–C20	113.6(6)
H19A–C19–H19B	107.7	H19A–C19–C20	108.8
H19B–C19–C20	108.8	C19–C20–H20A	109.5
C19–C20–H20B	109.5	C19–C20–H20C	109.5
H20A–C20–H20B	109.5	H20A–C20–H20C	109.5
H20B–C20–H20C	109.5	N2–C21–H21A	110.3
N2–C21–H21B	110.3	N2–C21–H21C	105.8
N2–C21–H21D	105.8	N2–C21–C22	107.2(8)
N2–C21–C22X	126.1(13)	H21A–C21–H21B	108.5
H21A–C21–C22	110.3	H21B–C21–C22	110.3
H21C–C21–H21D	106.2	H21C–C21–C22X	105.8
H21D–C21–C22X	105.8	C21–C22–H22A	109.5
C21–C22–H22B	109.5	C21–C22–H22C	109.5
H22A–C22–H22B	109.5	H22A–C22–H22C	109.5
H22B–C22–H22C	109.5	C21–C22X–H22D	109.5
C21–C22X–H22E	109.5	C21–C22X–H22F	109.5
H22D–C22X–H22E	109.5	H22D–C22X–H22F	109.5
H22E–C22X–H22F	109.5	N2–C23–H23A	109.0
N2–C23–H23B	109.0	N2–C23–H23C	107.5
N2–C23–H23D	107.5	N2–C23–C24	113.0(7)
N2–C23–C24X	119.5(10)	H23A–C23–H23B	107.8
H23A–C23–C24	109.0	H23B–C23–C24	109.0
H23C–C23–H23D	107.0	H23C–C23–C24X	107.5
H23D–C23–C24X	107.5	C23–C24–H24A	109.5
C23–C24–H24B	109.5	C23–C24–H24C	109.5
H24A–C24–H24B	109.5	H24A–C24–H24C	109.5
H24B–C24–H24C	109.5	C23–C24X–H24D	109.5
C23–C24X–H24E	109.5	C23–C24X–H24F	109.5
H24D–C24X–H24E	109.5	H24D–C24X–H24F	109.5
H24E–C24X–H24F	109.5		

Symmetry operations for equivalent atoms

a –x+1,–y+1,–z+1

Table S39. Torsion angles [°] for 6.

C6–C1–C2–C3	−1.0(8)	C6–C1–C2–C8	−176.1(5)
C7–C1–C2–C3	173.2(5)	C7–C1–C2–C8	−1.9(9)
C1–C2–C3–C4	4.0(8)	C8–C2–C3–C4	179.6(5)
C2–C3–C4–C5	−3.0(8)	C2–C3–C4–C9	−178.6(5)
C3–C4–C5–C6	−0.9(8)	C3–C4–C5–C10	−175.8(5)
C9–C4–C5–C6	174.1(5)	C9–C4–C5–C10	−0.7(9)
C4–C5–C6–C1	4.0(8)	C10–C5–C6–C1	179.2(5)
C2–C1–C6–C5	−3.0(8)	C7–C1–C6–C5	−177.7(5)
C2–C1–C7–O1	−135.8(6)	C2–C1–C7–O2	46.2(8)
C6–C1–C7–O1	38.4(7)	C6–C1–C7–O2	−139.6(5)
C1–C2–C8–O3	130.4(6)	C1–C2–C8–O4	−50.8(8)
C3–C2–C8–O3	−44.9(7)	C3–C2–C8–O4	133.9(5)
C3–C4–C9–O5	51.8(7)	C3–C4–C9–O6	−125.7(5)
C5–C4–C9–O5	−123.3(6)	C5–C4–C9–O6	59.2(8)
C4–C5–C10–O7	139.7(6)	C4–C5–C10–O8	−42.3(8)
C6–C5–C10–O7	−35.3(7)	C6–C5–C10–O8	142.7(5)
C1–C7–O2–Cu	10.0(7)	O1–C7–O2–Cu	−167.8(4)
C2–C8–O4–Cu	2.3(7)	O3–C8–O4–Cu	−178.9(4)
C4–C9–O6–Cua	−16.3(7)	O5–C9–O6–Cua	166.4(4)
C5–C10–O8–Cua	−13.2(7)	O7–C10–O8–Cua	164.7(4)
Cu–O9–C11–C12	−71.3(9)	Cu–O9–C11–C12X	138.2(11)
C15–N1–C13–C14	165.5(5)	C17–N1–C13–C14	−72.3(7)
C13–N1–C15–C16	−78.5(8)	C17–N1–C15–C16	158.4(6)
C13–N1–C17–C18	166.5(6)	C15–N1–C17–C18	−70.8(7)
C21–N2–C19–C20	−168.4(7)	C23–N2–C19–C20	63.0(8)
C19–N2–C21–C22	174.1(7)	C19–N2–C21–C22X	−136.7(19)
C23–N2–C21–C22	−58.8(10)	C23–N2–C21–C22X	−10(2)
C19–N2–C23–C24	60.0(10)	C19–N2–C23–C24X	−160.4(11)
C21–N2–C23–C24	−61.7(11)	C21–N2–C23–C24X	77.9(13)

Symmetry operations for equivalent atoms
a −x+1,−y+1,−z+1

Table S40. Anisotropic displacement parameters (Å^2) for 6. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu	0.0244(4)	0.0033(3)	0.0242(4)	–0.0006(2)	–0.0086(3)	–0.0021(3)
C1	0.020(3)	0.011(2)	0.021(2)	–0.0015(18)	–0.009(2)	–0.003(2)
C2	0.019(3)	0.008(2)	0.022(2)	–0.0014(18)	–0.008(2)	–0.004(2)
C3	0.023(3)	0.010(2)	0.018(3)	0.0010(18)	–0.008(2)	–0.006(2)
C4	0.019(3)	0.012(2)	0.020(2)	–0.0029(18)	–0.007(2)	–0.003(2)
C5	0.021(3)	0.009(2)	0.022(2)	–0.0015(18)	–0.009(2)	–0.006(2)
C6	0.026(3)	0.009(2)	0.023(3)	0.0009(19)	–0.013(2)	–0.005(2)
C7	0.021(3)	0.009(2)	0.024(3)	–0.0022(19)	–0.008(2)	–0.008(2)
C8	0.028(3)	0.005(2)	0.024(3)	–0.0008(19)	–0.012(2)	–0.003(2)
C9	0.025(3)	0.007(2)	0.022(3)	0.001(2)	–0.009(2)	–0.003(2)
C10	0.027(3)	0.008(2)	0.023(3)	0.0020(19)	–0.012(2)	–0.006(2)
O1	0.042(3)	0.020(2)	0.029(2)	–0.0072(17)	–0.021(2)	0.0082(19)
O2	0.027(2)	0.0087(18)	0.026(2)	–0.0059(15)	–0.0124(17)	0.0013(16)
O3	0.030(2)	0.0087(19)	0.035(2)	–0.0001(16)	–0.0025(18)	–0.0070(17)
O4	0.022(2)	0.0090(18)	0.034(2)	–0.0011(16)	–0.0073(17)	–0.0012(15)
O5	0.033(2)	0.024(2)	0.029(2)	–0.0071(17)	–0.0015(19)	–0.0144(19)
O6	0.029(2)	0.0130(19)	0.023(2)	–0.0056(15)	–0.0061(18)	–0.0096(17)
O7	0.053(3)	0.0066(19)	0.037(2)	0.0049(16)	–0.029(2)	–0.0078(19)
O8	0.036(2)	0.0056(18)	0.034(2)	0.0004(15)	–0.0197(19)	–0.0047(17)
O9	0.037(2)	0.0030(18)	0.035(2)	0.0004(16)	–0.0032(19)	–0.0031(17)
C11	0.061(4)	0.023(4)	0.060(4)	–0.010(3)	0.012(3)	–0.018(3)
C12	0.068(7)	0.035(7)	0.114(10)	–0.034(7)	–0.015(6)	–0.004(6)
C12X	0.081(12)	0.052(10)	0.064(9)	–0.021(8)	0.000(8)	–0.014(9)
N1	0.028(3)	0.020(2)	0.019(2)	0.0001(18)	–0.005(2)	–0.007(2)
C13	0.031(3)	0.029(3)	0.030(3)	–0.006(2)	–0.009(3)	–0.002(3)
C14	0.034(4)	0.055(4)	0.030(3)	0.007(3)	–0.006(3)	–0.020(3)
C15	0.067(5)	0.047(4)	0.033(4)	0.016(3)	–0.014(3)	–0.037(4)
C16	0.076(5)	0.054(5)	0.038(4)	0.015(3)	–0.025(4)	–0.037(4)
C17	0.039(4)	0.029(3)	0.038(3)	–0.004(3)	–0.019(3)	–0.007(3)
C18	0.068(5)	0.068(6)	0.072(5)	–0.042(5)	–0.038(4)	0.017(4)
N2	0.113(5)	0.015(3)	0.043(3)	0.011(2)	–0.041(3)	–0.025(3)
C19	0.113(6)	0.058(5)	0.081(6)	0.033(4)	–0.066(5)	–0.058(4)
C20	0.088(6)	0.088(6)	0.089(7)	0.009(5)	–0.045(5)	–0.046(5)
C21	0.111(6)	0.040(4)	0.075(5)	–0.004(4)	–0.044(4)	–0.015(4)
C22	0.078(6)	0.061(7)	0.052(6)	0.003(5)	–0.030(5)	–0.033(5)
C22X	0.087(11)	0.025(8)	0.044(11)	0.001(8)	–0.035(9)	–0.022(8)
C23	0.119(6)	0.033(4)	0.059(4)	0.017(3)	–0.055(4)	–0.036(4)
C24	0.107(10)	0.034(6)	0.065(7)	0.025(5)	–0.055(7)	–0.035(6)
C24X	0.125(10)	0.028(10)	0.072(12)	0.004(9)	–0.057(9)	–0.021(8)

Table S41. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for 6.

	x	y	z	U
H3	0.7521	0.5801	0.3048	0.020
H6	0.6318	0.3985	0.7029	0.022
H9	0.281(7)	1.043(3)	0.670(5)	0.044
H11A	0.1453	1.0850	0.8481	0.068
H11B	0.1611	0.9417	0.8830	0.068
H11C	0.1378	0.9291	0.8581	0.068
H11D	0.0845	1.0530	0.7858	0.068
H12A	–0.0382	1.0357	0.8534	0.116
H12B	0.0420	1.0804	0.7148	0.116
H12C	0.0578	0.9373	0.7497	0.116
H12D	0.0727	1.0944	0.9746	0.110
H12E	0.2309	1.0309	0.9370	0.110
H12F	0.1775	1.1548	0.8646	0.110
H1	0.7288	0.4652	0.8623	0.028
H13A	0.8927	0.2934	0.7407	0.038
H13B	0.9975	0.3105	0.7918	0.038
H14A	0.8694	0.4967	0.6498	0.061
H14B	1.0214	0.4128	0.5936	0.061
H14C	0.9799	0.5087	0.6964	0.061
H15A	0.8267	0.2355	0.9766	0.057
H15B	0.6995	0.3368	1.0591	0.057
H16A	0.5821	0.3323	0.9411	0.078
H16B	0.6352	0.1973	0.9961	0.078
H16C	0.7102	0.2352	0.8534	0.078
H17A	0.8970	0.5284	0.8924	0.041
H17B	0.9047	0.4163	0.9933	0.041
H18A	0.6673	0.6144	1.0131	0.104
H18B	0.7567	0.5966	1.0952	0.104
H18C	0.6734	0.5017	1.1135	0.104
H2	0.7406	0.0381	0.6661	0.064
H19A	0.5505	0.0101	0.6452	0.084
H19B	0.5311	–0.0806	0.7667	0.084
H20A	0.4770	0.0761	0.8910	0.121
H20B	0.3857	0.1201	0.8079	0.121
H20C	0.5145	0.1682	0.7720	0.121
H21A	0.7523	–0.2022	0.6342	0.088
H21B	0.7501	–0.0902	0.5317	0.088
H21C	0.8115	–0.0768	0.5251	0.088
H21D	0.7048	–0.1505	0.5981	0.088
H22A	0.9676	–0.2067	0.4998	0.088
H22B	0.9446	–0.0715	0.5362	0.088
H22C	0.9468	–0.1830	0.6382	0.088
H22D	0.9157	–0.2828	0.5211	0.071
H22E	0.9688	–0.2212	0.5965	0.071
H22F	0.8609	–0.2958	0.6703	0.071
H23A	0.7006	–0.0083	0.8741	0.074
H23B	0.8449	–0.0923	0.7927	0.074
H23C	0.7440	–0.1624	0.8395	0.074
H23D	0.6741	–0.0259	0.8848	0.074
H24A	0.7312	–0.2118	0.9584	0.091
H24B	0.6094	–0.1755	0.9102	0.091

H24C	0.7538	–0.2595	0.8287	0.091
H24D	0.8872	–0.0974	0.8955	0.104
H24E	0.9547	–0.1217	0.7497	0.104
H24F	0.8843	0.0156	0.7952	0.104

Table S42. Hydrogen bonds for 6 [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
O9–H9...O3b	0.836(10)	1.93(2)	2.734(5)	162(6)
N1–H1...O1	1.00	1.79	2.784(6)	173
N2–H2...O7	1.00	1.79	2.773(7)	166
N2–H2...O8	1.00	2.36	3.085(6)	129

Symmetry operations for equivalent atoms
b –x+1,–y+2,–z+1

Table S43. Crystal data and structure refinement for 7.

Identification code	7	
Chemical formula (moiety)	$4C_6H_{16}N^+ \cdot C_{22}H_{12}Cu_2O_{18}^{4-} \cdot 2CH_4O$	
Chemical formula (total)	$C_{48}H_{84}Cu_2N_4O_{20}$	
Formula weight	1164.27	
Temperature	160(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 11.5053(11) Å	α = 78.671(2)°
	b = 11.5543(11) Å	β = 64.251(2)°
	c = 12.0160(11) Å	γ = 71.747(2)°
Cell volume	1362.9(2) Å^3	
Z	1	
Calculated density	1.418 g/cm^3	
Absorption coefficient μ	0.858 mm^{-1}	
F(000)	618	
Crystal colour and size	blue, 0.480 × 0.440 × 0.240 mm^3	
Reflections for cell refinement	8941 (θ range 2.5 to 29.1°)	
Data collection method	Bruker SMART CCD diffractometer narrow-frame ω scans	
θ range for data collection	1.9 to 29.1°	
Index ranges	h −15 to 15, k −15 to 15, l −16 to 16	
Completeness to θ = 25.2°	98.9 %	
Reflections collected	11335	
Independent reflections	6487 (R_{int} = 0.0142)	
Reflections with $F^2>2\sigma$	5709	
Absorption correction	multi-scan	
Min. and max. transmission	0.680 and 0.820	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0694, 2.2682	
Data / restraints / parameters	6487 / 214 / 364	
Final R indices [$F^2>2\sigma$]	R1 = 0.0520, wR2 = 0.1342	
R indices (all data)	R1 = 0.0588, wR2 = 0.1368	
Goodness-of-fit on F^2	1.055	
Extinction coefficient	0.0043(14)	
Largest and mean shift/su	0.002 and 0.000	
Largest diff. peak and hole	1.11 and −0.90 e Å^{-3}	

Table S44. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for 7. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cu	0.36682(3)	0.78665(3)	0.62699(3)	0.01855(11)
C1	0.6162(2)	0.5673(2)	0.6064(2)	0.0187(5)
C2	0.6558(2)	0.6229(2)	0.4853(2)	0.0180(5)
C3	0.7240(3)	0.5488(2)	0.3857(2)	0.0198(5)
C4	0.7467(2)	0.4216(2)	0.4016(2)	0.0197(5)
C5	0.7052(2)	0.3666(2)	0.5224(2)	0.0196(5)
C6	0.6439(3)	0.4404(2)	0.6219(2)	0.0202(5)
C7	0.5556(3)	0.6346(2)	0.7231(2)	0.0207(5)
C8	0.6391(3)	0.7598(2)	0.4538(2)	0.0202(5)
C9	0.8271(3)	0.3541(2)	0.2835(2)	0.0243(5)
C10	0.7290(3)	0.2302(2)	0.5546(3)	0.0225(5)
O1	0.6028(2)	0.59158(18)	0.80265(19)	0.0299(4)
O2	0.45870(19)	0.72901(17)	0.73796(17)	0.0244(4)
O3	0.7392(2)	0.79261(17)	0.37657(19)	0.0288(4)
O4	0.52467(19)	0.83307(16)	0.50341(18)	0.0255(4)
O5	0.9357(2)	0.3759(2)	0.2151(2)	0.0450(6)
O6	0.7776(2)	0.28336(17)	0.25813(17)	0.0257(4)
O7	0.7548(2)	0.18893(17)	0.6477(2)	0.0335(5)
O8	0.7195(2)	0.16253(16)	0.48927(19)	0.0258(4)
O9	0.2576(2)	0.97159(17)	0.70646(19)	0.0297(4)
C11	0.1150(4)	1.0000(3)	0.7580(5)	0.0648(14)
N1	0.7776(3)	0.4005(2)	0.8710(2)	0.0314(5)
C12	0.8997(3)	0.3473(3)	0.7600(3)	0.0382(7)
C13	0.9485(4)	0.4454(4)	0.6633(3)	0.0439(8)
C14	0.8108(4)	0.4567(4)	0.9515(4)	0.0454(8)
C15	0.6895(4)	0.5223(4)	1.0555(3)	0.0496(9)
C16	0.6950(4)	0.3070(3)	0.9380(3)	0.0417(8)
C17	0.7658(4)	0.1951(3)	0.9927(4)	0.0531(10)
N2	0.7031(4)	–0.0393(3)	0.6991(3)	0.0497(8)
C18	0.7324(6)	–0.0840(4)	0.8118(4)	0.0451(11)
C19	0.6670(16)	–0.1907(10)	0.8848(11)	0.155(5)
C20	0.5505(6)	–0.0047(4)	0.7213(5)	0.0473(12)
C21	0.4641(6)	0.0954(6)	0.8046(6)	0.0705(16)
C22	0.7764(5)	–0.1257(4)	0.6010(5)	0.0522(12)
C23	0.9240(6)	–0.1538(6)	0.5669(7)	0.0749(17)
C18X	0.670(2)	–0.0555(16)	0.8438(13)	0.035(5)
C19X	0.6996(17)	–0.1959(14)	0.8681(17)	0.015(4)
C20X	0.597(2)	–0.070(3)	0.683(3)	0.075(8)
C21X	0.479(2)	0.023(2)	0.769(2)	0.044(6)
C22X	0.8447(18)	–0.106(2)	0.614(3)	0.071(8)
C23X	0.897(2)	–0.2403(16)	0.590(2)	0.037(5)
O10	1.1098(6)	0.2988(7)	–0.0223(8)	0.175(3)
C24	1.0988(10)	0.1906(8)	–0.0216(9)	0.130(3)

Table S45. Bond lengths [Å] and angles [°] for 7.

Cu–O2	1.9426(19)	Cu–O4	1.9352(19)
Cu–O6a	1.9320(19)	Cu–O8a	1.9497(19)
Cu–O9	2.2658(19)	C1–C2	1.406(3)
C1–C6	1.392(3)	C1–C7	1.515(3)
C2–C3	1.395(3)	C2–C8	1.523(3)
C3–H3	0.950	C3–C4	1.399(3)
C4–C5	1.402(4)	C4–C9	1.524(3)
C5–C6	1.395(3)	C5–C10	1.513(3)
C6–H6	0.950	C7–O1	1.246(3)
C7–O2	1.267(3)	C8–O3	1.240(3)
C8–O4	1.274(3)	C9–O5	1.234(4)
C9–O6	1.275(3)	C10–O7	1.248(3)
C10–O8	1.268(3)	O6–Cua	1.9319(19)
O8–Cua	1.9497(19)	O9–H9	0.835(10)
O9–C11	1.429(4)	C11–H11A	0.980
C11–H11B	0.980	C11–H11C	0.980
N1–H1	1.000	N1–C12	1.511(4)
N1–C14	1.493(4)	N1–C16	1.534(4)
C12–H12A	0.990	C12–H12B	0.990
C12–C13	1.505(5)	C13–H13A	0.980
C13–H13B	0.980	C13–H13C	0.980
C14–H14A	0.990	C14–H14B	0.990
C14–C15	1.510(5)	C15–H15A	0.980
C15–H15B	0.980	C15–H15C	0.980
C16–H16A	0.990	C16–H16B	0.990
C16–C17	1.496(5)	C17–H17A	0.980
C17–H17B	0.980	C17–H17C	0.980
N2–H2	1.000	N2–H2X	1.000
N2–C18	1.492(5)	N2–C20	1.583(6)
N2–C22	1.472(5)	N2–C18X	1.593(13)
N2–C20X	1.472(14)	N2–C22X	1.539(13)
C18–H18A	0.990	C18–H18B	0.990
C18–C19	1.561(8)	C19–H19A	0.980
C19–H19B	0.980	C19–H19C	0.980
C20–H20A	0.990	C20–H20B	0.990
C20–C21	1.482(8)	C21–H21A	0.980
C21–H21B	0.980	C21–H21C	0.980
C22–H22A	0.990	C22–H22B	0.990
C22–C23	1.503(7)	C23–H23A	0.980
C23–H23B	0.980	C23–H23C	0.980
C18X–H18C	0.990	C18X–H18D	0.990
C18X–C19X	1.545(14)	C19X–H19D	0.980
C19X–H19E	0.980	C19X–H19F	0.980
C20X–H20C	0.990	C20X–H20D	0.990
C20X–C21X	1.538(16)	C21X–H21D	0.980
C21X–H21E	0.980	C21X–H21F	0.980
C22X–H22C	0.990	C22X–H22D	0.990
C22X–C23X	1.519(15)	C23X–H23D	0.980
C23X–H23E	0.980	C23X–H23F	0.980
O10–H10	0.840	O10–C24	1.293(9)
C24–H24A	0.980	C24–H24B	0.980
C24–H24C	0.980		

O2–Cu–O4	88.69(9)	O2–Cu–O6a	90.31(9)
O2–Cu–O8a	177.12(8)	O2–Cu–O9	94.74(8)
O4–Cu–O6a	171.61(8)	O4–Cu–O8a	90.42(9)
O4–Cu–O9	96.67(8)	O6a–Cu–O8a	90.18(9)
O6a–Cu–O9	91.71(8)	O8a–Cu–O9	88.08(8)
C2–C1–C6	118.5(2)	C2–C1–C7	124.8(2)
C6–C1–C7	116.5(2)	C1–C2–C3	118.8(2)
C1–C2–C8	124.5(2)	C3–C2–C8	116.5(2)
C2–C3–H3	118.8	C2–C3–C4	122.4(2)
H3–C3–C4	118.8	C3–C4–C5	118.6(2)
C3–C4–C9	115.7(2)	C5–C4–C9	125.5(2)
C4–C5–C6	118.8(2)	C4–C5–C10	124.8(2)
C6–C5–C10	116.3(2)	C1–C6–C5	122.7(2)
C1–C6–H6	118.6	C5–C6–H6	118.6
C1–C7–O1	117.3(2)	C1–C7–O2	120.1(2)
O1–C7–O2	122.6(2)	C2–C8–O3	116.7(2)
C2–C8–O4	119.3(2)	O3–C8–O4	123.9(2)
C4–C9–O5	116.9(2)	C4–C9–O6	119.3(2)
O5–C9–O6	123.8(2)	C5–C10–O7	117.7(2)
C5–C10–O8	119.9(2)	O7–C10–O8	122.4(2)
Cu–O2–C7	123.90(17)	Cu–O4–C8	125.36(16)
Cua–O6–C9	126.39(17)	Cua–O8–C10	127.29(17)
Cu–O9–H9	123(3)	Cu–O9–C11	116.2(2)
H9–O9–C11	110(3)	O9–C11–H11A	109.5
O9–C11–H11B	109.5	O9–C11–H11C	109.5
H11A–C11–H11B	109.5	H11A–C11–H11C	109.5
H11B–C11–H11C	109.5	H1–N1–C12	106.0
H1–N1–C14	106.0	H1–N1–C16	106.0
C12–N1–C14	112.3(3)	C12–N1–C16	110.5(2)
C14–N1–C16	115.2(3)	N1–C12–H12A	109.3
N1–C12–H12B	109.3	N1–C12–C13	111.7(3)
H12A–C12–H12B	107.9	H12A–C12–C13	109.3
H12B–C12–C13	109.3	C12–C13–H13A	109.5
C12–C13–H13B	109.5	C12–C13–H13C	109.5
H13A–C13–H13B	109.5	H13A–C13–H13C	109.5
H13B–C13–H13C	109.5	N1–C14–H14A	108.9
N1–C14–H14B	108.9	N1–C14–C15	113.5(3)
H14A–C14–H14B	107.7	H14A–C14–C15	108.9
H14B–C14–C15	108.9	C14–C15–H15A	109.5
C14–C15–H15B	109.5	C14–C15–H15C	109.5
H15A–C15–H15B	109.5	H15A–C15–H15C	109.5
H15B–C15–H15C	109.5	N1–C16–H16A	108.8
N1–C16–H16B	108.8	N1–C16–C17	113.9(3)
H16A–C16–H16B	107.7	H16A–C16–C17	108.8
H16B–C16–C17	108.8	C16–C17–H17A	109.5
C16–C17–H17B	109.5	C16–C17–H17C	109.5
H17A–C17–H17B	109.5	H17A–C17–H17C	109.5
H17B–C17–H17C	109.5	H2–N2–C18	106.8
H2–N2–C20	106.8	H2–N2–C22	106.8
H2X–N2–C18X	106.3	H2X–N2–C20X	106.3
H2X–N2–C22X	106.3	C18–N2–C20	115.7(4)
C18–N2–C22	113.1(3)	C20–N2–C22	107.2(3)
C18X–N2–C20X	107.3(14)	C18X–N2–C22X	116.4(15)
C20X–N2–C22X	113.4(14)	N2–C18–H18A	109.5
N2–C18–H18B	109.5	N2–C18–C19	110.9(5)
H18A–C18–H18B	108.1	H18A–C18–C19	109.5

H18B–C18–C19	109.5	C18–C19–H19A	109.5
C18–C19–H19B	109.5	C18–C19–H19C	109.5
H19A–C19–H19B	109.5	H19A–C19–H19C	109.5
H19B–C19–H19C	109.5	N2–C20–H20A	108.6
N2–C20–H20B	108.6	N2–C20–C21	114.6(4)
H20A–C20–H20B	107.6	H20A–C20–C21	108.6
H20B–C20–C21	108.6	C20–C21–H21A	109.5
C20–C21–H21B	109.5	C20–C21–H21C	109.5
H21A–C21–H21B	109.5	H21A–C21–H21C	109.5
H21B–C21–H21C	109.5	N2–C22–H22A	109.6
N2–C22–H22B	109.6	N2–C22–C23	110.1(4)
H22A–C22–H22B	108.2	H22A–C22–C23	109.6
H22B–C22–C23	109.6	C22–C23–H23A	109.5
C22–C23–H23B	109.5	C22–C23–H23C	109.5
H23A–C23–H23B	109.5	H23A–C23–H23C	109.5
H23B–C23–H23C	109.5	N2–C18X–H18C	111.4
N2–C18X–H18D	111.4	N2–C18X–C19X	101.8(12)
H18C–C18X–H18D	109.3	H18C–C18X–C19X	111.4
H18D–C18X–C19X	111.4	C18X–C19X–H19D	109.5
C18X–C19X–H19E	109.5	C18X–C19X–H19F	109.5
H19D–C19X–H19E	109.5	H19D–C19X–H19F	109.5
H19E–C19X–H19F	109.5	N2–C20X–H20C	112.4
N2–C20X–H20D	112.4	N2–C20X–C21X	96.6(14)
H20C–C20X–H20D	110.0	H20C–C20X–C21X	112.4
H20D–C20X–C21X	112.4	C20X–C21X–H21D	109.5
C20X–C21X–H21E	109.5	C20X–C21X–H21F	109.5
H21D–C21X–H21E	109.5	H21D–C21X–H21F	109.5
H21E–C21X–H21F	109.5	N2–C22X–H22C	105.5
N2–C22X–H22D	105.5	N2–C22X–C23X	127.2(17)
H22C–C22X–H22D	106.1	H22C–C22X–C23X	105.5
H22D–C22X–C23X	105.5	C22X–C23X–H23D	109.5
C22X–C23X–H23E	109.5	C22X–C23X–H23F	109.5
H23D–C23X–H23E	109.5	H23D–C23X–H23F	109.5
H23E–C23X–H23F	109.5	H10–O10–C24	105.1
O10–C24–H24A	109.5	O10–C24–H24B	109.5
O10–C24–H24C	109.5	H24A–C24–H24B	109.5
H24A–C24–H24C	109.5	H24B–C24–H24C	109.5

Symmetry operations for equivalent atoms
a –x+1,–y+1,–z+1

Table S46. Torsion angles [°] for 7.

C6–C1–C2–C3	−1.6(4)	C6–C1–C2–C8	−176.6(2)
C7–C1–C2–C3	172.9(2)	C7–C1–C2–C8	−2.1(4)
C1–C2–C3–C4	4.3(4)	C8–C2–C3–C4	179.7(2)
C2–C3–C4–C5	−3.3(4)	C2–C3–C4–C9	−177.8(2)
C3–C4–C5–C6	−0.4(4)	C3–C4–C5–C10	−176.7(2)
C9–C4–C5–C6	173.5(2)	C9–C4–C5–C10	−2.7(4)
C2–C1–C6–C5	−2.1(4)	C7–C1–C6–C5	−177.0(2)
C4–C5–C6–C1	3.2(4)	C10–C5–C6–C1	179.7(2)
C2–C1–C7–O1	−132.1(3)	C2–C1–C7–O2	49.5(4)
C6–C1–C7–O1	42.4(3)	C6–C1–C7–O2	−136.0(3)
C1–C2–C8–O3	129.9(3)	C1–C2–C8–O4	−52.6(4)
C3–C2–C8–O3	−45.2(3)	C3–C2–C8–O4	132.2(3)
C3–C4–C9–O5	53.0(4)	C3–C4–C9–O6	−124.1(3)
C5–C4–C9–O5	−121.2(3)	C5–C4–C9–O6	61.8(4)
C4–C5–C10–O7	142.8(3)	C4–C5–C10–O8	−38.7(4)
C6–C5–C10–O7	−33.6(4)	C6–C5–C10–O8	145.0(3)
C1–C7–O2–Cu	6.8(3)	O1–C7–O2–Cu	−171.5(2)
C2–C8–O4–Cu	4.2(3)	O3–C8–O4–Cu	−178.5(2)
C4–C9–O6–Cua	−19.1(4)	O5–C9–O6–Cua	164.1(2)
C5–C10–O8–Cua	−17.2(4)	O7–C10–O8–Cua	161.3(2)
C14–N1–C12–C13	−75.0(4)	C16–N1–C12–C13	154.9(3)
C12–N1–C14–C15	173.8(3)	C16–N1–C14–C15	−58.5(4)
C12–N1–C16–C17	64.1(4)	C14–N1–C16–C17	−64.5(4)
C20–N2–C18–C19	52.2(8)	C22–N2–C18–C19	−72.0(9)
C18–N2–C20–C21	61.2(5)	C22–N2–C20–C21	−171.6(4)
C18–N2–C22–C23	−56.4(5)	C20–N2–C22–C23	174.9(4)
C20X–N2–C18X–C19X	71.6(19)	C22X–N2–C18X–C19X	−56.7(19)
C18X–N2–C20X–C21X	56(2)	C22X–N2–C20X–C21X	−173.7(19)
C18X–N2–C22X–C23X	78(3)	C20X–N2–C22X–C23X	−47(4)

Symmetry operations for equivalent atoms
a −x+1,−y+1,−z+1

Table S47. Anisotropic displacement parameters (Å^2) for 7. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu	0.02148(17)	0.01339(15)	0.01979(17)	–0.00207(10)	–0.00825(12)	–0.00267(11)
C1	0.0200(11)	0.0162(11)	0.0198(11)	–0.0019(9)	–0.0081(9)	–0.0040(9)
C2	0.0178(11)	0.0135(10)	0.0217(11)	–0.0019(8)	–0.0070(9)	–0.0037(9)
C3	0.0215(12)	0.0175(11)	0.0201(11)	–0.0015(9)	–0.0071(10)	–0.0062(9)
C4	0.0182(11)	0.0166(11)	0.0236(12)	–0.0050(9)	–0.0063(10)	–0.0045(9)
C5	0.0210(12)	0.0137(10)	0.0258(12)	–0.0012(9)	–0.0116(10)	–0.0034(9)
C6	0.0247(12)	0.0169(11)	0.0211(11)	0.0017(9)	–0.0115(10)	–0.0064(9)
C7	0.0244(12)	0.0164(10)	0.0210(11)	–0.0010(9)	–0.0088(10)	–0.0056(9)
C8	0.0263(13)	0.0149(10)	0.0207(11)	–0.0013(9)	–0.0103(10)	–0.0056(9)
C9	0.0270(13)	0.0185(11)	0.0232(12)	–0.0058(9)	–0.0052(10)	–0.0049(10)
C10	0.0259(13)	0.0151(11)	0.0283(13)	–0.0011(9)	–0.0133(11)	–0.0042(9)
O1	0.0366(11)	0.0272(10)	0.0262(10)	–0.0055(8)	–0.0188(9)	0.0025(8)
O2	0.0283(10)	0.0195(8)	0.0236(9)	–0.0048(7)	–0.0124(8)	0.0011(7)
O3	0.0271(10)	0.0183(9)	0.0328(10)	0.0005(7)	–0.0039(8)	–0.0086(8)
O4	0.0245(9)	0.0149(8)	0.0301(10)	0.0001(7)	–0.0075(8)	–0.0022(7)
O5	0.0367(13)	0.0522(14)	0.0400(13)	–0.0246(11)	0.0086(10)	–0.0255(11)
O6	0.0319(10)	0.0224(9)	0.0227(9)	–0.0051(7)	–0.0063(8)	–0.0112(8)
O7	0.0561(14)	0.0157(8)	0.0427(12)	0.0027(8)	–0.0354(11)	–0.0079(9)
O8	0.0366(11)	0.0143(8)	0.0328(10)	–0.0005(7)	–0.0205(9)	–0.0059(7)
O9	0.0332(11)	0.0148(8)	0.0315(10)	–0.0037(7)	–0.0049(9)	–0.0040(8)
C11	0.037(2)	0.0287(17)	0.083(3)	0.0010(18)	0.010(2)	–0.0018(15)
N1	0.0316(13)	0.0272(12)	0.0266(12)	–0.0004(9)	–0.0100(10)	0.0009(10)
C12	0.0327(16)	0.0398(17)	0.0332(16)	–0.0059(13)	–0.0094(13)	–0.0012(13)
C13	0.0313(16)	0.061(2)	0.0366(17)	0.0026(16)	–0.0111(14)	–0.0150(16)
C14	0.049(2)	0.0447(19)	0.0445(19)	–0.0107(15)	–0.0264(17)	0.0014(16)
C15	0.063(2)	0.0432(19)	0.0350(18)	–0.0048(15)	–0.0182(17)	–0.0047(17)
C16	0.0408(18)	0.0357(17)	0.0369(17)	–0.0020(13)	–0.0098(14)	–0.0033(14)
C17	0.059(2)	0.0365(18)	0.0396(19)	0.0015(15)	–0.0098(17)	0.0021(17)
N2	0.097(2)	0.0279(13)	0.0448(16)	0.0121(11)	–0.0433(17)	–0.0301(15)
C18	0.071(3)	0.035(2)	0.040(2)	0.0004(18)	–0.033(2)	–0.015(2)
C19	0.312(15)	0.127(7)	0.131(8)	0.094(6)	–0.165(9)	–0.150(9)
C20	0.072(3)	0.046(2)	0.048(3)	0.019(2)	–0.040(2)	–0.037(2)
C21	0.074(4)	0.080(4)	0.056(3)	–0.003(3)	–0.015(3)	–0.036(3)
C22	0.076(3)	0.0291(19)	0.070(3)	–0.0011(18)	–0.048(2)	–0.0125(19)
C23	0.073(4)	0.069(4)	0.092(5)	–0.004(3)	–0.040(3)	–0.021(3)
O10	0.109(4)	0.159(6)	0.255(9)	–0.081(6)	–0.037(5)	–0.046(4)
C24	0.158(8)	0.115(6)	0.183(9)	0.049(6)	–0.129(7)	–0.070(6)

Table S48. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for 7.

	x	y	z	U
H3	0.7562	0.5861	0.3041	0.024
H6	0.6200	0.4026	0.7036	0.024
H9	0.283(4)	1.035(2)	0.672(3)	0.045
H11A	0.0782	1.0815	0.7895	0.097
H11B	0.0846	0.9985	0.6939	0.097
H11C	0.0845	0.9395	0.8261	0.097
H1	0.7207	0.4689	0.8371	0.038
H12A	0.9718	0.2989	0.7872	0.046
H12B	0.8780	0.2916	0.7233	0.046
H13A	1.0275	0.4078	0.5929	0.066
H13B	0.8779	0.4926	0.6351	0.066
H13C	0.9717	0.4999	0.6989	0.066
H14A	0.8637	0.5153	0.8998	0.054
H14B	0.8672	0.3918	0.9874	0.054
H15A	0.7180	0.5570	1.1047	0.074
H15B	0.6341	0.5881	1.0208	0.074
H15C	0.6376	0.4645	1.1085	0.074
H16A	0.6114	0.3468	1.0050	0.050
H16B	0.6703	0.2822	0.8787	0.050
H17A	0.7074	0.1398	1.0338	0.080
H17B	0.8476	0.1538	0.9268	0.080
H17C	0.7886	0.2185	1.0533	0.080
H2	0.7343	0.0368	0.6647	0.060
H2X	0.6938	0.0499	0.6747	0.060
H18A	0.6976	–0.0159	0.8660	0.054
H18B	0.8303	–0.1126	0.7871	0.054
H19A	0.6876	–0.2185	0.9582	0.232
H19B	0.5700	–0.1619	0.9104	0.232
H19C	0.7025	–0.2585	0.8315	0.232
H20A	0.5436	0.0194	0.6403	0.057
H20B	0.5163	–0.0783	0.7568	0.057
H21A	0.3718	0.1112	0.8134	0.106
H21B	0.4681	0.0717	0.8860	0.106
H21C	0.4954	0.1695	0.7693	0.106
H22A	0.7568	–0.0898	0.5272	0.063
H22B	0.7468	–0.2021	0.6304	0.063
H23A	0.9719	–0.2113	0.5015	0.112
H23B	0.9532	–0.0782	0.5369	0.112
H23C	0.9432	–0.1903	0.6398	0.112
H18C	0.7275	–0.0220	0.8631	0.042
H18D	0.5748	–0.0158	0.8926	0.042
H19D	0.6824	–0.2177	0.9559	0.022
H19E	0.6421	–0.2264	0.8465	0.022
H19F	0.7935	–0.2326	0.8173	0.022
H20C	0.5925	–0.1554	0.7118	0.090
H20D	0.6050	–0.0538	0.5958	0.090
H21D	0.3953	0.0168	0.7706	0.066
H21E	0.4775	0.0054	0.8526	0.066
H21F	0.4898	0.1057	0.7381	0.066
H22C	0.8610	–0.0614	0.5312	0.085
H22D	0.9056	–0.0885	0.6431	0.085

H23D	0.9911	–0.2569	0.5317	0.055
H23E	0.8898	–0.2892	0.6683	0.055
H23F	0.8447	–0.2617	0.5551	0.055
H10	1.0577	0.3217	0.0489	0.262
H24A	1.1432	0.1646	–0.1064	0.194
H24B	1.0041	0.1920	0.0117	0.194
H24C	1.1408	0.1332	0.0303	0.194

Table S49. Hydrogen bonds for 7 [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
O9–H9...O3b	0.835(10)	1.934(19)	2.717(3)	156(4)
O10–H10...O5	0.84	1.96	2.803(8)	180
N1–H1...O1	1.00	1.75	2.745(3)	171
N2–H2...O7	1.00	1.81	2.778(3)	163
N2–H2X...O7	1.00	1.87	2.778(3)	150

Symmetry operations for equivalent atoms
b –x+1,–y+2,–z+1

Table S50. Crystal data and structure refinement for 8.

Identification code	8	
Chemical formula (moiety)	$2NH_4^+ \cdot CuN_4H_{12}^{2+} \cdot 2C_{10}H_{11}CuN_3O_8^{2-} \cdot 2H2O$	
Chemical formula (total)	$C_{20}H_{46}Cu_3N_{12}O_{18}$	
Formula weight	933.31	
Temperature	160(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P2_1/c$	
Unit cell parameters	a = 8.2343(7) Å	α = 90°
	b = 19.5788(16) Å	β = 100.371(2)°
	c = 10.9336(9) Å	γ = 90°
Cell volume	1733.9(2) Å^3	
Z	2	
Calculated density	1.788 g/cm^3	
Absorption coefficient μ	1.917 mm^{-1}	
F(000)	962	
Crystal colour and size	Blue, 0.270 × 0.080 × 0.040 mm^3	
Reflections for cell refinement	4625 (θ range 2.7 to 28.6°)	
Data collection method	Bruker SMART 1K CCD diffractometer narrow-frame ω scans	
θ range for data collection	2.1 to 28.7°	
Index ranges	h –10 to 10, k –24 to 25, l –14 to 14	
Completeness to θ = 25.2°	98.2 %	
Reflections collected	11979	
Independent reflections	3952 (R_{int} = 0.0429)	
Reflections with $F^2>2\sigma$	3125	
Absorption correction	multi-scan	
Min. and max. transmission	0.630 and 0.930	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0360, 3.5743	
Data / restraints / parameters	3952 / 0 / 304	
Final R indices [$F^2>2\sigma$]	R1 = 0.0451, wR2 = 0.0904	
R indices (all data)	R1 = 0.0651, wR2 = 0.0981	
Goodness-of-fit on F^2	1.094	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	0.65 and –0.75 e Å^{-3}	

Table S51. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for 8. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cu1	0.83314(5)	0.45250(2)	0.89782(4)	0.01185(11)
Cu2	0.5000	0.5000	0.5000	0.01365(14)
C1	0.8395(4)	0.66351(16)	1.0096(3)	0.0094(6)
C2	0.7750(4)	0.68894(16)	1.1110(3)	0.0100(6)
C3	0.8240(4)	0.75331(17)	1.1570(3)	0.0112(6)
C4	0.9423(4)	0.79108(16)	1.1097(3)	0.0105(6)
C5	1.0156(4)	0.76329(16)	1.0157(3)	0.0103(6)
C6	0.9604(4)	0.70035(16)	0.9644(3)	0.0117(6)
C7	0.7812(4)	0.59822(17)	0.9446(3)	0.0109(6)
C8	0.6659(4)	0.64542(17)	1.1778(3)	0.0116(6)
C9	0.9959(4)	0.86051(16)	1.1651(3)	0.0106(6)
C10	1.1592(4)	0.79754(17)	0.9718(3)	0.0133(7)
O1	0.6383(3)	0.59621(12)	0.8820(2)	0.0165(5)
O2	0.8864(3)	0.55000(11)	0.9523(2)	0.0110(5)
O3	0.5903(3)	0.67395(12)	1.2537(2)	0.0173(5)
O4	0.6609(3)	0.58208(12)	1.1559(2)	0.0196(6)
O5	0.8844(3)	0.90389(12)	1.1621(2)	0.0187(5)
O6	1.1460(3)	0.86896(12)	1.2108(2)	0.0175(5)
O7	1.1364(3)	0.85293(13)	0.9162(2)	0.0233(6)
O8	1.2942(3)	0.76500(14)	0.9959(3)	0.0231(6)
N1	0.7057(4)	0.44458(17)	1.0385(3)	0.0152(6)
N2	0.7626(4)	0.35864(16)	0.8355(3)	0.0163(6)
N3	0.9735(4)	0.46379(15)	0.7697(3)	0.0126(6)
N4	0.7369(4)	0.48656(18)	0.4760(3)	0.0193(7)
N5	0.5438(4)	0.60261(17)	0.5061(3)	0.0177(7)
N6	0.4291(4)	0.79176(17)	1.3051(3)	0.0181(7)
O9	0.5715(3)	0.48664(14)	0.7313(2)	0.0164(5)

Table S52. Bond lengths [Å] and angles [°] for 8.

Cu1–O2	2.024(2)	Cu1–N1	2.018(3)
Cu1–N2	2.009(3)	Cu1–N3	1.982(3)
Cu2–N4	2.031(3)	Cu2–N4a	2.031(3)
Cu2–N5	2.040(3)	Cu2–N5a	2.040(3)
C1–C2	1.404(5)	C1–C6	1.389(5)
C1–C7	1.499(4)	C2–C3	1.390(5)
C2–C8	1.518(5)	C3–H3	0.950
C3–C4	1.395(5)	C4–C5	1.393(5)
C4–C9	1.521(4)	C5–C6	1.396(4)
C5–C10	1.510(5)	C6–H6	0.950
C7–O1	1.250(4)	C7–O2	1.274(4)
C8–O3	1.254(4)	C8–O4	1.262(4)
C9–O5	1.247(4)	C9–O6	1.258(4)
C10–O7	1.241(4)	C10–O8	1.267(4)
N1–H1A	0.87(5)	N1–H1B	0.88(5)
N1–H1C	0.78(5)	N2–H2A	0.81(5)
N2–H2B	0.95(5)	N2–H2C	0.85(5)
N3–H3A	0.87(4)	N3–H3B	0.86(4)
N3–H3C	0.84(4)	N4–H4A	0.85(5)
N4–H4B	0.89(5)	N4–H4C	0.80(5)
N5–H5A	0.83(5)	N5–H5B	0.80(5)
N5–H5C	0.88(5)	N6–H6A	0.89(5)
N6–H6B	0.93(5)	N6–H6C	0.78(5)
N6–H6D	0.82(5)	O9–H9A	0.77(5)
O9–H9B	0.80(5)		

O2–Cu1–N1	87.88(12)	O2–Cu1–N2	175.24(11)
O2–Cu1–N3	88.84(11)	N1–Cu1–N2	91.71(14)
N1–Cu1–N3	175.21(13)	N2–Cu1–N3	91.85(14)
N4–Cu2–N4a	180.00	N4–Cu2–N5	87.90(14)
N4a–Cu2–N5	92.10(14)	N4–Cu2–N5a	92.10(14)
N4a–Cu2–N5a	87.90(14)	N5–Cu2–N5a	180.00
C2–C1–C6	119.6(3)	C2–C1–C7	122.8(3)
C6–C1–C7	117.6(3)	C1–C2–C3	118.8(3)
C1–C2–C8	121.5(3)	C3–C2–C8	119.5(3)
C2–C3–H3	119.2	C2–C3–C4	121.5(3)
H3–C3–C4	119.2	C3–C4–C5	119.4(3)
C3–C4–C9	119.9(3)	C5–C4–C9	120.7(3)
C4–C5–C6	119.2(3)	C4–C5–C10	121.9(3)
C6–C5–C10	118.8(3)	C1–C6–C5	121.2(3)
C1–C6–H6	119.4	C5–C6–H6	119.4
C1–C7–O1	118.4(3)	C1–C7–O2	116.4(3)
O1–C7–O2	125.1(3)	C2–C8–O3	118.4(3)
C2–C8–O4	117.5(3)	O3–C8–O4	124.0(3)
C4–C9–O5	116.0(3)	C4–C9–O6	118.0(3)
O5–C9–O6	125.9(3)	C5–C10–O7	119.0(3)
C5–C10–O8	114.8(3)	O7–C10–O8	126.2(3)
Cu1–O2–C7	124.8(2)	Cu1–N1–H1A	112(3)
Cu1–N1–H1B	111(3)	Cu1–N1–H1C	114(3)
H1A–N1–H1B	106(4)	H1A–N1–H1C	107(4)
H1B–N1–H1C	107(4)	Cu1–N2–H2A	109(3)
Cu1–N2–H2B	116(3)	Cu1–N2–H2C	116(3)
H2A–N2–H2B	102(4)	H2A–N2–H2C	102(4)
H2B–N2–H2C	110(4)	Cu1–N3–H3A	109(3)

Cu1–N3–H3B	104(3)	Cu1–N3–H3C	107(3)
H3A–N3–H3B	115(4)	H3A–N3–H3C	106(4)
H3B–N3–H3C	114(4)	Cu2–N4–H4A	109(3)
Cu2–N4–H4B	112(3)	Cu2–N4–H4C	114(3)
H4A–N4–H4B	113(4)	H4A–N4–H4C	105(5)
H4B–N4–H4C	103(4)	Cu2–N5–H5A	107(3)
Cu2–N5–H5B	110(3)	Cu2–N5–H5C	111(3)
H5A–N5–H5B	109(4)	H5A–N5–H5C	114(4)
H5B–N5–H5C	106(4)	H6A–N6–H6B	108(4)
H6A–N6–H6C	110(4)	H6A–N6–H6D	113(4)
H6B–N6–H6C	103(4)	H6B–N6–H6D	107(4)
H6C–N6–H6D	114(5)	H9A–O9–H9B	116(5)

Symmetry operations for equivalent atoms
a –x+1,–y+1,–z+1

Table S53. Torsion angles [°] for 8.

C6–C1–C2–C3	5.3(4)	C6–C1–C2–C8	−169.2(3)
C7–C1–C2–C3	−173.3(3)	C7–C1–C2–C8	12.2(5)
C1–C2–C3–C4	−3.8(5)	C8–C2–C3–C4	170.8(3)
C2–C3–C4–C5	−1.2(5)	C2–C3–C4–C9	−178.3(3)
C3–C4–C5–C6	4.7(5)	C3–C4–C5–C10	−172.2(3)
C9–C4–C5–C6	−178.2(3)	C9–C4–C5–C10	4.9(5)
C2–C1–C6–C5	−1.9(5)	C7–C1–C6–C5	176.8(3)
C4–C5–C6–C1	−3.2(5)	C10–C5–C6–C1	173.8(3)
C2–C1–C7–O1	68.8(4)	C2–C1–C7–O2	−115.1(3)
C6–C1–C7–O1	−109.9(4)	C6–C1–C7–O2	66.3(4)
C1–C2–C8–O3	−168.5(3)	C1–C2–C8–O4	13.5(4)
C3–C2–C8–O3	17.1(4)	C3–C2–C8–O4	−160.9(3)
C3–C4–C9–O5	−58.5(4)	C3–C4–C9–O6	120.7(3)
C5–C4–C9–O5	124.5(3)	C5–C4–C9–O6	−56.4(4)
C4–C5–C10–O7	−67.5(4)	C4–C5–C10–O8	113.1(4)
C6–C5–C10–O7	115.6(4)	C6–C5–C10–O8	−63.8(4)
C1–C7–O2–Cu1	169.8(2)	O1–C7–O2–Cu1	−14.3(5)

Table S54. Anisotropic displacement parameters (Å^2) for 8. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu1	0.0142(2)	0.0083(2)	0.0140(2)	–0.00134(16)	0.00482(15)	–0.00131(16)
Cu2	0.0105(3)	0.0112(3)	0.0188(3)	–0.0010(2)	0.0012(2)	0.0014(2)
C1	0.0091(14)	0.0072(15)	0.0111(16)	0.0017(12)	–0.0005(12)	0.0016(11)
C2	0.0058(14)	0.0093(16)	0.0145(17)	0.0007(12)	0.0008(12)	0.0000(11)
C3	0.0106(14)	0.0125(16)	0.0110(16)	–0.0006(12)	0.0030(12)	0.0007(12)
C4	0.0087(14)	0.0083(15)	0.0143(17)	–0.0009(12)	0.0012(12)	–0.0003(12)
C5	0.0098(15)	0.0096(15)	0.0109(16)	0.0015(12)	0.0002(12)	0.0001(12)
C6	0.0125(15)	0.0116(16)	0.0105(16)	0.0002(12)	0.0008(12)	0.0023(12)
C7	0.0134(15)	0.0106(16)	0.0098(16)	0.0004(12)	0.0052(12)	–0.0023(12)
C8	0.0105(15)	0.0140(16)	0.0102(16)	0.0014(13)	0.0016(12)	–0.0021(12)
C9	0.0164(16)	0.0103(15)	0.0056(15)	0.0011(12)	0.0033(12)	–0.0012(12)
C10	0.0195(17)	0.0142(17)	0.0070(16)	–0.0039(12)	0.0047(13)	–0.0090(13)
O1	0.0101(11)	0.0132(12)	0.0236(14)	–0.0036(10)	–0.0034(9)	0.0001(9)
O2	0.0110(11)	0.0086(11)	0.0127(11)	–0.0008(9)	0.0006(9)	0.0002(9)
O3	0.0187(13)	0.0147(12)	0.0215(14)	–0.0035(10)	0.0120(10)	–0.0019(10)
O4	0.0235(13)	0.0105(12)	0.0291(15)	–0.0046(10)	0.0160(11)	–0.0033(10)
O5	0.0173(12)	0.0126(12)	0.0251(14)	–0.0059(10)	0.0006(10)	0.0028(10)
O6	0.0114(11)	0.0173(12)	0.0223(14)	–0.0043(10)	–0.0007(10)	–0.0026(9)
O7	0.0317(15)	0.0180(14)	0.0212(14)	0.0049(11)	0.0077(11)	–0.0079(11)
O8	0.0153(13)	0.0261(15)	0.0307(16)	0.0014(12)	0.0118(11)	0.0002(11)
N1	0.0149(15)	0.0146(16)	0.0166(16)	0.0008(12)	0.0042(12)	–0.0012(12)
N2	0.0166(15)	0.0123(15)	0.0191(17)	–0.0016(12)	0.0005(12)	–0.0004(12)
N3	0.0135(14)	0.0077(14)	0.0167(16)	0.0013(11)	0.0032(11)	0.0008(11)
N4	0.0140(15)	0.0222(18)	0.0205(17)	–0.0016(14)	0.0000(12)	0.0018(13)
N5	0.0133(15)	0.0189(16)	0.0203(17)	–0.0024(13)	0.0011(13)	0.0021(12)
N6	0.0162(16)	0.0130(16)	0.0253(19)	–0.0055(13)	0.0042(13)	–0.0005(12)
O9	0.0206(13)	0.0114(13)	0.0177(14)	–0.0010(10)	0.0051(10)	–0.0042(10)

Table S55. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for 8.

	x	y	z	U
H3	0.7758	0.7720	1.2223	0.013
H6	1.0062	0.6824	0.8974	0.014
H1A	0.761(5)	0.422(2)	1.101(4)	0.023
H1B	0.687(5)	0.485(2)	1.068(4)	0.023
H1C	0.620(6)	0.427(2)	1.020(4)	0.023
H2A	0.669(6)	0.361(2)	0.796(4)	0.025
H2B	0.753(5)	0.325(2)	0.897(4)	0.025
H2C	0.814(5)	0.342(2)	0.783(4)	0.025
H3A	0.944(5)	0.434(2)	0.711(4)	0.019
H3B	0.959(5)	0.506(2)	0.747(4)	0.019
H3C	1.070(6)	0.454(2)	0.803(4)	0.019
H4A	0.769(6)	0.447(3)	0.499(4)	0.029
H4B	0.803(6)	0.519(2)	0.513(4)	0.029
H4C	0.749(6)	0.489(2)	0.405(5)	0.029
H5A	0.460(6)	0.621(2)	0.523(4)	0.027
H5B	0.621(6)	0.611(2)	0.560(4)	0.027
H5C	0.572(5)	0.617(2)	0.436(4)	0.027
H6A	0.503(6)	0.824(2)	1.331(4)	0.027
H6B	0.397(5)	0.772(2)	1.375(4)	0.027
H6C	0.471(6)	0.761(2)	1.277(4)	0.027
H6D	0.346(6)	0.807(2)	1.261(4)	0.027
H9A	0.507(6)	0.464(2)	0.754(4)	0.025
H9B	0.584(6)	0.524(2)	0.763(4)	0.025

Table S56. Hydrogen bonds for 8 [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
N1–H1A...O6b	0.87(5)	2.31(5)	3.161(4)	166(4)
N1–H1B...O4	0.88(5)	2.16(5)	3.034(4)	174(4)
N1–H1C...O1c	0.78(5)	2.59(5)	3.210(4)	138(4)
N2–H2A...O3c	0.81(5)	2.21(5)	2.963(4)	154(4)
N2–H2A...O9	0.81(5)	2.65(4)	3.067(4)	114(4)
N2–H2B...O8d	0.95(5)	2.19(5)	3.128(4)	167(4)
N2–H2C...O7e	0.85(5)	2.29(5)	3.017(4)	144(4)
N3–H3A...O7e	0.87(4)	2.13(4)	3.000(4)	173(4)
N3–H3B...O5f	0.86(4)	2.04(4)	2.885(4)	166(4)
N3–H3C...O2d	0.84(4)	2.64(4)	3.063(4)	113(3)
N3–H3C...O4d	0.84(4)	2.29(5)	3.107(4)	166(4)
N4–H4A...O7e	0.85(5)	2.14(5)	2.980(4)	171(4)
N4–H4B...O5f	0.89(5)	2.23(5)	3.054(4)	154(4)
N5–H5A...O8g	0.83(5)	2.60(5)	3.297(4)	142(4)
N5–H5B...O5f	0.80(5)	2.27(5)	3.011(4)	154(4)
N5–H5C...O3h	0.88(5)	2.31(5)	3.177(4)	166(4)
N6–H6A...O1i	0.89(5)	1.94(5)	2.822(4)	171(4)
N6–H6B...O8j	0.93(5)	1.85(5)	2.767(5)	170(4)
N6–H6C...O3	0.78(5)	2.01(5)	2.769(4)	164(5)
N6–H6D...O6k	0.82(5)	2.05(5)	2.814(4)	157(4)
O9–H9A...O4c	0.77(5)	2.04(5)	2.800(4)	168(5)
O9–H9B...O1	0.80(5)	1.92(5)	2.701(4)	162(4)

Symmetry operations for equivalent atoms

b –x+2,y–1/2,–z+5/2 c –x+1,–y+1,–z+2 d –x+2,–y+1,–z+2
e –x+2,y–1/2,–z+3/2 f x,–y+3/2,z–1/2 g x–1,–y+3/2,z–1/2
h x,y,z–1 i x,–y+3/2,z+1/2 j x–1,–y+3/2,z+1/2
k x–1,y,z

Table S57. Crystal data and structure refinement for 9.

Identification code	9	
Chemical formula (moiety)	$C_{30}H_{26}Cu_2N_4O_{10}\cdot 4H_2O$	
Chemical formula (total)	$C_{30}H_{34}Cu_2N_4O_{14}$	
Formula weight	801.69	
Temperature	160(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 8.9464(9) Å	α = 82.360(2)°
	b = 11.1622(11) Å	β = 81.293(2)°
	c = 17.4780(17) Å	γ = 82.365(2)°
Cell volume	1698.6(3) Å^3	
Z	2	
Calculated density	1.567 g/cm^3	
Absorption coefficient μ	1.326 mm^{-1}	
F(000)	824	
Crystal colour and size	Blue, 0.200 × 0.200 × 0.080 mm^3	
Reflections for cell refinement	4519 (θ range 2.3 to 28.4°)	
Data collection method	Bruker SMART 1K CCD diffractometer narrow-frame ω scans	
θ range for data collection	1.9 to 25.0°	
Index ranges	h –10 to 10, k –13 to 13, l –20 to 20	
Completeness to θ = 25.0°	99.0 %	
Reflections collected	12220	
Independent reflections	5926 (R_{int} = 0.0873)	
Reflections with $F^2>2\sigma$	3285	
Absorption correction	multi-scan	
Min. and max. transmission	0.780 and 0.900	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0463,	
Data / restraints / parameters	5926 / 438 / 488	
Final R indices [$F^2>2\sigma$]	R1 = 0.0638, wR2 = 0.1210	
R indices (all data)	R1 = 0.1394, wR2 = 0.1489	
Goodness-of-fit on F^2	1.081	
Extinction coefficient	0.0032(6)	
Largest and mean shift/su	0.000 and 0.000	
Largest diff. peak and hole	0.75 and –0.69 e Å^{-3}	

Table S58. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for 9. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cu1	0.28804(10)	0.71317(8)	0.27010(5)	0.0114(3)
Cu2	0.74348(10)	0.30428(8)	0.26723(5)	0.0089(3)
C1	0.4934(8)	0.5468(6)	0.0714(4)	0.0069(15)
C2	0.5425(8)	0.4233(6)	0.0653(4)	0.0077(14)
C3	0.5470(7)	0.3784(6)	–0.0058(4)	0.0085(15)
C4	0.4815(8)	0.6065(6)	0.1460(4)	0.0081(15)
C5	0.5978(8)	0.3354(6)	0.1313(4)	0.0084(15)
O1	0.5837(6)	0.6652(4)	0.1527(3)	0.0141(12)
O2	0.3555(5)	0.5999(4)	0.1912(3)	0.0104(11)
O3	0.6298(6)	0.2269(4)	0.1230(3)	0.0216(13)
O4	0.6053(5)	0.3832(4)	0.1933(3)	0.0111(11)
C6	0.0350(8)	0.9300(6)	0.4368(4)	0.0063(14)
C7	–0.0302(8)	1.0510(6)	0.4251(4)	0.0080(15)
C8	–0.0617(7)	1.1189(6)	0.4880(4)	0.0066(15)
C9	0.0697(9)	0.8445(6)	0.3739(4)	0.0106(15)
C10	–0.0655(8)	1.1090(6)	0.3454(4)	0.0094(15)
O5	–0.0319(6)	0.7851(4)	0.3643(3)	0.0133(12)
O6	0.2088(6)	0.8327(4)	0.3432(3)	0.0161(12)
O7	–0.0413(6)	1.0454(4)	0.2913(3)	0.0171(12)
O8	–0.1210(5)	1.2204(4)	0.3412(3)	0.0117(11)
N1	0.2830(7)	0.8476(5)	0.1822(3)	0.0132(14)
C11	0.1917(9)	0.8484(8)	0.1290(5)	0.027(2)
C12	0.1948(11)	0.9337(8)	0.0626(5)	0.035(2)
C13	0.2910(11)	1.0202(8)	0.0530(5)	0.035(2)
C14	0.3842(10)	1.0201(7)	0.1082(5)	0.030(2)
C15	0.3788(9)	0.9338(7)	0.1718(5)	0.0207(18)
N2	0.2515(7)	0.5747(5)	0.3519(3)	0.0131(14)
C16	0.1846(9)	0.4803(7)	0.3374(5)	0.0186(18)
C17	0.1384(9)	0.3903(7)	0.3960(5)	0.024(2)
C18	0.1681(10)	0.3947(8)	0.4716(5)	0.027(2)
C19	0.2388(9)	0.4892(7)	0.4857(5)	0.0231(19)
C20	0.2790(9)	0.5756(7)	0.4248(4)	0.0170(17)
N3	0.9191(7)	0.3546(5)	0.1879(3)	0.0117(14)
C21	1.0522(9)	0.2861(7)	0.1751(5)	0.0211(19)
C22	1.1697(9)	0.3227(7)	0.1208(5)	0.027(2)
C23	1.1531(9)	0.4361(7)	0.0788(4)	0.0189(18)
C24	1.0167(8)	0.5076(7)	0.0929(4)	0.0152(17)
C25	0.9043(8)	0.4646(6)	0.1476(4)	0.0119(16)
N4	0.5711(7)	0.2304(5)	0.3371(3)	0.0152(14)
C26	0.4724(8)	0.1710(7)	0.3117(5)	0.0194(18)
C27	0.3676(9)	0.1054(8)	0.3600(5)	0.028(2)
C28	0.3643(9)	0.1028(7)	0.4388(5)	0.0264(19)
C29	0.4615(9)	0.1649(8)	0.4675(5)	0.029(2)
C30	0.5621(9)	0.2291(8)	0.4152(4)	0.0222(19)
O9	0.5283(6)	0.7067(5)	0.3023(3)	0.0200(13)
O10	0.7262(6)	0.4790(4)	0.3251(3)	0.0169(12)
O11	0.9357(8)	0.6411(5)	0.2561(3)	0.0321(15)
O12	0.7684(7)	1.0131(5)	0.1895(4)	0.0309(16)
O13	0.8371(6)	0.7964(5)	0.1209(4)	0.0283(15)
O14	0.6715(6)	0.8856(5)	0.3447(3)	0.0252(14)

Table S59. Bond lengths [Å] and angles [°] for 9.

Cu1–O2	1.968(5)	Cu1–O6	1.960(5)
Cu1–N1	2.002(6)	Cu1–N2	1.986(6)
Cu1–O9	2.293(6)	Cu2–O4	1.966(5)
Cu2–O8a	1.968(5)	Cu2–N3	2.019(6)
Cu2–N4	2.012(6)	Cu2–O10	2.290(5)
C1–C2	1.403(9)	C1–C3b	1.391(9)
C1–C4	1.525(9)	C2–C3	1.393(9)
C2–C5	1.510(9)	C3–C1b	1.391(9)
C3–H3	0.950	C4–O1	1.221(8)
C4–O2	1.280(8)	C5–O3	1.230(8)
C5–O4	1.284(8)	C6–C7	1.400(9)
C6–C8c	1.397(9)	C6–C9	1.521(9)
C7–C8	1.391(9)	C7–C10	1.517(9)
C8–C6c	1.397(9)	C8–H8	0.950
C9–O5	1.237(8)	C9–O6	1.275(8)
C10–O7	1.233(8)	C10–O8	1.273(8)
O8–Cu2d	1.967(5)	N1–C11	1.325(9)
N1–C15	1.348(9)	C11–H11	0.950
C11–C12	1.400(11)	C12–H12	0.950
C12–C13	1.355(12)	C13–H13	0.950
C13–C14	1.367(11)	C14–H14	0.950
C14–C15	1.370(10)	C15–H15	0.950
N2–C16	1.348(9)	N2–C20	1.335(9)
C16–H16	0.950	C16–C17	1.392(10)
C17–H17	0.950	C17–C18	1.395(10)
C18–H18	0.950	C18–C19	1.367(11)
C19–H19	0.950	C19–C20	1.377(10)
C20–H20	0.950	N3–C21	1.333(9)
N3–C25	1.332(9)	C21–H21	0.950
C21–C22	1.372(10)	C22–H22	0.950
C22–C23	1.379(10)	C23–H23	0.950
C23–C24	1.375(10)	C24–H24	0.950
C24–C25	1.368(10)	C25–H25	0.950
N4–C26	1.330(9)	N4–C30	1.353(9)
C26–H26	0.950	C26–C27	1.381(10)
C27–H27	0.950	C27–C28	1.369(11)
C28–H28	0.950	C28–C29	1.368(12)
C29–H29	0.950	C29–C30	1.381(10)
C30–H30	0.950	O9–H9A	0.837(10)
O9–H9B	0.839(10)	O10–H10A	0.839(10)
O10–H10B	0.839(10)	O11–H11A	0.838(10)
O11–H11B	0.838(10)	O12–H12A	0.842(10)
O12–H12B	0.841(10)	O13–H13A	0.841(10)
O13–H13B	0.838(10)	O14–H14A	0.841(10)
O14–H14B	0.841(10)		

O2–Cu1–O6	175.4(2)	O2–Cu1–N1	87.4(2)
O2–Cu1–N2	90.6(2)	O2–Cu1–O9	92.95(19)
O6–Cu1–N1	89.2(2)	O6–Cu1–N2	92.1(2)
O6–Cu1–O9	90.9(2)	N1–Cu1–N2	168.2(3)
N1–Cu1–O9	102.8(2)	N2–Cu1–O9	88.9(2)
O4–Cu2–O8a	178.2(2)	O4–Cu2–N3	88.1(2)
O4–Cu2–N4	91.2(2)	O4–Cu2–O10	91.44(19)
O8a–Cu2–N3	92.9(2)	O8a–Cu2–N4	87.5(2)

O8a–Cu2–O10	90.09(19)	N3–Cu2–N4	170.7(3)
N3–Cu2–O10	92.0(2)	N4–Cu2–O10	97.2(2)
C2–C1–C3b	118.9(6)	C2–C1–C4	124.3(6)
C3b–C1–C4	116.7(6)	C1–C2–C3	119.3(6)
C1–C2–C5	123.5(6)	C3–C2–C5	117.1(6)
C1b–C3–C2	121.7(7)	C1b–C3–H3	119.1
C2–C3–H3	119.1	C1–C4–O1	117.7(6)
C1–C4–O2	115.0(6)	O1–C4–O2	126.9(7)
C2–C5–O3	119.6(6)	C2–C5–O4	115.0(6)
O3–C5–O4	125.4(6)	Cu1–O2–C4	121.2(4)
Cu2–O4–C5	120.3(4)	C7–C6–C8c	118.5(6)
C7–C6–C9	124.3(6)	C8c–C6–C9	117.0(6)
C6–C7–C8	119.0(6)	C6–C7–C10	121.3(6)
C8–C7–C10	119.8(6)	C6c–C8–C7	122.5(6)
C6c–C8–H8	118.7	C7–C8–H8	118.7
C6–C9–O5	118.1(6)	C6–C9–O6	114.2(6)
O5–C9–O6	127.2(7)	C7–C10–O7	118.3(6)
C7–C10–O8	115.8(6)	O7–C10–O8	125.9(7)
Cu1–O6–C9	122.1(5)	Cu2d–O8–C10	126.4(4)
Cu1–N1–C11	119.9(5)	Cu1–N1–C15	121.7(5)
C11–N1–C15	118.2(7)	N1–C11–H11	119.0
N1–C11–C12	122.0(8)	H11–C11–C12	119.0
C11–C12–H12	120.4	C11–C12–C13	119.3(8)
H12–C12–C13	120.4	C12–C13–H13	120.6
C12–C13–C14	118.7(8)	H13–C13–C14	120.6
C13–C14–H14	120.0	C13–C14–C15	120.0(8)
H14–C14–C15	120.0	N1–C15–C14	121.8(8)
N1–C15–H15	119.1	C14–C15–H15	119.1
Cu1–N2–C16	120.7(5)	Cu1–N2–C20	122.0(5)
C16–N2–C20	117.0(7)	N2–C16–H16	118.9
N2–C16–C17	122.1(7)	H16–C16–C17	118.9
C16–C17–H17	120.4	C16–C17–C18	119.1(8)
H17–C17–C18	120.4	C17–C18–H18	120.8
C17–C18–C19	118.5(8)	H18–C18–C19	120.8
C18–C19–H19	120.6	C18–C19–C20	118.9(8)
H19–C19–C20	120.6	N2–C20–C19	124.3(8)
N2–C20–H20	117.9	C19–C20–H20	117.9
Cu2–N3–C21	123.9(5)	Cu2–N3–C25	118.5(5)
C21–N3–C25	117.5(7)	N3–C21–H21	118.7
N3–C21–C22	122.7(7)	H21–C21–C22	118.7
C21–C22–H22	120.2	C21–C22–C23	119.5(8)
H22–C22–C23	120.2	C22–C23–H23	121.1
C22–C23–C24	117.8(7)	H23–C23–C24	121.1
C23–C24–H24	120.3	C23–C24–C25	119.4(7)
H24–C24–C25	120.3	N3–C25–C24	123.1(7)
N3–C25–H25	118.4	C24–C25–H25	118.4
Cu2–N4–C26	123.6(5)	Cu2–N4–C30	119.2(5)
C26–N4–C30	116.8(7)	N4–C26–H26	118.0
N4–C26–C27	124.0(8)	H26–C26–C27	118.0
C26–C27–H27	121.1	C26–C27–C28	117.8(8)
H27–C27–C28	121.1	C27–C28–H28	119.9
C27–C28–C29	120.2(8)	H28–C28–C29	119.9
C28–C29–H29	120.8	C28–C29–C30	118.4(8)
H29–C29–C30	120.8	N4–C30–C29	122.7(8)
N4–C30–H30	118.6	C29–C30–H30	118.6
Cu1–O9–H9A	82(5)	Cu1–O9–H9B	122(5)

H9A–O9–H9B	107.4(18)	Cu2–O10–H10A	119(5)
Cu2–O10–H10B	106(5)	H10A–O10–H10B	107.5(18)
H11A–O11–H11B	107.6(18)	H12A–O12–H12B	106.4(18)
H13A–O13–H13B	107.2(18)	H14A–O14–H14B	106.6(18)

Symmetry operations for equivalent atoms
a x+1,y−1,z b −x+1,−y+1,−z c −x,−y+2,−z+1
d x−1,y+1,z

Table S60. Torsion angles [°] for 9.

C3b–C1–C2–C3	−1.1(11)	C3b–C1–C2–C5	176.3(6)
C4–C1–C2–C3	179.2(6)	C4–C1–C2–C5	−3.4(11)
C1–C2–C3–C1b	1.2(11)	C5–C2–C3–C1b	−176.4(6)
C2–C1–C4–O1	100.6(8)	C2–C1–C4–O2	−86.6(8)
C3b–C1–C4–O1	−79.0(8)	C3b–C1–C4–O2	93.7(7)
C1–C2–C5–O3	175.4(7)	C1–C2–C5–O4	−3.7(10)
C3–C2–C5–O3	−7.2(10)	C3–C2–C5–O4	173.7(6)
C1–C4–O2–Cu1	−159.3(4)	O1–C4–O2–Cu1	12.6(10)
C2–C5–O4–Cu2	−156.0(4)	O3–C5–O4–Cu2	24.9(10)
C8c–C6–C7–C8	1.9(11)	C8c–C6–C7–C10	−178.7(6)
C9–C6–C7–C8	177.7(6)	C9–C6–C7–C10	−2.9(11)
C6–C7–C8–C6c	−2.0(11)	C10–C7–C8–C6c	178.6(6)
C7–C6–C9–O5	−87.8(9)	C7–C6–C9–O6	99.9(8)
C8c–C6–C9–O5	88.0(8)	C8c–C6–C9–O6	−84.2(8)
C6–C7–C10–O7	3.0(10)	C6–C7–C10–O8	−178.3(6)
C8–C7–C10–O7	−177.5(7)	C8–C7–C10–O8	1.2(10)
C6–C9–O6–Cu1	172.5(4)	O5–C9–O6–Cu1	1.1(10)
C7–C10–O8–Cu2d	−152.1(5)	O7–C10–O8–Cu2d	26.5(11)
Cu1–N1–C11–C12	−173.8(7)	C15–N1–C11–C12	1.4(12)
N1–C11–C12–C13	−1.8(14)	C11–C12–C13–C14	1.1(14)
C12–C13–C14–C15	−0.2(14)	Cu1–N1–C15–C14	174.6(6)
C11–N1–C15–C14	−0.4(11)	C13–C14–C15–N1	−0.2(13)
Cu1–N2–C16–C17	−171.0(6)	C20–N2–C16–C17	3.2(11)
N2–C16–C17–C18	−2.8(12)	C16–C17–C18–C19	1.4(12)
C17–C18–C19–C20	−0.5(12)	Cu1–N2–C20–C19	171.8(6)
C16–N2–C20–C19	−2.3(11)	C18–C19–C20–N2	1.0(12)
Cu2–N3–C21–C22	−179.9(6)	C25–N3–C21–C22	−2.5(11)
N3–C21–C22–C23	1.9(13)	C21–C22–C23–C24	−0.7(12)
C22–C23–C24–C25	0.2(11)	Cu2–N3–C25–C24	179.6(5)
C21–N3–C25–C24	2.0(10)	C23–C24–C25–N3	−0.9(11)
Cu2–N4–C26–C27	170.4(6)	C30–N4–C26–C27	−2.7(11)
N4–C26–C27–C28	0.8(12)	C26–C27–C28–C29	0.7(12)
C27–C28–C29–C30	−0.2(12)	Cu2–N4–C30–C29	−170.2(6)
C26–N4–C30–C29	3.2(11)	C28–C29–C30–N4	−1.9(12)

Symmetry operations for equivalent atoms
b −x+1,−y+1,−z c −x,−y+2,−z+1 d x−1,y+1,z

Table S61. Anisotropic displacement parameters (Å^2) for 9. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu1	0.0153(6)	0.0097(5)	0.0074(5)	–0.0019(4)	0.0021(4)	0.0025(4)
Cu2	0.0109(5)	0.0091(5)	0.0059(5)	0.0026(4)	–0.0023(4)	–0.0005(4)
C1	0.004(3)	0.010(2)	0.007(2)	–0.0023(19)	–0.002(2)	–0.001(2)
C2	0.005(3)	0.009(2)	0.009(2)	–0.0005(18)	–0.002(2)	–0.002(2)
C3	0.008(3)	0.009(3)	0.009(2)	0.000(2)	–0.001(2)	0.000(2)
C4	0.010(2)	0.005(2)	0.009(2)	–0.001(2)	–0.0044(19)	0.001(2)
C5	0.006(3)	0.011(2)	0.007(2)	0.0030(19)	–0.002(2)	0.000(2)
O1	0.018(3)	0.013(3)	0.014(3)	–0.007(2)	–0.001(2)	–0.006(2)
O2	0.012(3)	0.009(3)	0.010(2)	–0.003(2)	–0.0003(19)	0.000(2)
O3	0.035(4)	0.008(2)	0.022(3)	0.005(2)	–0.012(3)	0.000(2)
O4	0.012(3)	0.013(3)	0.008(2)	0.001(2)	–0.004(2)	–0.002(2)
C6	0.006(3)	0.006(2)	0.007(2)	–0.0020(19)	0.000(2)	–0.0031(19)
C7	0.008(3)	0.009(2)	0.007(2)	–0.0038(19)	0.000(2)	–0.001(2)
C8	0.008(3)	0.003(2)	0.008(2)	0.000(2)	–0.001(2)	0.002(2)
C9	0.014(2)	0.009(3)	0.008(3)	0.000(2)	–0.003(2)	0.001(2)
C10	0.011(3)	0.009(2)	0.008(2)	–0.0033(19)	0.000(2)	–0.002(2)
O5	0.019(3)	0.012(3)	0.010(3)	–0.002(2)	–0.006(2)	–0.001(2)
O6	0.016(3)	0.015(3)	0.016(3)	–0.008(2)	0.003(2)	0.000(2)
O7	0.038(3)	0.009(3)	0.006(3)	–0.001(2)	–0.006(2)	–0.003(2)
O8	0.014(3)	0.010(2)	0.010(3)	–0.002(2)	–0.005(2)	0.002(2)
N1	0.017(3)	0.008(3)	0.014(3)	0.000(2)	–0.001(2)	–0.001(2)
C11	0.024(5)	0.029(5)	0.028(4)	0.002(3)	–0.008(3)	–0.007(4)
C12	0.054(6)	0.031(5)	0.023(4)	0.003(4)	–0.021(4)	–0.001(4)
C13	0.052(6)	0.023(5)	0.026(5)	0.010(4)	–0.014(4)	0.002(4)
C14	0.045(5)	0.012(4)	0.033(4)	0.004(3)	–0.008(4)	–0.006(4)
C15	0.027(4)	0.012(4)	0.023(4)	–0.002(3)	–0.002(3)	–0.001(3)
N2	0.013(3)	0.012(3)	0.013(3)	0.000(2)	0.001(2)	0.002(2)
C16	0.022(4)	0.012(4)	0.021(4)	0.001(3)	–0.006(3)	0.001(3)
C17	0.030(5)	0.023(4)	0.021(4)	0.003(3)	–0.003(3)	–0.010(4)
C18	0.033(5)	0.024(4)	0.022(4)	0.005(3)	0.000(3)	–0.005(4)
C19	0.030(5)	0.027(4)	0.011(4)	0.009(3)	–0.007(3)	–0.005(4)
C20	0.023(4)	0.012(4)	0.015(3)	–0.001(3)	–0.003(3)	0.005(3)
N3	0.015(3)	0.011(3)	0.009(3)	–0.001(2)	–0.002(2)	–0.001(2)
C21	0.021(4)	0.010(4)	0.030(5)	–0.002(3)	0.002(3)	0.001(3)
C22	0.018(4)	0.024(4)	0.033(5)	0.001(3)	0.006(3)	0.003(3)
C23	0.015(4)	0.019(4)	0.022(4)	0.002(3)	0.000(3)	–0.007(3)
C24	0.012(4)	0.018(4)	0.017(4)	–0.002(3)	–0.005(3)	–0.004(3)
C25	0.012(4)	0.010(3)	0.015(4)	–0.005(3)	–0.001(3)	–0.002(3)
N4	0.016(3)	0.015(3)	0.013(3)	0.006(2)	–0.004(2)	–0.001(3)
C26	0.013(4)	0.025(4)	0.019(4)	0.001(3)	0.001(3)	–0.005(3)
C27	0.019(4)	0.029(5)	0.035(4)	0.003(4)	0.000(3)	–0.006(4)
C28	0.014(4)	0.025(5)	0.032(4)	0.008(3)	0.010(3)	0.003(3)
C29	0.025(4)	0.035(5)	0.020(4)	0.011(3)	0.003(3)	0.004(4)
C30	0.021(4)	0.033(5)	0.011(3)	0.004(3)	–0.005(3)	0.000(4)
O9	0.022(3)	0.025(3)	0.014(3)	–0.011(3)	–0.001(2)	–0.001(3)
O10	0.027(3)	0.013(3)	0.013(3)	–0.003(2)	–0.008(3)	–0.001(2)
O11	0.048(4)	0.027(4)	0.026(4)	–0.015(3)	–0.014(3)	0.001(3)
O12	0.048(4)	0.012(3)	0.037(4)	0.004(3)	–0.025(3)	–0.003(3)

O13	0.021(3)	0.027(4)	0.039(4)	–0.002(3)	–0.006(3)	–0.009(3)
O14	0.019(3)	0.025(4)	0.029(4)	0.000(3)	0.001(3)	0.001(3)

Table S62. Hydrogen coordinates and isotropic displacement parameters (Å^2) for 9.

	x	y	z	U
H3	0.5785	0.2944	–0.0095	0.010
H8	–0.1030	1.2018	0.4796	0.008
H11	0.1221	0.7893	0.1363	0.032
H12	0.1302	0.9309	0.0246	0.043
H13	0.2936	1.0799	0.0088	0.042
H14	0.4526	1.0798	0.1025	0.036
H15	0.4445	0.9347	0.2096	0.025
H16	0.1683	0.4751	0.2855	0.022
H17	0.0874	0.3267	0.3846	0.029
H18	0.1398	0.3334	0.5124	0.033
H19	0.2599	0.4952	0.5366	0.028
H20	0.3295	0.6400	0.4353	0.020
H21	1.0663	0.2087	0.2048	0.025
H22	1.2619	0.2702	0.1122	0.032
H23	1.2332	0.4639	0.0413	0.023
H24	1.0006	0.5862	0.0650	0.018
H25	0.8112	0.5155	0.1573	0.014
H26	0.4741	0.1738	0.2570	0.023
H27	0.3000	0.0635	0.3393	0.034
H28	0.2942	0.0578	0.4737	0.032
H29	0.4598	0.1638	0.5220	0.035
H30	0.6277	0.2742	0.4348	0.027
H9A	0.552(8)	0.715(6)	0.2538(8)	0.030
H9B	0.557(8)	0.766(4)	0.319(3)	0.030
H10A	0.794(5)	0.525(5)	0.311(4)	0.025
H10B	0.643(3)	0.519(5)	0.316(4)	0.025
H11A	0.962(10)	0.691(5)	0.282(4)	0.048
H11B	0.905(10)	0.680(5)	0.216(3)	0.048
H12A	0.736(9)	1.076(4)	0.162(4)	0.046
H12B	0.821(8)	1.037(6)	0.220(4)	0.046
H13A	0.750(4)	0.778(6)	0.119(5)	0.042
H13B	0.826(7)	0.856(5)	0.146(4)	0.042
H14A	0.753(4)	0.842(5)	0.353(5)	0.038
H14B	0.696(7)	0.948(4)	0.316(4)	0.038

Table S63. Hydrogen bonds for 9 [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
O9–H9A...O1	0.837(10)	1.89(3)	2.678(7)	155(6)
O9–H9B...O14	0.839(10)	1.93(2)	2.746(8)	165(7)
O10–H10A...O11	0.839(10)	1.98(2)	2.806(8)	167(7)
O10–H10B...O9	0.839(10)	2.21(4)	2.916(7)	142(6)
O11–H11A...O5e	0.838(10)	1.90(3)	2.709(7)	161(8)
O11–H11B...O13	0.838(10)	2.082(17)	2.916(9)	173(7)
O12–H12A...O3f	0.842(10)	1.92(3)	2.738(7)	165(9)
O12–H12B...O7e	0.841(10)	1.91(2)	2.729(7)	165(7)
O13–H13A...O1	0.841(10)	2.04(4)	2.807(7)	151(8)
O13–H13B...O12	0.838(10)	1.97(2)	2.796(8)	168(8)
O14–H14A...O5e	0.841(10)	1.98(2)	2.793(7)	163(6)
O14–H14B...O7e	0.841(10)	2.67(5)	3.272(7)	130(5)
O14–H14B...O12	0.841(10)	2.25(5)	2.954(8)	141(7)

Symmetry operations for equivalent atoms
e x+1,y,z f x,y+1,z

Table S64. Crystal data and structure refinement for 10.

Identification code	10	
Chemical formula (moiety)	$C_{33}H_{34}Cu_2N_4O_{11}$	
Chemical formula (total)	$C_{33}H_{34}Cu_2N_4O_{11}$	
Formula weight	789.72	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 8.7980(3) Å	α = 94.840(3)°
	b = 10.6480(4) Å	β = 90.453(3)°
	c = 19.1470(8) Å	γ = 110.355(4)°
Cell volume	1674.37(12) Å^3	
Z	2	
Calculated density	1.566 g/cm^3	
Absorption coefficient μ	1.337 mm^{-1}	
F(000)	812	
Crystal colour and size	blue, 0.250 × 0.200 × 0.200 mm^3	
Reflections for cell refinement	7450 (θ range 2.8 to 29.4°)	
Data collection method	Oxford Diffraction Gemini A Ultra diffractomer thick-slice ω scans	
θ range for data collection	2.8 to 26.4°	
Index ranges	h −9 to 10, k −13 to 13, l −23 to 23	
Completeness to θ = 25.2°	97.9 %	
Reflections collected	13658	
Independent reflections	6640 (R_{int} = 0.0391)	
Reflections with $F^2>2\sigma$	4652	
Absorption correction	multi-scan	
Min. and max. transmission	0.70 and 0.79	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0515, 0.5893	
Data / restraints / parameters	6640 / 3 / 472	
Final R indices [$F^2>2\sigma$]	R1 = 0.0451, wR2 = 0.0963	
R indices (all data)	R1 = 0.0750, wR2 = 0.1039	
Goodness-of-fit on F^2	1.016	
Largest and mean shift/su	0.000 and 0.000	
Largest diff. peak and hole	0.55 and −0.84 e Å^{-3}	

Table S65. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for 10. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cu1	0.39681(5)	0.47379(4)	0.21811(2)	0.01463(12)
Cu2	0.5000	1.0000	0.0000	0.01935(16)
Cu3	1.0000	1.0000	0.5000	0.01349(14)
C1	0.1129(4)	0.5134(3)	0.05452(16)	0.0125(7)
C2	0.1475(4)	0.6072(3)	0.00472(16)	0.0124(7)
C3	0.0346(4)	0.5931(3)	–0.04888(16)	0.0128(7)
C4	0.2260(4)	0.5332(3)	0.11720(17)	0.0145(7)
C5	0.3104(4)	0.7175(3)	0.00520(17)	0.0160(8)
O1	0.2650(3)	0.6404(2)	0.15486(12)	0.0201(6)
O2	0.2702(3)	0.4340(2)	0.12847(11)	0.0173(5)
O3	0.4331(3)	0.6852(2)	0.00251(13)	0.0223(6)
O4	0.3087(3)	0.8376(2)	0.00601(12)	0.0202(6)
C6	0.5081(4)	0.5355(3)	0.43083(16)	0.0101(7)
C7	0.6311(4)	0.6088(3)	0.48067(16)	0.0109(7)
C8	0.6197(4)	0.5717(3)	0.54912(16)	0.0112(7)
C9	0.5004(4)	0.5749(3)	0.35753(16)	0.0128(7)
C10	0.7774(4)	0.7235(3)	0.46053(17)	0.0124(7)
O5	0.4900(3)	0.6842(2)	0.34764(12)	0.0204(6)
O6	0.4979(3)	0.4811(2)	0.30986(11)	0.0155(5)
O7	0.8296(3)	0.7153(2)	0.40084(12)	0.0178(5)
O8	0.8352(3)	0.8208(2)	0.50809(11)	0.0137(5)
N1	0.1853(3)	0.4259(3)	0.26872(14)	0.0184(7)
C11	0.1217(4)	0.5196(4)	0.29140(18)	0.0201(8)
C12	–0.0140(5)	0.4883(5)	0.3324(2)	0.0375(11)
C13	–0.0858(5)	0.3590(6)	0.3492(2)	0.0449(13)
C14	–0.0202(5)	0.2636(5)	0.3264(2)	0.0438(12)
C15	0.1139(5)	0.2997(4)	0.2861(2)	0.0296(9)
N2	0.6129(3)	0.5680(3)	0.17598(14)	0.0183(6)
C16	0.7507(4)	0.6214(4)	0.21576(19)	0.0262(9)
C17	0.8972(4)	0.6898(4)	0.1890(2)	0.0285(9)
C18	0.9049(5)	0.7089(4)	0.1186(2)	0.0285(9)
C19	0.7649(5)	0.6558(4)	0.0777(2)	0.0256(9)
C20	0.6233(4)	0.5859(4)	0.10741(18)	0.0201(8)
N3	0.5962(3)	0.9811(3)	0.09453(15)	0.0188(6)
C21	0.5014(5)	0.9082(3)	0.14230(19)	0.0240(9)
C22	0.5622(5)	0.8859(4)	0.2052(2)	0.0293(9)
C23	0.7258(5)	0.9423(4)	0.2206(2)	0.0306(10)
C24	0.8242(5)	1.0185(4)	0.1723(2)	0.0308(10)
C25	0.7563(4)	1.0353(4)	0.11049(19)	0.0234(8)
N4	0.8181(3)	1.0670(3)	0.47746(14)	0.0143(6)
C26	0.7013(4)	0.9998(4)	0.42802(18)	0.0180(8)
C27	0.5748(4)	1.0422(4)	0.41174(19)	0.0224(8)
C28	0.5620(4)	1.1538(4)	0.4488(2)	0.0260(9)
C29	0.6794(4)	1.2232(4)	0.5002(2)	0.0255(9)
C30	0.8058(4)	1.1780(4)	0.51239(18)	0.0197(8)
O9	0.4124(3)	0.2568(3)	0.20193(13)	0.0312(7)
C31	0.5554(7)	0.2414(5)	0.2302(3)	0.0617(17)
O10	1.0131(3)	0.9579(3)	0.36899(14)	0.0281(6)
C32	1.1553(5)	0.9772(4)	0.3318(2)	0.0335(10)
O11	0.3504(3)	1.1345(3)	0.06634(13)	0.0247(6)
C33	0.1815(4)	1.1049(4)	0.0573(2)	0.0324(10)

Table S66. Bond lengths [Å] and angles [°] for 10.

Cu1–O2	1.971(2)	Cu1–O6	1.946(2)
Cu1–N1	2.028(3)	Cu1–N2	2.026(3)
Cu1–O9	2.357(3)	Cu2–O4	1.961(2)
Cu2–O4a	1.961(2)	Cu2–N3	2.047(3)
Cu2–N3a	2.047(3)	Cu3–O8	1.973(2)
Cu3–O8b	1.973(2)	Cu3–N4	2.023(3)
Cu3–N4b	2.023(3)	C1–C2	1.398(4)
C1–C3c	1.391(4)	C1–C4	1.505(4)
C2–C3	1.384(4)	C2–C5	1.503(4)
C3–C1c	1.391(4)	C3–H3	0.950
C4–O1	1.235(4)	C4–O2	1.279(4)
C5–O3	1.241(4)	C5–O4	1.283(4)
C6–C7	1.401(4)	C6–C8d	1.379(4)
C6–C9	1.506(4)	C7–C8	1.395(4)
C7–C10	1.513(4)	C8–C6d	1.379(4)
C8–H8	0.950	C9–O5	1.229(4)
C9–O6	1.289(4)	C10–O7	1.243(4)
C10–O8	1.276(4)	N1–C11	1.347(5)
N1–C15	1.343(5)	C11–H11A	0.950
C11–C12	1.392(5)	C12–H12	0.950
C12–C13	1.368(7)	C13–H13	0.950
C13–C14	1.376(7)	C14–H34	0.950
C14–C15	1.372(6)	C15–H35	0.950
N2–C16	1.344(4)	N2–C20	1.342(4)
C16–H36	0.950	C16–C17	1.369(5)
C17–H37	0.950	C17–C18	1.379(5)
C18–H38	0.950	C18–C19	1.369(5)
C19–H39	0.950	C19–C20	1.366(5)
C20–H20	0.950	N3–C21	1.348(4)
N3–C25	1.344(4)	C21–H21	0.950
C21–C22	1.385(5)	C22–H22	0.950
C22–C23	1.371(6)	C23–H23	0.950
C23–C24	1.384(6)	C24–H24	0.950
C24–C25	1.374(5)	C25–H25	0.950
N4–C26	1.350(4)	N4–C30	1.346(4)
C26–H26	0.950	C26–C27	1.380(5)
C27–H27	0.950	C27–C28	1.371(5)
C28–H28	0.950	C28–C29	1.383(5)
C29–H29	0.950	C29–C30	1.382(5)
C30–H30	0.950	O9–H9	0.842(10)
O9–C31	1.432(5)	C31–H31A	0.980
C31–H31B	0.980	C31–H31C	0.980
O10–H10	0.835(10)	O10–C32	1.404(5)
C32–H32A	0.980	C32–H32B	0.980
C32–H32C	0.980	O11–H11	0.841(10)
O11–C33	1.413(5)	C33–H33A	0.980
C33–H33B	0.980	C33–H33C	0.980

O2–Cu1–O6	169.89(10)	O2–Cu1–N1	88.60(10)
O2–Cu1–N2	95.07(10)	O2–Cu1–O9	88.33(9)
O6–Cu1–N1	85.60(10)	O6–Cu1–N2	92.53(10)
O6–Cu1–O9	84.32(9)	N1–Cu1–N2	166.01(12)
N1–Cu1–O9	98.16(11)	N2–Cu1–O9	95.44(11)
O4–Cu2–O4a	180.00	O4–Cu2–N3	92.69(10)

O4–Cu2–N3a	87.31(10)	O4a–Cu2–N3a	92.69(10)
O4a–Cu2–N3	87.31(10)	N3–Cu2–N3a	180.00
O8–Cu3–O8b	180.00	O8–Cu3–N4	88.44(10)
O8b–Cu3–N4b	88.44(10)	O8–Cu3–N4b	91.56(10)
O8b–Cu3–N4	91.56(10)	N4–Cu3–N4b	180.00
C2–C1–C3c	119.1(3)	C2–C1–C4	120.8(3)
C3c–C1–C4	119.8(3)	C1–C2–C3	119.6(3)
C1–C2–C5	121.0(3)	C3–C2–C5	119.2(3)
C1c–C3–C2	121.3(3)	C1c–C3–H3	119.4
C2–C3–H3	119.4	C1–C4–O1	118.6(3)
C1–C4–O2	116.5(3)	O1–C4–O2	124.9(3)
C2–C5–O3	118.1(3)	C2–C5–O4	116.0(3)
O3–C5–O4	125.8(3)	Cu1–O2–C4	109.6(2)
Cu2–O4–C5	125.3(2)	C7–C6–C8d	118.9(3)
C7–C6–C9	123.1(3)	C8d–C6–C9	117.7(3)
C6–C7–C8	118.9(3)	C6–C7–C10	120.9(3)
C8–C7–C10	120.1(3)	C6d–C8–C7	122.1(3)
C6d–C8–H8	118.9	C7–C8–H8	118.9
C6–C9–O5	120.7(3)	C6–C9–O6	112.9(3)
O5–C9–O6	126.3(3)	C7–C10–O7	118.5(3)
C7–C10–O8	115.2(3)	O7–C10–O8	126.3(3)
Cu1–O6–C9	119.4(2)	Cu3–O8–C10	128.6(2)
Cu1–N1–C11	121.9(2)	Cu1–N1–C15	119.3(3)
C11–N1–C15	118.5(3)	N1–C11–H11A	119.3
N1–C11–C12	121.5(4)	H11A–C11–C12	119.3
C11–C12–H12	120.4	C11–C12–C13	119.2(4)
H12–C12–C13	120.4	C12–C13–H13	120.4
C12–C13–C14	119.3(4)	H13–C13–C14	120.4
C13–C14–H34	120.4	C13–C14–C15	119.3(4)
H34–C14–C15	120.4	N1–C15–C14	122.3(4)
N1–C15–H35	118.8	C14–C15–H35	118.8
Cu1–N2–C16	121.7(2)	Cu1–N2–C20	121.3(2)
C16–N2–C20	116.9(3)	N2–C16–H36	118.6
N2–C16–C17	122.9(3)	H36–C16–C17	118.6
C16–C17–H37	120.3	C16–C17–C18	119.3(3)
H37–C17–C18	120.3	C17–C18–H38	120.9
C17–C18–C19	118.2(4)	H38–C18–C19	120.9
C18–C19–H39	120.2	C18–C19–C20	119.5(4)
H39–C19–C20	120.2	N2–C20–C19	123.1(3)
N2–C20–H20	118.4	C19–C20–H20	118.4
Cu2–N3–C21	120.9(2)	Cu2–N3–C25	121.9(2)
C21–N3–C25	117.2(3)	N3–C21–H21	118.5
N3–C21–C22	123.0(3)	H21–C21–C22	118.5
C21–C22–H22	120.5	C21–C22–C23	119.0(4)
H22–C22–C23	120.5	C22–C23–H23	120.7
C22–C23–C24	118.5(3)	H23–C23–C24	120.7
C23–C24–H24	120.2	C23–C24–C25	119.5(4)
H24–C24–C25	120.2	N3–C25–C24	122.8(4)
N3–C25–H25	118.6	C24–C25–H25	118.6
Cu3–N4–C26	121.2(2)	Cu3–N4–C30	121.5(2)
C26–N4–C30	117.3(3)	N4–C26–H26	118.7
N4–C26–C27	122.7(3)	H26–C26–C27	118.7
C26–C27–H27	120.3	C26–C27–C28	119.4(3)
H27–C27–C28	120.3	C27–C28–H28	120.6
C27–C28–C29	118.8(3)	H28–C28–C29	120.6
C28–C29–H29	120.5	C28–C29–C30	118.9(4)

H29–C29–C30	120.5	N4–C30–C29	122.9(3)
N4–C30–H30	118.6	C29–C30–H30	118.6
Cu1–O9–H9	115(3)	Cu1–O9–C31	116.5(2)
H9–O9–C31	111(3)	O9–C31–H31A	109.5
O9–C31–H31B	109.5	O9–C31–H31C	109.5
H31A–C31–H31B	109.5	H31A–C31–H31C	109.5
H31B–C31–H31C	109.5	H10–O10–C32	119(3)
O10–C32–H32A	109.5	O10–C32–H32B	109.5
O10–C32–H32C	109.5	H32A–C32–H32B	109.5
H32A–C32–H32C	109.5	H32B–C32–H32C	109.5
H11–O11–C33	112(3)	O11–C33–H33A	109.5
O11–C33–H33B	109.5	O11–C33–H33C	109.5
H33A–C33–H33B	109.5	H33A–C33–H33C	109.5
H33B–C33–H33C	109.5		

Symmetry operations for equivalent atoms

a –x+1,–y+2,–z b –x+2,–y+2,–z+1 c –x,–y+1,–z

d –x+1,–y+1,–z+1

Table S67. Torsion angles [°] for 10.

C3c–C1–C2–C3	0.3(5)	C3c–C1–C2–C5	−175.0(3)
C4–C1–C2–C3	−174.1(3)	C4–C1–C2–C5	10.6(5)
C1–C2–C3–C1c	−0.3(5)	C5–C2–C3–C1c	175.1(3)
C2–C1–C4–O1	53.6(4)	C2–C1–C4–O2	−128.7(3)
C3c–C1–C4–O1	−120.8(3)	C3c–C1–C4–O2	57.0(4)
C1–C2–C5–O3	55.6(4)	C1–C2–C5–O4	−126.7(3)
C3–C2–C5–O3	−119.7(4)	C3–C2–C5–O4	58.0(4)
C1–C4–O2–Cu1	−173.7(2)	O1–C4–O2–Cu1	3.9(4)
C2–C5–O4–Cu2	−175.4(2)	O3–C5–O4–Cu2	2.2(5)
C8d–C6–C7–C8	−0.6(5)	C8d–C6–C7–C10	177.4(3)
C9–C6–C7–C8	174.0(3)	C9–C6–C7–C10	−8.1(5)
C6–C7–C8–C6d	0.6(5)	C10–C7–C8–C6d	−177.4(3)
C7–C6–C9–O5	−60.1(5)	C7–C6–C9–O6	123.1(3)
C8d–C6–C9–O5	114.4(3)	C8d–C6–C9–O6	−62.3(4)
C6–C7–C10–O7	−33.7(4)	C6–C7–C10–O8	146.3(3)
C8–C7–C10–O7	144.2(3)	C8–C7–C10–O8	−35.8(4)
C6–C9–O6–Cu1	153.4(2)	O5–C9–O6–Cu1	−23.2(4)
C7–C10–O8–Cu3	−169.47(19)	O7–C10–O8–Cu3	10.5(5)
Cu1–N1–C11–C12	−173.1(3)	C15–N1–C11–C12	0.5(5)
N1–C11–C12–C13	−0.9(6)	C11–C12–C13–C14	1.3(6)
C12–C13–C14–C15	−1.2(6)	Cu1–N1–C15–C14	173.4(3)
C11–N1–C15–C14	−0.4(5)	C13–C14–C15–N1	0.8(6)
Cu1–N2–C16–C17	−177.5(3)	C20–N2–C16–C17	−0.8(6)
N2–C16–C17–C18	1.8(6)	C16–C17–C18–C19	−1.3(6)
C17–C18–C19–C20	−0.1(6)	Cu1–N2–C20–C19	176.0(3)
C16–N2–C20–C19	−0.7(5)	C18–C19–C20–N2	1.2(6)
Cu2–N3–C21–C22	176.1(3)	C25–N3–C21–C22	−1.1(5)
N3–C21–C22–C23	1.3(6)	C21–C22–C23–C24	−0.6(6)
C22–C23–C24–C25	−0.2(6)	Cu2–N3–C25–C24	−176.9(3)
C21–N3–C25–C24	0.3(5)	C23–C24–C25–N3	0.4(6)
Cu3–N4–C26–C27	179.5(3)	C30–N4–C26–C27	1.3(5)
N4–C26–C27–C28	−2.7(5)	C26–C27–C28–C29	1.9(5)
C27–C28–C29–C30	0.1(5)	Cu3–N4–C30–C29	−177.3(3)
C26–N4–C30–C29	0.8(5)	C28–C29–C30–N4	−1.6(5)

Symmetry operations for equivalent atoms

c −x,−y+1,−z d −x+1,−y+1,−z+1

Table S68. Anisotropic displacement parameters (Å^2) for 10. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu1	0.0159(2)	0.0181(2)	0.0100(2)	0.00208(17)	−0.00411(16)	0.00594(18)
Cu2	0.0191(3)	0.0153(3)	0.0199(3)	0.0046(3)	−0.0067(2)	0.0008(3)
Cu3	0.0100(3)	0.0098(3)	0.0188(3)	0.0012(2)	−0.0033(2)	0.0012(2)
C1	0.0140(16)	0.0126(17)	0.0116(16)	−0.0003(13)	−0.0043(13)	0.0060(14)
C2	0.0120(16)	0.0105(17)	0.0121(16)	0.0017(13)	−0.0024(13)	0.0007(13)
C3	0.0142(17)	0.0120(17)	0.0126(16)	0.0043(13)	−0.0023(13)	0.0044(14)
C4	0.0115(17)	0.0167(19)	0.0114(16)	0.0055(14)	−0.0017(13)	−0.0010(14)
C5	0.0163(18)	0.0153(19)	0.0119(17)	0.0048(14)	−0.0070(13)	−0.0010(15)
O1	0.0209(13)	0.0175(14)	0.0171(12)	0.0003(11)	−0.0085(10)	0.0012(11)
O2	0.0180(12)	0.0210(13)	0.0134(12)	0.0032(10)	−0.0055(10)	0.0071(11)
O3	0.0136(13)	0.0231(14)	0.0290(14)	0.0080(11)	−0.0030(10)	0.0036(11)
O4	0.0171(12)	0.0125(13)	0.0267(14)	0.0064(11)	−0.0060(10)	−0.0010(10)
C6	0.0123(16)	0.0091(16)	0.0093(15)	−0.0015(13)	−0.0006(12)	0.0047(13)
C7	0.0111(16)	0.0097(17)	0.0104(16)	−0.0003(13)	−0.0017(12)	0.0022(13)
C8	0.0108(16)	0.0100(17)	0.0103(16)	−0.0006(13)	−0.0042(12)	0.0011(13)
C9	0.0063(16)	0.0159(19)	0.0125(16)	0.0032(14)	−0.0017(12)	−0.0013(13)
C10	0.0100(16)	0.0115(17)	0.0173(18)	0.0049(14)	−0.0027(13)	0.0051(13)
O5	0.0291(14)	0.0156(13)	0.0162(12)	0.0057(10)	−0.0034(10)	0.0065(11)
O6	0.0196(12)	0.0184(13)	0.0092(11)	−0.0004(10)	−0.0037(9)	0.0082(10)
O7	0.0149(12)	0.0186(13)	0.0164(13)	0.0009(10)	0.0032(10)	0.0015(10)
O8	0.0130(11)	0.0079(12)	0.0164(12)	0.0006(10)	−0.0029(9)	−0.0010(9)
N1	0.0159(15)	0.0243(17)	0.0130(15)	0.0047(13)	−0.0057(12)	0.0041(13)
C11	0.0190(19)	0.021(2)	0.0210(19)	0.0052(16)	0.0064(15)	0.0070(16)
C12	0.039(3)	0.060(3)	0.023(2)	0.004(2)	0.0007(18)	0.030(2)
C13	0.021(2)	0.079(4)	0.023(2)	0.009(2)	0.0051(18)	0.001(2)
C14	0.039(3)	0.042(3)	0.032(2)	0.009(2)	0.002(2)	−0.009(2)
C15	0.029(2)	0.031(2)	0.023(2)	0.0044(18)	−0.0048(17)	0.0035(18)
N2	0.0189(15)	0.0234(17)	0.0149(15)	0.0028(13)	−0.0001(12)	0.0102(13)
C16	0.024(2)	0.038(2)	0.0170(19)	0.0015(17)	−0.0054(15)	0.0112(18)
C17	0.0168(19)	0.036(2)	0.031(2)	0.0000(19)	−0.0051(16)	0.0069(17)
C18	0.023(2)	0.027(2)	0.040(2)	0.0067(19)	0.0119(17)	0.0142(17)
C19	0.032(2)	0.028(2)	0.022(2)	0.0087(17)	0.0089(16)	0.0159(18)
C20	0.0219(19)	0.026(2)	0.0159(18)	0.0025(15)	−0.0022(15)	0.0129(16)
N3	0.0216(16)	0.0140(16)	0.0178(15)	−0.0002(12)	−0.0036(12)	0.0031(13)
C21	0.029(2)	0.0126(19)	0.0225(19)	0.0012(15)	−0.0034(16)	−0.0021(16)
C22	0.043(2)	0.018(2)	0.020(2)	0.0025(16)	−0.0018(17)	0.0034(18)
C23	0.048(3)	0.029(2)	0.019(2)	0.0007(18)	−0.0081(18)	0.020(2)
C24	0.026(2)	0.044(3)	0.027(2)	−0.0011(19)	−0.0091(17)	0.0175(19)
C25	0.024(2)	0.024(2)	0.023(2)	−0.0006(16)	−0.0028(15)	0.0094(17)
N4	0.0136(14)	0.0110(15)	0.0176(14)	0.0035(12)	0.0006(11)	0.0030(12)
C26	0.0169(18)	0.0186(19)	0.0170(18)	0.0032(15)	−0.0021(14)	0.0039(15)
C27	0.0185(19)	0.026(2)	0.0221(19)	0.0028(16)	−0.0044(15)	0.0075(16)
C28	0.0180(19)	0.033(2)	0.034(2)	0.0098(18)	0.0010(16)	0.0161(17)
C29	0.027(2)	0.021(2)	0.033(2)	−0.0002(17)	0.0018(17)	0.0150(17)
C30	0.0182(18)	0.021(2)	0.0217(19)	0.0010(15)	−0.0003(14)	0.0086(15)
O9	0.0496(18)	0.0289(16)	0.0197(14)	−0.0060(12)	−0.0138(13)	0.0217(14)
C31	0.085(4)	0.057(3)	0.061(3)	−0.029(3)	−0.045(3)	0.056(3)
O10	0.0256(15)	0.0209(15)	0.0343(15)	0.0033(13)	0.0047(12)	0.0033(12)
C32	0.026(2)	0.036(3)	0.034(2)	0.010(2)	0.0044(18)	0.004(2)

O11	0.0201(14)	0.0246(15)	0.0256(14)	0.0037(12)	0.0002(11)	0.0030(12)
C33	0.020(2)	0.036(3)	0.034(2)	0.000(2)	0.0001(17)	0.0023(19)

Table S69. Hydrogen coordinates and isotropic displacement parameters (Å^2) for 10.

	x	y	z	U
H3	0.0583	0.6574	–0.0825	0.015
H8	0.7026	0.6220	0.5830	0.013
H11A	0.1707	0.6090	0.2791	0.024
H12	–0.0563	0.5559	0.3485	0.045
H13	–0.1799	0.3353	0.3764	0.054
H34	–0.0673	0.1737	0.3383	0.053
H35	0.1577	0.2331	0.2700	0.036
H36	0.7464	0.6111	0.2646	0.031
H37	0.9925	0.7238	0.2186	0.034
H38	1.0047	0.7577	0.0989	0.034
H39	0.7662	0.6674	0.0290	0.031
H20	0.5277	0.5482	0.0781	0.024
H21	0.3877	0.8704	0.1324	0.029
H22	0.4917	0.8325	0.2372	0.035
H23	0.7706	0.9293	0.2636	0.037
H24	0.9378	1.0589	0.1817	0.037
H25	0.8253	1.0874	0.0777	0.028
H26	0.7063	0.9201	0.4034	0.022
H27	0.4974	0.9945	0.3752	0.027
H28	0.4740	1.1829	0.4393	0.031
H29	0.6733	1.3008	0.5266	0.031
H30	0.8876	1.2274	0.5469	0.024
H9	0.389(5)	0.219(4)	0.1608(10)	0.047
H31A	0.5339	0.1462	0.2359	0.093
H31B	0.5860	0.2939	0.2759	0.093
H31C	0.6442	0.2734	0.1982	0.093
H10	0.952(4)	0.8794(19)	0.374(2)	0.042
H32A	1.1959	0.9041	0.3387	0.034(12)
H32B	1.2377	1.0634	0.3491	0.053(14)
H32C	1.1314	0.9775	0.2818	0.047(13)
H11	0.405(4)	1.199(3)	0.0440(19)	0.037
H33A	0.1522	1.1779	0.0812	0.046(13)
H33B	0.1230	1.0204	0.0773	0.050(14)
H33C	0.1523	1.0960	0.0072	0.056(14)

Table S70. Hydrogen bonds for 10 [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
O9–H9...O11e	0.842(10)	1.924(11)	2.765(4)	176(5)
O10–H10...O7	0.835(10)	1.826(13)	2.651(3)	169(4)
O11–H11...O3a	0.841(10)	1.825(16)	2.641(3)	163(4)

Symmetry operations for equivalent atoms

a –x+1,–y+2,–z e x,y–1,z