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SUPPLEMENTARY MATERIAL TO

Synthesis, characterization, electrochemical studies and X-ray structures of mixed-ligand polypyridyl copper(II) complexes with the acetate

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ANALYTICAL AND SPECTRAL DATA OF **1** AND **2**

*$[Cu(phen)_2(CH_3COO)](ClO_4)\cdot 2H_2O$ (**1**).* Yield: 30 %; Anal. Calcd. for $C_{26}H_{23}N_4O_8ClCu$ (FW: 618.47): C, 48.59; H, 3.43; N, 9.06 %. Found: C, 48.83; H, 3.16; N, 9.13 %; IR (ATR, cm^{-1}):[1] 3382 (*br*), 1587 (*m*), 1428 (*s*), 1314 (*w*); (ClO_4): 1059 (*vs*), 720 (*m*); UV–Vis (CH_3CN, λ_{max} / cm^{-1} (nm)): 14514 (689), 37175 (269), 43478 (230), 48781 (205); μ_{eff} (at 299 K): 1.83 μ_B.

*$[Cu(bipy)_2(CH_3COO)](ClO_4)\cdot H_2O$ (**2**).* Yield: 44 %; Anal. Calcd. for $C_{22}H_{21}N_4O_7ClCu$: C, 49.80; H, 3.83; N, 10.42 %. Found: C, 49.57; H, 3.59; N, 10.49 %; IR (ATR, cm^{-1}):[1] 3399 (*br*), 1571 (*m*), 1441 (*s*), 1319 (*w*); (ClO_4): 1080 (*vs*), 768 (*m*). UV–Vis (CH_3CN, λ_{max} / cm^{-1} (nm)): 14535 (688), 37037 (270), 44053 (230), 48780 (205); μ_{eff} (at 297 K): 1.72 μ_B.

TABLE S-I. Crystal data and structural refinement for **1** and **2**

Compound	$[Cu(phen)_2(CH_3COO)](ClO_4)\cdot 2H_2O$	$[Cu(bipy)_2(CH_3COO)](ClO_4)\cdot H_2O$
CCDC deposit No.	1418811	1418812
Identification code	shelx	shelx
Color/Shape	Bluish–green/block	Blue/rod
Chemical formula	$C_{26}H_{23}ClCuN_4O_8$	$C_{22}H_{21}ClCuN_4O_7$
Formula weight	618.47	552.42
Temperature, K	100(2)	100(2)
Wavelength, Å	0.71073	0.71073
Crystal system	Monoclinic	Triclinic
Space group	Pn	P-1

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TABLE S-I. Continued

Unit cell dimensions	a = 9.3682(6)Å b = 8.3029(5) Å c = 16.8784(10) Å β = 103.3014(18)°	a = 8.2822(4) Å b = 9.4748(4) Å c = 14.7992(6) Å α = 78.729(2)° β = 82.881(2)° γ = 85.092(2)°
Volume, Å^3	1277.64(14)	1127.90(9)
Z	2	2
Density (calculated), kg m^{-3}	1.608	1.627
Absorption coefficient, mm^{-1}	1.019	1.140
F(000)	634	566
Crystal size, mm^3	0.300×0.260×0.200	0.500×0.240×0.200
θ range for data collection, °	2.292–30.570	2.20–30.58
Index ranges	–13<=h<=13, –11<=k<=11, –23<=l<=24	–11<=h<=11, –13<=k<=13, –21<=l<=21
Reflections collected	9896	58024
Independent reflections	6312 [R(int) = 0.0196]	6914 [R(int) = 0.0421]
Completeness to theta = 25.500°	99.3 %	100 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.6516	0.7461 and 0.6323
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/ /parameters	6312/8/379	6914/68/339
Goodness-of-fit on F^2	1.070	1.083
Final R indices ($I > 2\sigma(I)$)	R1 = 0.0325, wR2 = 0.0772	R1 = 0.0357, wR2 = 0.0776
R indices (all data)	R1 = 0.0377, wR2 = 0.0802	R1 = 0.0451, wR2 = 0.0814
Absolute structure parameter[2]	0.521(12)	–
Extinction coefficient	n/a	
Largest diff. peak and hole	0.601 and –0.278 e.Å^{-3}	0.563 and –0.384 e.Å^{-3}

TABLE S-II. Atomic coordinates (×10^4) and equivalent isotropic displacement parameters (10^3 Å^2) for [Cu(phen)$_2$(CH$_3$COO)](ClO$_4$)·2H$_2$O (**1**). *U*(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

Atom	*x*	*y*	*z*	*U*(eq)
Cu	2292(1)	4985(1)	6297(1)	14(1)
O(1)	1792(2)	2888(2)	6743(1)	18(1)
O(2)	2670(2)	2136(3)	5695(1)	22(1)
N(1)	2082(3)	6422(3)	7371(2)	15(1)
N(2)	4366(4)	4921(3)	6963(2)	15(1)
N(3)	2796(3)	6505(3)	5453(2)	15(1)
N(4)	267(3)	5241(3)	5589(2)	15(1)
C(11A)	2151(4)	1802(3)	6284(2)	17(1)
C(12A)	1924(5)	80(3)	6503(3)	29(1)
C(1)	936(4)	7070(4)	7596(2)	19(1)
C(2)	1063(4)	7973(4)	8309(2)	23(1)
C(3)	2437(4)	8247(4)	8792(2)	23(1)
C(4)	3674(4)	7578(4)	8582(2)	19(1)
C(5)	5144(4)	7732(4)	9065(2)	23(1)
C(6)	6279(4)	6974(4)	8862(2)	22(1)
C(7)	6068(3)	5989(4)	8148(2)	18(1)
C(8)	7201(3)	5104(4)	7933(2)	20(1)
C(9)	6889(3)	4130(4)	7262(2)	22(1)
C(10)	5447(3)	4077(4)	6778(2)	20(1)
C(11)	4643(3)	5846(3)	7643(2)	15(1)
C(12)	3432(3)	6649(3)	7864(2)	16(1)
C(13)	4077(3)	7101(3)	5387(2)	18(1)
C(14)	4234(4)	8132(4)	4763(2)	21(1)
C(15)	3011(4)	8568(4)	4175(2)	20(1)
C(16)	1629(3)	7948(3)	4217(2)	16(1)
C(17)	288(4)	8283(3)	3629(2)	19(1)
C(18)	–1007(4)	7639(4)	3702(2)	19(1)
C(19)	–1082(3)	6602(3)	4370(2)	16(1)
C(20)	–2379(3)	5868(3)	4481(2)	18(1)
C(21)	–2324(3)	4854(4)	5123(2)	18(1)
C(22)	–970(3)	4551(4)	5672(2)	19(1)
C(23)	215(3)	6243(3)	4946(2)	14(1)
C(24)	1589(3)	6920(3)	4871(2)	14(1)
Cl(1)	7284(1)	–404(1)	6606(1)	23(1)
O(3)	7603(3)	803(4)	6059(2)	41(1)
O(4)	7490(3)	–1975(3)	6296(2)	38(1)
O(5)	5799(3)	–209(3)	6682(2)	36(1)
O(6)	8281(3)	–210(3)	7390(2)	36(1)
O(1W)	4978(3)	2019(3)	4944(2)	31(1)
O(2W)	176(3)	2583(4)	7910(2)	33(1)

TABLE S-III. Bond lengths (Å) and angles (°) for [Cu(phen)$_2$(CH$_3$COO)](ClO$_4$)·2H$_2$O (**1**)

Cu–O(1)	1.995(2)	O(2)–C(11A)–O(1)	122.3(3)
Cu–N(4)	2.007(3)	O(2)–C(11A)–C(12A)	121.0(3)
Cu–N(2)	2.009(3)	O(1)–C(11A)–C(12A)	116.6(3)
Cu–N(3)	2.038(2)	C(11A)–C(12A)–H(12A)	109.5

TABLE S-III. Continued

Cu–N(1)	2.217(3)	C(11A)–C(12A)–H(12B)	109.5
O(1)–C(11A)	1.282(4)	H(12A)–C(12A)–H(12B)	109.5
O(2)–C(11A)	1.236(4)	C(11A)–C(12A)–H(12C)	109.5
N(1)–C(1)	1.332(4)	H(12A)–C(12A)–H(12C)	109.5
N(1)–C(12)	1.357(4)	H(12B)–C(12A)–H(12C)	109.5
N(2)–C(10)	1.327(4)	N(1)–C(1)–C(2)	123.1(3)
N(2)–C(11)	1.356(4)	N(1)–C(1)–H(1A)	118.5
N(3)–C(13)	1.327(4)	C(2)–C(1)–H(1A)	118.5
N(3)–C(24)	1.361(4)	C(3)–C(2)–C(1)	118.8(3)
N(4)–C(22)	1.329(4)	C(3)–C(2)–H(2A)	120.6
N(4)–C(23)	1.359(4)	C(1)–C(2)–H(2A)	120.6
C(11A)–C(12A)	1.504(4)	C(2)–C(3)–C(4)	119.9(3)
C(12A)–H(12A)	0.9800	C(2)–C(3)–H(3A)	120.0
C(12A)–H(12B)	0.9800	C(4)–C(3)–H(3A)	120.0
C(12A)–H(12C)	0.9800	C(3)–C(4)–C(12)	117.1(3)
C(1)–C(2)	1.400(5)	C(3)–C(4)–C(5)	124.1(3)
C(1)–H(1A)	0.9500	C(12)–C(4)–C(5)	118.7(3)
C(2)–C(3)	1.375(5)	C(6)–C(5)–C(4)	121.7(3)
C(2)–H(2A)	0.9500	C(6)–C(5)–H(5A)	119.2
C(3)–C(4)	1.403(4)	C(4)–C(5)–H(5A)	119.2
C(3)–H(3A)	0.9500	C(5)–C(6)–C(7)	121.1(3)
C(4)–C(12)	1.410(4)	C(5)–C(6)–H(6A)	119.5
C(4)–C(5)	1.436(5)	C(7)–C(6)–H(6A)	119.5
C(5)–C(6)	1.346(5)	C(8)–C(7)–C(11)	117.7(3)
C(5)–H(5A)	0.9500	C(8)–C(7)–C(6)	123.4(3)
C(6)–C(7)	1.432(4)	C(11)–C(7)–C(6)	118.9(3)
C(6)–H(6A)	0.9500	C(9)–C(8)–C(7)	119.5(3)
C(7)–C(8)	1.406(4)	C(9)–C(8)–H(8A)	120.2
C(7)–C(11)	1.414(4)	C(7)–C(8)–H(8A)	120.2
C(8)–C(9)	1.367(5)	C(8)–C(9)–C(10)	119.5(3)
C(8)–H(8A)	0.9500	C(8)–C(9)–H(9A)	120.2
C(9)–C(10)	1.409(4)	C(10)–C(9)–H(9A)	120.2
C(9)–H(9A)	0.9500	N(2)–C(10)–C(9)	121.9(3)
C(10)–H(10A)	0.9500	N(2)–C(10)–H(10A)	119.0
C(11)–C(12)	1.437(4)	C(9)–C(10)–H(10A)	119.0
C(13)–C(14)	1.392(4)	N(2)–C(11)–C(7)	121.9(3)
C(13)–H(13A)	0.9500	N(2)–C(11)–C(12)	118.2(3)
C(14)–C(15)	1.381(5)	C(7)–C(11)–C(12)	119.8(3)
C(14)–H(14A)	0.9500	N(1)–C(12)–C(4)	123.0(3)
C(15)–C(16)	1.410(4)	N(1)–C(12)–C(11)	117.2(3)
C(15)–H(15A)	0.9500	C(4)–C(12)–C(11)	119.7(3)
C(16)–C(24)	1.402(4)	N(3)–C(13)–C(14)	123.3(3)
C(16)–C(17)	1.437(4)	N(3)–C(13)–H(13A)	118.4
C(17)–C(18)	1.356(4)	C(14)–C(13)–H(13A)	118.4
C(17)–H(17A)	0.9500	C(15)–C(14)–C(13)	119.4(3)
C(18)–C(19)	1.434(4)	C(15)–C(14)–H(14A)	120.3
C(18)–H(18A)	0.9500	C(13)–C(14)–H(14A)	120.3

TABLE S-III. Continued

C(19)–C(23)	1.403(4)	C(14)–C(15)–C(16)	119.2(3)
C(19)–C(20)	1.410(4)	C(14)–C(15)–H(15A)	120.4
C(20)–C(21)	1.364(5)	C(16)–C(15)–H(15A)	120.4
C(20)–H(20A)	0.9500	C(24)–C(16)–C(15)	116.9(3)
C(21)–C(22)	1.411(4)	C(24)–C(16)–C(17)	118.9(3)
C(21)–H(21A)	0.9500	C(15)–C(16)–C(17)	124.2(3)
C(22)–H(22A)	0.9500	C(18)–C(17)–C(16)	121.3(3)
C(23)–C(24)	1.437(4)	C(18)–C(17)–H(17A)	119.3
Cl(1)–O(4)	1.434(2)	C(16)–C(17)–H(17A)	119.3
Cl(1)–O(5)	1.436(3)	C(17)–C(18)–C(19)	121.0(3)
Cl(1)–O(3)	1.439(3)	C(17)–C(18)–H(18A)	119.5
Cl(1)–O(6)	1.442(3)	C(19)–C(18)–H(18A)	119.5
O(1W)–H(1W1)	0.85(2)	C(23)–C(19)–C(20)	116.8(3)
O(1W)–H(1W2)	0.84(2)	C(23)–C(19)–C(18)	118.8(3)
O(2W)–H(2W1)	0.84(2)	C(20)–C(19)–C(18)	124.4(3)
O(2W)–H(2W2)	0.83(2)	C(21)–C(20)–C(19)	119.8(3)
O(1)–Cu–N(4)	92.60(10)	C(21)–C(20)–H(20A)	120.1
O(1)–Cu–N(2)	92.65(10)	C(19)–C(20)–H(20A)	120.1
N(4)–Cu–N(2)	174.75(12)	C(20)–C(21)–C(22)	119.7(3)
O(1)–Cu–N(3)	156.38(9)	C(20)–C(21)–H(21A)	120.1
N(4)–Cu–N(3)	81.81(11)	C(22)–C(21)–H(21A)	120.1
N(2)–Cu–N(3)	93.33(11)	N(4)–C(22)–C(21)	121.9(3)
O(1)–Cu–N(1)	95.09(9)	N(4)–C(22)–H(22A)	119.1
N(4)–Cu–N(1)	100.38(11)	C(21)–C(22)–H(22A)	119.1
N(2)–Cu–N(1)	79.22(11)	N(4)–C(23)–C(19)	123.3(3)
N(3)–Cu–N(1)	108.48(9)	N(4)–C(23)–C(24)	116.3(3)
C(11A)–O(1)–Cu	105.61(19)	C(19)–C(23)–C(24)	120.4(3)
C(1)–N(1)–C(12)	118.0(3)	N(3)–C(24)–C(16)	123.7(3)
C(1)–N(1)–Cu	132.8(2)	N(3)–C(24)–C(23)	116.7(3)
C(12)–N(1)–Cu	109.27(19)	C(16)–C(24)–C(23)	119.6(3)
C(10)–N(2)–C(11)	119.4(3)	O(4)–Cl(1)–O(5)	110.43(17)
C(10)–N(2)–Cu	125.1(2)	O(4)–Cl(1)–O(3)	109.61(19)
C(11)–N(2)–Cu	115.5(2)	O(5)–Cl(1)–O(3)	109.10(17)
C(13)–N(3)–C(24)	117.5(3)	O(4)–Cl(1)–O(6)	108.83(16)
C(13)–N(3)–Cu	130.5(2)	O(5)–Cl(1)–O(6)	109.93(19)
C(24)–N(3)–Cu	112.00(19)	O(3)–Cl(1)–O(6)	108.92(19)
C(22)–N(4)–C(23)	118.5(3)	H(1W1)–O(1W)–H(1W2)	101(3)
C(22)–N(4)–Cu	128.3(2)	H(2W1)–O(2W)–H(2W2)	104(3)
C(23)–N(4)–Cu	113.3(2)		

TABLE S-IV. Anisotropic displacement parameters (10^3 Å^2) for **1**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^2U^{11}+\ldots+2hkabU1^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu	12(1)	16(1)	13(1)	2(1)	2(1)	0(1)
O(1)	21(1)	15(1)	19(1)	2(1)	5(1)	0(1)
O(2)	20(1)	29(1)	18(1)	2(1)	5(1)	2(1)

TABLE S-IV. Continued

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	16(1)	15(1)	15(1)	2(1)	3(1)	0(1)
N(2)	14(1)	17(1)	12(1)	2(1)	0(1)	1(1)
N(3)	14(1)	13(1)	16(1)	–1(1)	4(1)	–1(1)
N(4)	14(1)	16(1)	15(1)	1(1)	5(1)	0(1)
C(11A)	16(1)	18(1)	14(1)	1(1)	–1(1)	0(1)
C(12A)	40(2)	17(1)	30(2)	1(1)	11(2)	0(1)
C(1)	21(2)	19(1)	18(2)	5(1)	5(1)	3(1)
C(2)	28(2)	22(1)	22(2)	3(1)	12(1)	7(1)
C(3)	33(2)	19(1)	17(2)	0(1)	8(1)	5(1)
C(4)	27(2)	14(1)	15(1)	3(1)	3(1)	0(1)
C(5)	32(2)	18(1)	15(1)	–1(1)	–2(1)	–3(1)
C(6)	24(2)	20(1)	17(2)	3(1)	–5(1)	–4(1)
C(7)	17(2)	19(1)	16(1)	3(1)	0(1)	–4(1)
C(8)	13(1)	26(2)	21(2)	7(1)	0(1)	–1(1)
C(9)	15(1)	30(2)	23(2)	6(1)	5(1)	3(1)
C(10)	16(1)	25(2)	19(2)	1(1)	5(1)	1(1)
C(11)	16(1)	14(1)	15(1)	4(1)	2(1)	–2(1)
C(12)	17(1)	13(1)	16(1)	2(1)	2(1)	–1(1)
C(13)	14(1)	20(1)	21(2)	–1(1)	4(1)	–2(1)
C(14)	20(2)	21(1)	23(2)	–1(1)	9(1)	–6(1)
C(15)	27(2)	17(1)	19(2)	1(1)	11(1)	–4(1)
C(16)	21(2)	13(1)	14(1)	–2(1)	4(1)	0(1)
C(17)	25(2)	16(1)	15(1)	2(1)	1(1)	3(1)
C(18)	20(2)	19(1)	16(2)	1(1)	–2(1)	2(1)
C(19)	14(1)	17(1)	16(1)	–3(1)	0(1)	1(1)
C(20)	13(1)	20(1)	21(2)	–5(1)	1(1)	2(1)
C(21)	12(1)	22(2)	22(2)	–4(1)	6(1)	–2(1)
C(22)	17(2)	19(1)	20(2)	2(1)	4(1)	–1(1)
C(23)	14(1)	13(1)	13(1)	–1(1)	2(1)	0(1)
C(24)	17(1)	12(1)	14(1)	–2(1)	3(1)	–1(1)
Cl(1)	19(1)	24(1)	24(1)	–6(1)	–2(1)	2(1)
O(3)	37(2)	47(2)	37(2)	12(1)	4(1)	–1(1)
O(4)	29(2)	30(1)	50(2)	–16(1)	–5(1)	8(1)
O(5)	22(1)	41(2)	44(2)	–5(1)	7(1)	6(1)
O(6)	33(2)	41(2)	26(1)	–9(1)	–10(1)	3(1)
O(1W)	30(1)	36(1)	27(1)	2(1)	10(1)	–5(1)
O(2W)	22(1)	50(2)	27(1)	–6(1)	8(1)	–8(1)

TABLE S-V. Hydrogen coordinates ($\times 14^4$) and isotropic displacement parameters (10^3 Å^2) for $[Cu(phen)_2(CH_3COO)](ClO_4)\cdot 2H_2O$ (**1**)

Atom	*x*	*y*	*z*	*U*(eq)
H(12A)	2737	–580	6410	43
H(12B)	998	–318	6165	43
H(12C)	1890	16	7078	43
H(1A)	–14	6910	7256	23

TABLE S-V. Continued

Atom	*x*	*y*	*z*	*U*(eq)
H(2A)	216	8390	8456	27
H(3A)	2548	8889	9269	27
H(5A)	5319	8385	9540	27
H(6A)	7237	7095	9199	27
H(8A)	8177	5183	8251	24
H(9A)	7639	3494	7124	27
H(10A)	5244	3417	6305	24
H(13A)	4930	6810	5787	22
H(14A)	5175	8533	4742	25
H(15A)	3099	9276	3747	24
H(17A)	309	8969	3182	23
H(18A)	–1876	7879	3303	23
H(20A)	–3288	6078	4110	22
H(21A)	–3194	4355	5201	22
H(22A)	–942	3834	6114	23
H(1W1)	5680(50)	1460(70)	5220(40)	110(30)
H(1W2)	4270(50)	1700(70)	5130(40)	100(20)
H(2W1)	690(50)	2550(60)	7560(30)	59(17)
H(2W2)	–330(50)	1760(40)	7830(30)	50(15)

TABLE S-VI. Torsion angles (°) for[$Cu(phen)_2(CH_3COO)](ClO_4)\cdot 2H_2O$ (**1**)

Cu–O(1)–C(11A)–O(2)	–1.0(4)	C(7)–C(11)–C(12)–C(4)	0.2(4)
Cu–O(1)–C(11A)–C(12A)	178.4(3)	C(24)–N(3)–C(13)–C(14)	0.7(4)
C(12)–N(1)–C(1)–C(2)	0.4(4)	Cu–N(3)–C(13)–C(14)	179.7(2)
Cu–N(1)–C(1)–C(2)	–178.8(2)	N(3)–C(13)–C(14)–C(15)	–0.2(5)
N(1)–C(1)–C(2)–C(3)	1.8(5)	C(13)–C(14)–C(15)–C(16)	–0.4(4)
C(1)–C(2)–C(3)–C(4)	–2.2(5)	C(14)–C(15)–C(16)–C(24)	0.5(4)
C(2)–C(3)–C(4)–C(12)	0.5(4)	C(14)–C(15)–C(16)–C(17)	–178.4(3)
C(2)–C(3)–C(4)–C(5)	–177.0(3)	C(24)–C(16)–C(17)–C(18)	0.7(4)
C(3)–C(4)–C(5)–C(6)	175.4(3)	C(15)–C(16)–C(17)–C(18)	179.5(3)
C(12)–C(4)–C(5)–C(6)	–2.1(5)	C(16)–C(17)–C(18)–C(19)	0.2(5)
C(4)–C(5)–C(6)–C(7)	0.5(5)	C(17)–C(18)–C(19)–C(23)	–0.9(4)
C(5)–C(6)–C(7)–C(8)	–176.5(3)	C(17)–C(18)–C(19)–C(20)	–179.0(3)
C(5)–C(6)–C(7)–C(11)	1.4(4)	C(23)–C(19)–C(20)–C(21)	–0.5(4)
C(11)–C(7)–C(8)–C(9)	–1.2(4)	C(18)–C(19)–C(20)–C(21)	177.7(3)
C(6)–C(7)–C(8)–C(9)	176.7(3)	C(19)–C(20)–C(21)–C(22)	0.1(4)
C(7)–C(8)–C(9)–C(10)	2.5(5)	C(23)–N(4)–C(22)–C(21)	–1.2(5)
C(11)–N(2)–C(10)–C(9)	–1.0(5)	Cu–N(4)–C(22)–C(21)	179.8(2)
Cu–N(2)–C(10)–C(9)	178.0(2)	C(20)–C(21)–C(22)–N(4)	0.7(5)
C(8)–C(9)–C(10)–N(2)	–1.5(5)	C(22)–N(4)–C(23)–C(19)	0.8(4)
C(10)–N(2)–C(11)–C(7)	2.4(4)	Cu–N(4)–C(23)–C(19)	180.0(2)
Cu–N(2)–C(11)–C(7)	–176.6(2)	C(22)–N(4)–C(23)–C(24)	–178.2(3)
C(10)–N(2)–C(11)–C(12)	–175.3(3)	Cu–N(4)–C(23)–C(24)	0.9(3)
Cu–N(2)–C(11)–C(12)	5.7(3)	C(20)–C(19)–C(23)–N(4)	0.0(4)

TABLE S-VI. Continued

C(8)–C(7)–C(11)–N(2)	–1.3(4)	C(18)–C(19)–C(23)–N(4)	–178.3(3)
C(6)–C(7)–C(11)–N(2)	–179.3(3)	C(20)–C(19)–C(23)–C(24)	179.0(3)
C(8)–C(7)–C(11)–C(12)	176.3(3)	C(18)–C(19)–C(23)–C(24)	0.7(4)
C(6)–C(7)–C(11)–C(12)	–1.7(4)	C(13)–N(3)–C(24)–C(16)	–0.6(4)
C(1)–N(1)–C(12)–C(4)	–2.2(4)	Cu–N(3)–C(24)–C(16)	–179.8(2)
Cu–N(1)–C(12)–C(4)	177.2(2)	C(13)–N(3)–C(24)–C(23)	179.1(2)
C(1)–N(1)–C(12)–C(11)	175.6(2)	Cu–N(3)–C(24)–C(23)	0.0(3)
Cu–N(1)–C(12)–C(11)	–5.0(3)	C(15)–C(16)–C(24)–N(3)	0.1(4)
C(3)–C(4)–C(12)–N(1)	1.7(4)	C(17)–C(16)–C(24)–N(3)	179.0(3)
C(5)–C(4)–C(12)–N(1)	179.4(3)	C(15)–C(16)–C(24)–C(23)	–179.7(3)
C(3)–C(4)–C(12)–C(11)	–176.0(3)	C(17)–C(16)–C(24)–C(23)	–0.8(4)
C(5)–C(4)–C(12)–C(11)	1.7(4)	N(4)–C(23)–C(24)–N(3)	–0.6(4)
N(2)–C(11)–C(12)–N(1)	0.0(4)	C(19)–C(23)–C(24)–N(3)	–179.7(3)
C(7)–C(11)–C(12)–N(1)	–177.7(3)	N(4)–C(23)–C(24)–C(16)	179.2(3)
N(2)–C(11)–C(12)–C(4)	177.9(3)	C(19)–C(23)–C(24)–C(16)	0.1(4)

TABLE S-VII. Hydrogen bonds for $[Cu(phen)_2(CH_3COO)](ClO_4)\cdot 2H_2O$ (**1**); symmetry transformations used to generate equivalent atoms: #1 *x*–1, *y*+1, *z*; #2 *x*–1/2, –*y*+1, *z*+1/2; #3 *x*+1, *y*, *z*; #4 *x*, *y*+1, *z*; #5 *x*–1, *y*, *z*

D–H···A	*d*(D–H) / Å	*d*(H···A) / Å	*d*(D···A) / Å	<(DHA) / °
C(2)–H(2A)···O(6)#1	0.95	2.53	3.101(4)	119.2
C(2)–H(2A)···O(1W)#2	0.95	2.59	3.153(4)	117.9
C(9)–H(9A) ··O(2W)#3	0.95	2.56	3.283(4)	133.5
C(10)–H(10A)···O(2)	0.95	2.62	3.243(4)	123.6
C(10)–H(10A)···O(1W)	0.95	2.53	3.474(4)	169.7
C(13)–H(13A)···N(2)	0.95	2.68	3.177(4)	113.5
C(13)–H(13A)···O(4)#4	0.95	2.56	3.302(4)	135.0
C(21)–H(21A)···O(1W)#5	0.95	2.56	3.416(4)	150.5
C(22)–H(22A)···O(1)	0.95	2.66	3.118(4)	110.4
O(1W)–H(1W1)···O(3)	0.85(2)	2.09(3)	2.912(4)	162(7)
O(1W)–H(1W2)···O(2)	0.84(2)	1.98(4)	2.747(4)	151(6)
O(2W)–H(2W1)···O(1)	0.84(2)	1.93(2)	2.758(3)	169(5)
O(2W)–H(2W2)···O(6)#5	0.83(2)	2.11(3)	2.930(4)	170(5)

TABLE S-VIII. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (10^3 Å^2) for $[Cu(bipy)_2(CH_3COO)](ClO_4)H_2O$ (**2**). *U*(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

Atom	*x*	*y*	*z*	*U*(eq)
Cu	5317(1)	4840(1)	7450(1)	14(1)
Cl(1)	339(1)	–375(1)	7208(1)	21(1)
O(11)	1427(2)	–1065(2)	6565(1)	36(1)
O(12)	1148(2)	775(2)	7437(1)	42(1)
O(13)	–1104(2)	209(2)	6787(1)	37(1)
O(14)	–83(3)	–1404(2)	8035(1)	45(1)
O(11A)	1276(12)	–797(13)	6409(5)	36(1)
O(12A)	717(15)	1053(5)	7273(9)	42(1)

TABLE S-VIII. Continued

Atom	*x*	*y*	*z*	*U*(eq)
O(13A)	–1371(3)	–383(14)	7122(9)	37(1)
O(14A)	729(17)	–1368(10)	8029(5)	45(1)
O(1)	3129(1)	5531(1)	7058(1)	17(1)
O(2)	2394(2)	4246(2)	8442(1)	30(1)
O(1W)	2286(2)	1305(2)	9032(1)	30(1)
N(1)	5532(2)	3434(1)	6597(1)	14(1)
N(2)	6868(2)	5964(2)	6279(1)	15(1)
N(3)	6693(2)	3667(2)	8423(1)	14(1)
N(4)	5323(2)	6280(1)	8251(1)	15(1)
C(1)	4781(2)	2193(2)	6797(1)	17(1)
C(2)	4932(2)	1227(2)	6197(1)	20(1)
C(3)	5892(2)	1568(2)	5356(1)	20(1)
C(4)	6635(2)	2865(2)	5133(1)	18(1)
C(5)	6430(2)	3790(2)	5766(1)	14(1)
C(6)	7155(2)	5214(2)	5584(1)	15(1)
C(7)	8065(2)	5748(2)	4752(1)	21(1)
C(8)	8725(2)	7078(2)	4645(1)	24(1)
C(9)	8442(2)	7847(2)	5356(1)	22(1)
C(10)	7498(2)	7254(2)	6161(1)	18(1)
C(11)	7313(2)	2299(2)	8480(1)	17(1)
C(12)	8199(2)	1609(2)	9190(1)	20(1)
C(13)	8469(2)	2359(2)	9867(1)	21(1)
C(14)	7840(2)	3776(2)	9816(1)	17(1)
C(15)	6958(2)	4400(2)	9084(1)	14(1)
C(16)	6249(2)	5903(2)	8955(1)	14(1)
C(17)	6513(2)	6878(2)	9502(1)	18(1)
C(18)	5791(2)	8266(2)	9313(1)	20(1)
C(19)	4814(2)	8637(2)	8598(1)	20(1)
C(20)	4604(2)	7613(2)	8078(1)	18(1)
C(11A)	2049(2)	5009(2)	7699(1)	18(1)
C(12A)	301(2)	5339(3)	7513(2)	32(1)

TABLE S-IX. Bond lengths (Å) and angles (°) for $[Cu(bipy)_2(CH_3COO)](ClO_4)\cdot H_2O$ (**2**)

Cu–N(4)	1.9750(14)	O(14A)–Cl(1)–O(12A)	109.41(9)
Cu–O(1)	1.9896(12)	O(11)–Cl(1)–O(12A)	115.7(6)
Cu–N(1)	1.9899(13)	O(13)–Cl(1)–O(12)	109.43(7)
Cu–N(3)	2.0422(14)	O(14)–Cl(1)–O(12)	109.40(7)
Cu–N(2)	2.1786(14)	O(13A)–Cl(1)–O(12)	126.4(5)
Cl(1)–O(13)	1.4341(11)	O(11A)–Cl(1)–O(12)	107.2(6)
Cl(1)–O(14)	1.4343(11)	O(14A)–Cl(1)–O(12)	93.0(5)
Cl(1)–O(13A)	1.4378(12)	O(11)–Cl(1)–O(12)	108.89(7)
Cl(1)–O(11A)	1.4367(12)	O(12A)–Cl(1)–O(12)	19.4(5)
Cl(1)–O(14A)	1.4377(12)	C(11A)–O(1)–Cu	108.47(10)
Cl(1)–O(11)	1.4404(11)	H(1W1)–O(1W)–H(1W2)	104(3)
Cl(1)–O(12A)	1.4382(12)	C(1)–N(1)–C(5)	119.38(14)

TABLE S-IX. Continued

Cl(1)–O(12)	1.4416(11)	C(1)–N(1)–Cu	122.99(11)
O(1)–C(11A)	1.275(2)	C(5)–N(1)–Cu	117.58(11)
O(2)–C(11A)	1.244(2)	C(10)–N(2)–C(6)	118.56(14)
O(1W)–H(1W1)	0.88(3)	C(10)–N(2)–Cu	129.68(12)
O(1W)–H(1W2)	0.87(3)	C(6)–N(2)–Cu	111.73(10)
N(1)–C(1)	1.341(2)	C(11)–N(3)–C(15)	118.58(14)
N(1)–C(5)	1.354(2)	C(11)–N(3)–Cu	128.08(11)
N(2)–C(10)	1.342(2)	C(15)–N(3)–Cu	113.33(10)
N(2)–C(6)	1.347(2)	C(20)–N(4)–C(16)	119.89(14)
N(3)–C(11)	1.343(2)	C(20)–N(4)–Cu	124.14(11)
N(3)–C(15)	1.353(2)	C(16)–N(4)–Cu	115.65(11)
N(4)–C(20)	1.341(2)	N(1)–C(1)–C(2)	122.50(15)
N(4)–C(16)	1.345(2)	N(1)–C(1)–H(1A)	118.7
C(1)–C(2)	1.383(2)	C(2)–C(1)–H(1A)	118.7
C(1)–H(1A)	0.9500	C(1)–C(2)–C(3)	118.26(16)
C(2)–C(3)	1.387(2)	C(1)–C(2)–H(2A)	120.9
C(2)–H(2A)	0.9500	C(3)–C(2)–H(2A)	120.9
C(3)–C(4)	1.385(2)	C(4)–C(3)–C(2)	119.69(16)
C(3)–H(3A)	0.9500	C(4)–C(3)–H(3A)	120.2
C(4)–C(5)	1.391(2)	C(2)–C(3)–H(3A)	120.2
C(4)–H(4A)	0.9500	C(3)–C(4)–C(5)	119.12(15)
C(5)–C(6)	1.487(2)	C(3)–C(4)–H(4A)	120.4
C(6)–C(7)	1.390(2)	C(5)–C(4)–H(4A)	120.4
C(7)–C(8)	1.390(2)	N(1)–C(5)–C(4)	120.99(15)
C(7)–H(7A)	0.9500	N(1)–C(5)–C(6)	115.88(14)
C(8)–C(9)	1.379(3)	C(4)–C(5)–C(6)	123.14(14)
C(8)–H(8A)	0.9500	N(2)–C(6)–C(7)	121.88(15)
C(9)–C(10)	1.389(2)	N(2)–C(6)–C(5)	115.60(14)
C(9)–H(9A)	0.9500	C(7)–C(6)–C(5)	122.52(15)
C(10)–H(10A)	0.9500	C(8)–C(7)–C(6)	118.81(16)
C(11)–C(12)	1.383(2)	C(8)–C(7)–H(7A)	120.6
C(11)–H(11A)	0.9500	C(6)–C(7)–H(7A)	120.6
C(12)–C(13)	1.385(3)	C(9)–C(8)–C(7)	119.55(16)
C(12)–H(12A)	0.9500	C(9)–C(8)–H(8A)	120.2
C(13)–C(14)	1.389(2)	C(7)–C(8)-H(8A)	120.2
C(13)–H(13A)	0.9500	C(8)–C(9)–C(10)	118.28(16)
C(14)–C(15)	1.389(2)	C(8)–C(9)–H(9A)	120.9
C(14)–H(14A)	0.9500	C(10)–C(9)–H(9A)	120.9
C(15)–C(16)	1.479(2)	N(2)–C(10)–C(9)	122.90(16)
C(16)–C(17)	1.389(2)	N(2)–C(10)–H(10A)	118.6
C(17)–C(18)	1.388(2)	C(9)–C(10)–H(10A)	118.6
C(17)–H(17A)	0.9500	N(3)–C(11)–C(12)	122.60(16)
C(18)–C(19)	1.385(3)	N(3)–C(11)–H(11A)	118.7
C(18)–H(18A)	0.9500	C(12)–C(11)–H(11A)	118.7
C(19)–C(20)	1.384(2)	C(11)–C(12)–C(13)	118.76(16)
C(19)–H(19A)	0.9500	C(11)–C(12)–H(12A)	120.6
C(20)–H(20A)	0.9500	C(13)–C(12)–H(12A)	120.6

TABLE S-IX. Continued

C(11A)–C(12A)	1.502(3)	C(12)–C(13)–C(14)	119.31(15)
C(12A)–H(12B)	0.9800	C(12)–C(13)–H(13A)	120.3
C(12A)–H(12C)	0.9800	C(14)–C(13)–H(13A)	120.3
C(12A)–H(12D)	0.9800	C(15)–C(14)–C(13)	118.80(16)
N(4)–Cu–O(1)	94.13(5)	C(15)–C(14)–H(14A)	120.6
N(4)–Cu–N(1)	174.48(6)	C(13)–C(14)–H(14A)	120.6
O(1)–Cu–N(1)	89.80(5)	N(3)–C(15)–C(14)	121.94(15)
N(4)–Cu–N(3)	81.11(5)	N(3)–C(15)–C(16)	114.66(13)
O(1)–Cu–N(3)	149.08(5)	C(14)–C(15)–C(16)	123.40(14)
N(1)–Cu–N(3)	97.46(5)	N(4)–C(16)–C(17)	121.39(15)
N(4)–Cu–N(2)	96.31(5)	N(4)–C(16)–C(15)	114.87(14)
O(1)–Cu–N(2)	100.18(5)	C(17)–C(16)–C(15)	123.74(14)
N(1)–Cu–N(2)	79.16(5)	C(18)–C(17)–C(16)	118.68(15)
N(3)–Cu–N(2)	110.70(5)	C(18)–C(17)–H(17A)	120.7
O(13)–Cl(1)–O(14)	110.03(7)	C(16)–C(17)–H(17A)	120.7
O(13)–Cl(1)–O(13A)	28.3(5)	C(19)–C(18)–C(17)	119.57(16)
O(14)–Cl(1)–O(13A)	82.3(5)	C(19)–C(18)–H(18A)	120.2
O(13)–Cl(1)–O(11A)	98.3(5)	C(17)–C(18)–H(18A)	120.2
O(14)–Cl(1)–O(11A)	121.6(5)	C(20)–C(19)–C(18)	118.79(16)
O(13A)–Cl(1)–O(11A)	109.54(9)	C(20)–C(19)–H(19A)	120.6
O(13)–Cl(1)–O(14A)	137.1(5)	C(18)–C(19)–H(19A)	120.6
O(14)–Cl(1)–O(14A)	27.2(5)	N(4)–C(20)–C(19)	121.67(16)
O(13A)–Cl(1)–O(14A)	109.44(9)	N(4)–C(20)–H(20A)	119.2
O(11A)–Cl(1)–O(14A)	109.55(9)	C(19)–C(20)–H(20A)	119.2
O(13)–Cl(1)–O(11)	109.48(7)	O(2)–C(11A)–O(1)	122.79(16)
O(14)–Cl(1)–O(11)	109.59(7)	O(2)–C(11A)–C(12A)	120.44(16)
O(13A)–Cl(1)–O(11)	115.8(5)	O(1)–C(11A)–C(12A)	116.76(15)
O(11A)–Cl(1)–O(11)	13.4(5)	C(11A)–C(12A)–H(12B)	109.5
O(14A)–Cl(1)–O(11)	96.2(5)	C(11A)–C(12A)–H(12C)	109.5
O(13)–Cl(1)–O(12A)	90.1(5)	H(12B)–C(12A)–H(12C)	109.5
O(14)–Cl(1)–O(12A)	119.9(5)	C(11A)–C(12A)–H(12D)	109.5
O(13A)–Cl(1)–O(12A)	109.40(9)	H(12B)–C(12A)–H(12D)	109.5
O(11A)–Cl(1)–O(12A)	109.49(9)	H(12C)–C(12A)–H(12D)	109.5

TABLE S-X. Anisotropic displacement parameters (10^3 Å^2) for $Cu(bipy)_2(CH_3COO)](ClO_4)\cdot H_2O$ (**2**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^2U^{11} + \cdots + 2hkabU^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu	15(1)	13(1)	14(1)	–4(1)	–3(1)	1(1)
Cl(1)	24(1)	22(1)	17(1)	–2(1)	–4(1)	–5(1)
O(11)	36(1)	43(1)	29(1)	–11(1)	1(1)	5(1)
O(12)	58(1)	53(1)	25(1)	–12(1)	–6(1)	–36(1)
O(13)	31(1)	34(1)	49(1)	–14(1)	–18(1)	9(1)
O(14)	64(2)	39(1)	25(1)	7(1)	5(1)	–14(1)
O(11A)	36(1)	43(1)	29(1)	–11(1)	1(1)	5(1)
O(12A)	58(1)	53(1)	25(1)	–12(1)	–6(1)	–36(1)

TABLE S-X. Continued

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(13A)	31(1)	34(1)	49(1)	–14(1)	–18(1)	9(1)
O(14A)	64(2)	39(1)	25(1)	7(1)	5(1)	–14(1)
O(1)	15(1)	20(1)	14(1)	–2(1)	–1(1)	0(1)
O(2)	42(1)	30(1)	18(1)	6(1)	–10(1)	–16(1)
O(1W)	36(1)	25(1)	32(1)	–10(1)	–14(1)	6(1)
N(1)	13(1)	14(1)	14(1)	–3(1)	–2(1)	–2(1)
N(2)	14(1)	15(1)	17(1)	–3(1)	–4(1)	–1(1)
N(3)	14(1)	14(1)	15(1)	–3(1)	–1(1)	–1(1)
N(4)	16(1)	13(1)	15(1)	–3(1)	–2(1)	1(1)
C(1)	18(1)	17(1)	16(1)	–2(1)	0(1)	–4(1)
C(2)	23(1)	17(1)	21(1)	–5(1)	–2(1)	–6(1)
C(3)	25(1)	20(1)	18(1)	–8(1)	–3(1)	–3(1)
C(4)	19(1)	19(1)	15(1)	–4(1)	–1(1)	–2(1)
C(5)	13(1)	15(1)	14(1)	–3(1)	–3(1)	–1(1)
C(6)	14(1)	14(1)	16(1)	–1(1)	–4(1)	–1(1)
C(7)	26(1)	19(1)	17(1)	–2(1)	–1(1)	–3(1)
C(8)	27(1)	22(1)	21(1)	4(1)	0(1)	–6(1)
C(9)	22(1)	17(1)	25(1)	2(1)	–7(1)	–5(1)
C(10)	19(1)	16(1)	22(1)	–3(1)	–6(1)	–3(1)
C(11)	17(1)	14(1)	20(1)	–4(1)	–1(1)	1(1)
C(12)	19(1)	16(1)	25(1)	–1(1)	–2(1)	3(1)
C(13)	19(1)	22(1)	19(1)	2(1)	–4(1)	2(1)
C(14)	18(1)	20(1)	14(1)	–2(1)	–3(1)	–1(1)
C(15)	12(1)	14(1)	14(1)	–2(1)	1(1)	–2(1)
C(16)	14(1)	13(1)	14(1)	–2(1)	1(1)	–1(1)
C(17)	19(1)	19(1)	16(1)	–5(1)	–3(1)	–2(1)
C(18)	23(1)	18(1)	21(1)	–9(1)	0(1)	–3(1)
C(19)	24(1)	13(1)	22(1)	–4(1)	1(1)	1(1)
C(20)	19(1)	17(1)	19(1)	–2(1)	–3(1)	2(1)
C(11A)	19(1)	19(1)	15(1)	–5(1)	–2(1)	–4(1)
C(12A)	16(1)	49(1)	30(1)	–6(1)	2(1)	–4(1)

TABLE S-XI. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters (10^3 Å^2) for $Cu(bipy)_2(CH_3COO)](ClO_4)\cdot H_2O$ (**2**)

Atom	*x*	*y*	*z*	*U*(eq)
H(1W1)	2220(40)	2250(30)	8850(20)	47(8)
H(1W2)	1760(40)	990(30)	8640(20)	50(8)
H(1A)	4121	1970	7372	21
H(2A)	4392	353	6356	24
H(3A)	6039	914	4937	24
H(4A)	7276	3119	4554	21
H(7A)	8232	5212	4265	25
H(8A)	9368	7455	4087	29
H(9A)	8880	8759	5296	26
H(10A)	7290	7785	6650	22

TABLE S-XI. Continued

Atom	*x*	*y*	*z*	*U*(eq)
H(11A)	7136	1786	8014	20
H(12A)	8616	638	9214	24
H(13A)	9077	1909	10361	25
H(14A)	8010	4308	10273	21
H(17A)	7174	6602	9996	21
H(18A)	5966	8956	9672	24
H(19A)	4296	9577	8466	24
H(20A)	3935	7861	7587	22
H(12B)	–304	5767	8016	48
H(12C)	–184	4446	7477	48
H(12D)	250	6019	6925	48

TABLE S-XII. Torsion angles (°) for $[Cu(bipy)_2(CH_3COO)](ClO_4)\cdot H_2O$ (**2**)

N(4)–Cu–O(1)–C(11A)	–80.21(11)	C(3)–C(4)–C(5)–N(1)	0.6(2)
N(1)–Cu–O(1)–C(11A)	103.66(11)	C(3)–C(4)–C(5)–C(6)	–179.03(15)
N(3)–Cu–O(1)–C(11A)	–0.64(17)	C(10)–N(2)–C(6)–C(7)	–0.7(2)
N(2)–Cu–O(1)–C(11A)	–177.38(11)	Cu–N(2)–C(6)–C(7)	177.53(13)
N(4)–Cu–N(1)–C(1)	146.8(5)	C(10)–N(2)–C(6)–C(5)	179.57(14)
O(1)–Cu–N(1)–C(1)	–77.67(13)	Cu–N(2)–C(6)–C(5)	–2.16(17)
N(3)–Cu–N(1)–C(1)	72.18(13)	N(1)–C(5)–C(6)–N(2)	1.7(2)
N(2)–Cu–N(1)–C(1)	–178.07(14)	C(4)–C(5)–C(6)–N(2)	–178.62(15)
N(4)–Cu–N(1)–C(5)	–35.8(6)	N(1)–C(5)–C(6)–C(7)	–177.99(15)
O(1)–Cu–N(1)–C(5)	99.69(12)	C(4)–C(5)–C(6)–C(7)	1.7(2)
N(3)–Cu–N(1)–C(5)	–110.45(12)	N(2)–C(6)–C(7)–C(8)	1.5(3)
N(2)–Cu–N(1)–C(5)	–0.71(11)	C(5)–C(6)–C(7)–C(8)	–178.83(16)
N(4)–Cu–N(2)–C(10)	–3.57(15)	C(6)–C(7)–C(8)–C(9)	–1.2(3)
O(1)–Cu–N(2)–C(10)	91.79(14)	C(7)–C(8)–C(9)–C(10)	0.1(3)
N(1)–Cu–N(2)–C(10)	179.62(15)	C(6)–N(2)–C(10)–C(9)	–0.4(2)
N(3)–Cu–N(2)–C(10)	–86.42(15)	Cu–N(2)–C(10)–C(9)	–178.28(12)
N(4)–Cu–N(2)–C(6)	178.41(11)	C(8)–C(9)–C(10)–N(2)	0.7(3)
O(1)–Cu–N(2)–C(6)	–86.23(11)	C(15)–N(3)–C(11)–C(12)	0.5(2)
N(1)–Cu–N(2)–C(6)	1.60(11)	Cu–N(3)–C(11)–C(12)	–178.40(12)
N(3)–Cu–N(2)–C(6)	95.56(11)	N(3)–C(11)–C(12)–C(13)	–0.5(3)
N(4)–Cu–N(3)–C(11)	177.52(15)	C(11)–C(12)–C(13)–C(14)	0.2(3)
O(1)–Cu–N(3)–C(11)	94.37(16)	C(12)–C(13)–C(14)–C(15)	–0.1(3)
N(1)–Cu–N(3)–C(11)	–7.87(14)	C(11)–N(3)–C(15)–C(14)	–0.4(2)
N(2)–Cu–N(3)–C(11)	–89.06(14)	Cu–N(3)–C(15)–C(14)	178.70(12)
N(4)–Cu–N(3)–C(15)	–1.45(11)	C(11)–N(3)–C(15)–C(16)	179.18(14)
O(1)–Cu–N(3)–C(15)	–84.60(14)	Cu–N(3)–C(15)–C(16)	–1.74(16)
N(1)–Cu–N(3)–C(15)	173.16(11)	C(13)–C(14)–C(15)–N(3)	0.2(2)
N(2)–Cu–N(3)–C(15)	91.97(11)	C(13)–C(14)–C(15)–C(16)	–179.35(15)
O(1)–Cu–N(4)–C(20)	–32.56(14)	C(20)–N(4)–C(16)–C(17)	–1.4(2)
N(1)–Cu–N(4)–C(20)	102.8(6)	Cu–N(4)–C(16)–C(17)	172.32(12)
N(3)–Cu–N(4)–C(20)	178.20(14)	C(20)–N(4)–C(16)–C(15)	179.25(14)
N(2)–Cu–N(4)–C(20)	68.17(14)	Cu–N(4)–C(16)–C(15)	–6.99(17)

TABLE S-XII. Continued

O(1)–Cu–N(4)–C(16)	153.98(11)	N(3)–C(15)–C(16)–N(4)	5.7(2)
N(1)–Cu–N(4)–C(16)	–70.7(6)	C(14)–C(15)–C(16)–N(4)	–174.74(15)
N(3)–Cu–N(4)–C(16)	4.74(11)	N(3)–C(15)–C(16)–C(17)	–173.58(15)
N(2)–Cu–N(4)–C(16)	–105.29(12)	C(14)–C(15)–C(16)–C(17)	6.0(2)
C(5)–N(1)–C(1)–C(2)	2.3(2)	N(4)–C(16)–C(17)–C(18)	0.3(2)
Cu–N(1)–C(1)–C(2)	179.64(13)	C(15)–C(16)–C(17)–C(18)	179.59(15)
N(1)–C(1)–C(2)–C(3)	–0.3(3)	C(16)–C(17)–C(18)–C(19)	0.9(3)
C(1)–C(2)–C(3)–C(4)	–1.5(3)	C(17)–C(18)–C(19)–C(20)	–1.0(3)
C(2)–C(3)–C(4)–C(5)	1.4(3)	C(16)–N(4)–C(20)–C(19)	1.3(2)
C(1)–N(1)–C(5)–C(4)	–2.5(2)	Cu–N(4)–C(20)–C(19)	–171.91(13)
Cu–N(1)–C(5)–C(4)	–179.92(12)	C(18)–C(19)–C(20)–N(4)	0.0(3)
C(1)–N(1)–C(5)–C(6)	177.23(14)	Cu–O(1)–C(11A)–O(2)	2.4(2)
Cu–N(1)–C(5)–C(6)	–0.23(18)	Cu–O(1)–C(11A)–C(12A)	–176.70(14)

TABLE S-XIII. Hydrogen bonds for $[Cu(bipy)_2(CH_3COO)](ClO_4)\cdot H_2O$ (**2**)

D–H···A	*d*(D–H) / Å	*d*(H···A) / Å	*d*(D···A) / Å	<(DHA) / °
O(1W)–H(1W1)···O(2)	0.88(3)	1.88(3)	2.758(2)	172(3)
O(1W)–H(1W2)···O(12)	0.87(3)	1.97(3)	2.793(2)	158(3)
O(1W)–H(1W2)···O(12A)	0.87(3)	2.29(3)	3.107(11)	156(3)

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