SUPPLEMENTARY MATERIAL TO

Synthesis, Characterization, electrochemical studies and X-ray structures of Mixed–Ligand complexes of $[Cu(phen)_2(CH_3COO)].2H_2O(ClO_4)$ and $Cu(bipy)_2(CH_3COO)]H_2O(ClO_4)$

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CCDC 1418811 and 1418812 are for $[Cu(phen)_2(CH_3COO)].2H_2O(ClO_4)$ **(1)** and $Cu(bipy)_2(CH_3COO)](ClO_4)H_2O$ **(2)** respectively

Table S1. Crystal data and structure refinement for $[Cu(phen)_2(CH_3COO)].2H_2O(ClO_4)$ **(1)**.

Identification code	shelx	
Empirical formula	C26 H23 Cl Cu N4 O8	
Formula weight	618.47	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P n	
Unit cell dimensions	a = 9.3682(6) Å	α = 90°.
	b = 8.3029(5) Å	β= 103.3014(18)°.
	c = 16.8784(10) Å	γ = 90°.
Volume	1277.64(14) $Å^3$	
Z	2	
Density (calculated)	1.608 Mg/m^3	
Absorption coefficient	1.019 mm^{-1}	
F(000)	634	
Crystal size	0.300 x 0.260 x 0.200 mm^3	
Theta range for data collection	2.292 to 30.570°.	
Index ranges	-13<=h<=13, -11<=k<=11, -23<=l<=24	
Reflections collected	9896	
Independent reflections	6312 [R(int) = 0.0196]	

Completeness to theta = 25.500°	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.6516
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6312 / 8 / 379
Goodness-of-fit on F^2	1.070
Final R indices [I>2sigma(I)]	R1 = 0.0325, wR2 = 0.0772
R indices (all data)	R1 = 0.0377, wR2 = 0.0802
Absolute structure parameter	0.521(12)
Extinction coefficient	n/a
Largest diff. peak and hole	0.601 and -0.278 e.$Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[Cu(phen)_2(CH_3COO)].2H_2O(ClO_4)$ **(1)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	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 S3. Bond lengths [Å] and angles [°] for $[Cu(phen)_2(CH_3COO)].2H_2O(ClO_4)$ **(1)**.

Cu-O(1)	1.995(2)
Cu-N(4)	2.007(3)
Cu-N(2)	2.009(3)
Cu-N(3)	2.038(2)
Cu-N(1)	2.217(3)
O(1)-C(11A)	1.282(4)
O(2)-C(11A)	1.236(4)
N(1)-C(1)	1.332(4)
N(1)-C(12)	1.357(4)
N(2)-C(10)	1.327(4)
N(2)-C(11)	1.356(4)
N(3)-C(13)	1.327(4)
N(3)-C(24)	1.361(4)
N(4)-C(22)	1.329(4)
N(4)-C(23)	1.359(4)
C(11A)-C(12A)	1.504(4)
C(12A)-H(12A)	0.9800
C(12A)-H(12B)	0.9800
C(12A)-H(12C)	0.9800
C(1)-C(2)	1.400(5)
C(1)-H(1A)	0.9500
C(2)-C(3)	1.375(5)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.403(4)
C(3)-H(3A)	0.9500
C(4)-C(12)	1.410(4)
C(4)-C(5)	1.436(5)
C(5)-C(6)	1.346(5)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.432(4)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.406(4)

C(7)-C(11)	1.414(4)
C(8)-C(9)	1.367(5)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.409(4)
C(9)-H(9A)	0.9500
C(10)-H(10A)	0.9500
C(11)-C(12)	1.437(4)
C(13)-C(14)	1.392(4)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.381(5)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.410(4)
C(15)-H(15A)	0.9500
C(16)-C(24)	1.402(4)
C(16)-C(17)	1.437(4)
C(17)-C(18)	1.356(4)
C(17)-H(17A)	0.9500
C(18)-C(19)	1.434(4)
C(18)-H(18A)	0.9500
C(19)-C(23)	1.403(4)
C(19)-C(20)	1.410(4)
C(20)-C(21)	1.364(5)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.411(4)
C(21)-H(21A)	0.9500
C(22)-H(22A)	0.9500
C(23)-C(24)	1.437(4)
Cl(1)-O(4)	1.434(2)
Cl(1)-O(5)	1.436(3)
Cl(1)-O(3)	1.439(3)
Cl(1)-O(6)	1.442(3)
O(1W)-H(1W1)	0.85(2)
O(1W)-H(1W2)	0.84(2)
O(2W)-H(2W1)	0.84(2)
O(2W)-H(2W2)	0.83(2)
O(1)-Cu-N(4)	92.60(10)

O(1)-Cu-N(2)	92.65(10)
N(4)-Cu-N(2)	174.75(12)
O(1)-Cu-N(3)	156.38(9)
N(4)-Cu-N(3)	81.81(11)
N(2)-Cu-N(3)	93.33(11)
O(1)-Cu-N(1)	95.09(9)
N(4)-Cu-N(1)	100.38(11)
N(2)-Cu-N(1)	79.22(11)
N(3)-Cu-N(1)	108.48(9)
C(11A)-O(1)-Cu	105.61(19)
C(1)-N(1)-C(12)	118.0(3)
C(1)-N(1)-Cu	132.8(2)
C(12)-N(1)-Cu	109.27(19)
C(10)-N(2)-C(11)	119.4(3)
C(10)-N(2)-Cu	125.1(2)
C(11)-N(2)-Cu	115.5(2)
C(13)-N(3)-C(24)	117.5(3)
C(13)-N(3)-Cu	130.5(2)
C(24)-N(3)-Cu	112.00(19)
C(22)-N(4)-C(23)	118.5(3)
C(22)-N(4)-Cu	128.3(2)
C(23)-N(4)-Cu	113.3(2)
O(2)-C(11A)-O(1)	122.3(3)
O(2)-C(11A)-C(12A)	121.0(3)
O(1)-C(11A)-C(12A)	116.6(3)
C(11A)-C(12A)-H(12A)	109.5
C(11A)-C(12A)-H(12B)	109.5
H(12A)-C(12A)-H(12B)	109.5
C(11A)-C(12A)-H(12C)	109.5
H(12A)-C(12A)-H(12C)	109.5
H(12B)-C(12A)-	109.5

H(12C)	
N(1)-C(1)-C(2)	123.1(3)
N(1)-C(1)-H(1A)	118.5
C(2)-C(1)-H(1A)	118.5
C(3)-C(2)-C(1)	118.8(3)
C(3)-C(2)-H(2A)	120.6
C(1)-C(2)-H(2A)	120.6
C(2)-C(3)-C(4)	119.9(3)
C(2)-C(3)-H(3A)	120.0
C(4)-C(3)-H(3A)	120.0
C(3)-C(4)-C(12)	117.1(3)
C(3)-C(4)-C(5)	124.1(3)
C(12)-C(4)-C(5)	118.7(3)
C(6)-C(5)-C(4)	121.7(3)
C(6)-C(5)-H(5A)	119.2
C(4)-C(5)-H(5A)	119.2
C(5)-C(6)-C(7)	121.1(3)
C(5)-C(6)-H(6A)	119.5
C(7)-C(6)-H(6A)	119.5
C(8)-C(7)-C(11)	117.7(3)
C(8)-C(7)-C(6)	123.4(3)
C(11)-C(7)-C(6)	118.9(3)
C(9)-C(8)-C(7)	119.5(3)
C(9)-C(8)-H(8A)	120.2
C(7)-C(8)-H(8A)	120.2
C(8)-C(9)-C(10)	119.5(3)
C(8)-C(9)-H(9A)	120.2
C(10)-C(9)-H(9A)	120.2
N(2)-C(10)-C(9)	121.9(3)
N(2)-C(10)-H(10A)	119.0
C(9)-C(10)-H(10A)	119.0
N(2)-C(11)-C(7)	121.9(3)
N(2)-C(11)-C(12)	118.2(3)
C(7)-C(11)-C(12)	119.8(3)
N(1)-C(12)-C(4)	123.0(3)
N(1)-C(12)-C(11)	117.2(3)

C(4)-C(12)-C(11)	119.7(3)
N(3)-C(13)-C(14)	123.3(3)
N(3)-C(13)-H(13A)	118.4
C(14)-C(13)-H(13A)	118.4
C(15)-C(14)-C(13)	119.4(3)
C(15)-C(14)-H(14A)	120.3
C(13)-C(14)-H(14A)	120.3
C(14)-C(15)-C(16)	119.2(3)
C(14)-C(15)-H(15A)	120.4
C(16)-C(15)-H(15A)	120.4
C(24)-C(16)-C(15)	116.9(3)
C(24)-C(16)-C(17)	118.9(3)
C(15)-C(16)-C(17)	124.2(3)
C(18)-C(17)-C(16)	121.3(3)
C(18)-C(17)-H(17A)	119.3
C(16)-C(17)-H(17A)	119.3
C(17)-C(18)-C(19)	121.0(3)
C(17)-C(18)-H(18A)	119.5
C(19)-C(18)-H(18A)	119.5
C(23)-C(19)-C(20)	116.8(3)
C(23)-C(19)-C(18)	118.8(3)
C(20)-C(19)-C(18)	124.4(3)
C(21)-C(20)-C(19)	119.8(3)
C(21)-C(20)-H(20A)	120.1
C(19)-C(20)-H(20A)	120.1
C(20)-C(21)-C(22)	119.7(3)
C(20)-C(21)-H(21A)	120.1
C(22)-C(21)-H(21A)	120.1
N(4)-C(22)-C(21)	121.9(3)
N(4)-C(22)-H(22A)	119.1
C(21)-C(22)-H(22A)	119.1
N(4)-C(23)-C(19)	123.3(3)
N(4)-C(23)-C(24)	116.3(3)
C(19)-C(23)-C(24)	120.4(3)
N(3)-C(24)-C(16)	123.7(3)
N(3)-C(24)-C(23)	116.7(3)

C(16)-C(24)-C(23)	119.6(3)
O(4)-Cl(1)-O(5)	110.43(17)
O(4)-Cl(1)-O(3)	109.61(19)
O(5)-Cl(1)-O(3)	109.10(17)
O(4)-Cl(1)-O(6)	108.83(16)
O(5)-Cl(1)-O(6)	109.93(19)
O(3)-Cl(1)-O(6)	108.92(19)
H(1W1)-O(1W)-H(1W2)	101(3)
H(2W1)-O(2W)-H(2W2)	104(3)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Cu(phen)_2(CH_3COO)].2H_2O(ClO_4)$ **(1)**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	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)
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 S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[Cu(phen)_2(CH_3COO)].2H_2O(ClO_4)$ **(1)**.

	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
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)

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136 Table S6. Torsion angles [°] for[Cu(phen)$_2$(CH_3COO)].2H_2O(ClO_4) **(1)**.

Cu-O(1)-C(11A)-O(2)	-1.0(4)
Cu-O(1)-C(11A)-C(12A)	178.4(3)
C(12)-N(1)-C(1)-C(2)	0.4(4)
Cu-N(1)-C(1)-C(2)	-178.8(2)
N(1)-C(1)-C(2)-C(3)	1.8(5)
C(1)-C(2)-C(3)-C(4)	-2.2(5)
C(2)-C(3)-C(4)-C(12)	0.5(4)
C(2)-C(3)-C(4)-C(5)	-177.0(3)
C(3)-C(4)-C(5)-C(6)	175.4(3)
C(12)-C(4)-C(5)-C(6)	-2.1(5)
C(4)-C(5)-C(6)-C(7)	0.5(5)
C(5)-C(6)-C(7)-C(8)	-176.5(3)
C(5)-C(6)-C(7)-C(11)	1.4(4)
C(11)-C(7)-C(8)-C(9)	-1.2(4)
C(6)-C(7)-C(8)-C(9)	176.7(3)
C(7)-C(8)-C(9)-C(10)	2.5(5)
C(11)-N(2)-C(10)-C(9)	-1.0(5)
Cu-N(2)-C(10)-C(9)	178.0(2)
C(8)-C(9)-C(10)-N(2)	-1.5(5)
C(10)-N(2)-C(11)-C(7)	2.4(4)
Cu-N(2)-C(11)-C(7)	-176.6(2)
C(10)-N(2)-C(11)-C(12)	-175.3(3)
Cu-N(2)-C(11)-C(12)	5.7(3)
C(8)-C(7)-C(11)-N(2)	-1.3(4)
C(6)-C(7)-C(11)-N(2)	-179.3(3)
C(8)-C(7)-C(11)-C(12)	176.3(3)
C(6)-C(7)-C(11)-C(12)	-1.7(4)
C(1)-N(1)-C(12)-C(4)	-2.2(4)
Cu-N(1)-C(12)-C(4)	177.2(2)
C(1)-N(1)-C(12)-C(11)	175.6(2)
Cu-N(1)-C(12)-C(11)	-5.0(3)

C(3)-C(4)-C(12)-N(1)	1.7(4)
C(5)-C(4)-C(12)-N(1)	179.4(3)
C(3)-C(4)-C(12)-C(11)	-176.0(3)
C(5)-C(4)-C(12)-C(11)	1.7(4)
N(2)-C(11)-C(12)-N(1)	0.0(4)
C(7)-C(11)-C(12)-N(1)	-177.7(3)
N(2)-C(11)-C(12)-C(4)	177.9(3)
C(7)-C(11)-C(12)-C(4)	0.2(4)
C(24)-N(3)-C(13)-C(14)	0.7(4)
Cu-N(3)-C(13)-C(14)	179.7(2)
N(3)-C(13)-C(14)-C(15)	-0.2(5)
C(13)-C(14)-C(15)-C(16)	-0.4(4)
C(14)-C(15)-C(16)-C(24)	0.5(4)
C(14)-C(15)-C(16)-C(17)	-178.4(3)
C(24)-C(16)-C(17)-C(18)	0.7(4)
C(15)-C(16)-C(17)-C(18)	179.5(3)
C(16)-C(17)-C(18)-C(19)	0.2(5)
C(17)-C(18)-C(19)-C(23)	-0.9(4)
C(17)-C(18)-C(19)-C(20)	-179.0(3)
C(23)-C(19)-C(20)-C(21)	-0.5(4)
C(18)-C(19)-C(20)-C(21)	177.7(3)
C(19)-C(20)-C(21)-C(22)	0.1(4)
C(23)-N(4)-C(22)-C(21)	-1.2(5)
Cu-N(4)-C(22)-C(21)	179.8(2)
C(20)-C(21)-C(22)-N(4)	0.7(5)
C(22)-N(4)-C(23)-C(19)	0.8(4)
Cu-N(4)-C(23)-C(19)	180.0(2)
C(22)-N(4)-C(23)-C(24)	-178.2(3)
Cu-N(4)-C(23)-C(24)	0.9(3)
C(20)-C(19)-C(23)-N(4)	0.0(4)
C(18)-C(19)-C(23)-N(4)	-178.3(3)
C(20)-C(19)-C(23)-C(24)	179.0(3)
C(18)-C(19)-C(23)-C(24)	0.7(4)
C(13)-N(3)-C(24)-C(16)	-0.6(4)
Cu-N(3)-C(24)-C(16)	-179.8(2)
C(13)-N(3)-C(24)-C(23)	179.1(2)

Cu-N(3)-C(24)-C(23)	0.0(3)
C(15)-C(16)-C(24)-N(3)	0.1(4)
C(17)-C(16)-C(24)-N(3)	179.0(3)
C(15)-C(16)-C(24)-C(23)	-179.7(3)
C(17)-C(16)-C(24)-C(23)	-0.8(4)
N(4)-C(23)-C(24)-N(3)	-0.6(4)
C(19)-C(23)-C(24)-N(3)	-179.7(3)
N(4)-C(23)-C(24)-C(16)	179.2(3)
C(19)-C(23)-C(24)-C(16)	0.1(4)

Symmetry transformations used to generate equivalent atoms:

Table S7. Hydrogen bonds for $[Cu(phen)_2(CH_3COO)].2H_2O(ClO_4)$ **(1)** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(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)

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

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152 Table S8. Crystal data and structure refinement for $Cu(bipy)_2(CH_3COO)](ClO_4)H_2O$ **(2)**.

Identification code	shelxl	
Empirical formula	C22 H21 Cl Cu N4 O7	
Formula weight	552.42	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.2822(4) Å	α= 78.729(2)°.
	b = 9.4748(4) Å	β= 82.881(2)°.
	c = 14.7992(6) Å	γ = 85.092(2)°.
Volume	1127.90(9) $Å^3$	
Z	2	
Density (calculated)	1.627 Mg/m^3	
Absorption coefficient	1.140 mm^{-1}	
F(000)	566	
Crystal size	0.500 x 0.240 x 0.200 mm^3	
Theta range for data collection	2.20 to 30.58°.	
Index ranges	-11<=h<=11, -13<=k<=13, -21<=l<=21	
Reflections collected	58024	
Independent reflections	6914 [R(int) = 0.0421]	
Completeness to theta = 25.50°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6323	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6914 / 68 / 339	
Goodness-of-fit on F^2	1.083	

Final R indices [I>2sigma(I)]	R1 = 0.0357, wR2 = 0.0776
R indices (all data)	R1 = 0.0451, wR2 = 0.0814
Largest diff. peak and hole	0.563 and -0.384 e.Å^{-3}

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) 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.

	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)
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)

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179 Table S10. Bond lengths [Å] and angles [°] for $Cu(bipy)_2(CH_3COO)](ClO_4)H_2O$ **(2)**.

Cu-N(4)	1.9750(14)
Cu-O(1)	1.9896(12)
Cu-N(1)	1.9899(13)
Cu-N(3)	2.0422(14)
Cu-N(2)	2.1786(14)
Cl(1)-O(13)	1.4341(11)
Cl(1)-O(14)	1.4343(11)
Cl(1)-O(13A)	1.4378(12)
Cl(1)-O(11A)	1.4367(12)
Cl(1)-O(14A)	1.4377(12)
Cl(1)-O(11)	1.4404(11)
Cl(1)-O(12A)	1.4382(12)
Cl(1)-O(12)	1.4416(11)
O(1)-C(11A)	1.275(2)
O(2)-C(11A)	1.244(2)
O(1W)-H(1W1)	0.88(3)
O(1W)-H(1W2)	0.87(3)
N(1)-C(1)	1.341(2)
N(1)-C(5)	1.354(2)
N(2)-C(10)	1.342(2)
N(2)-C(6)	1.347(2)
N(3)-C(11)	1.343(2)
N(3)-C(15)	1.353(2)
N(4)-C(20)	1.341(2)
N(4)-C(16)	1.345(2)
C(1)-C(2)	1.383(2)
C(1)-H(1A)	0.9500
C(2)-C(3)	1.387(2)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.385(2)

C(3)-H(3A)	0.9500
C(4)-C(5)	1.391(2)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.487(2)
C(6)-C(7)	1.390(2)
C(7)-C(8)	1.390(2)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.379(3)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.389(2)
C(9)-H(9A)	0.9500
C(10)-H(10A)	0.9500
C(11)-C(12)	1.383(2)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.385(3)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.389(2)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.389(2)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.479(2)
C(16)-C(17)	1.389(2)
C(17)-C(18)	1.388(2)
C(17)-H(17A)	0.9500
C(18)-C(19)	1.385(3)
C(18)-H(18A)	0.9500
C(19)-C(20)	1.384(2)
C(19)-H(19A)	0.9500
C(20)-H(20A)	0.9500
C(11A)-C(12A)	1.502(3)
C(12A)-H(12B)	0.9800
C(12A)-H(12C)	0.9800
C(12A)-H(12D)	0.9800
N(4)-Cu-O(1)	94.13(5)
N(4)-Cu-N(1)	174.48(6)
O(1)-Cu-N(1)	89.80(5)

N(4)-Cu-N(3)	81.11(5)
O(1)-Cu-N(3)	149.08(5)

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N(1)-Cu-N(3)	97.46(5)
N(4)-Cu-N(2)	96.31(5)
O(1)-Cu-N(2)	100.18(5)
N(1)-Cu-N(2)	79.16(5)
N(3)-Cu-N(2)	110.70(5)
O(13)-Cl(1)-O(14)	110.03(7)
O(13)-Cl(1)-O(13A)	28.3(5)
O(14)-Cl(1)-O(13A)	82.3(5)
O(13)-Cl(1)-O(11A)	98.3(5)
O(14)-Cl(1)-O(11A)	121.6(5)
O(13A)-Cl(1)-O(11A)	109.54(9)
O(13)-Cl(1)-O(14A)	137.1(5)
O(14)-Cl(1)-O(14A)	27.2(5)
O(13A)-Cl(1)-O(14A)	109.44(9)
O(11A)-Cl(1)-O(14A)	109.55(9)
O(13)-Cl(1)-O(11)	109.48(7)
O(14)-Cl(1)-O(11)	109.59(7)
O(13A)-Cl(1)-O(11)	115.8(5)
O(11A)-Cl(1)-O(11)	13.4(5)
O(14A)-Cl(1)-O(11)	96.2(5)
O(13)-Cl(1)-O(12A)	90.1(5)
O(14)-Cl(1)-O(12A)	119.9(5)
O(13A)-Cl(1)-O(12A)	109.40(9)
O(11A)-Cl(1)-O(12A)	109.49(9)
O(14A)-Cl(1)-O(12A)	109.41(9)
O(11)-Cl(1)-O(12A)	115.7(6)
O(13)-Cl(1)-O(12)	109.43(7)
O(14)-Cl(1)-O(12)	109.40(7)
O(13A)-Cl(1)-O(12)	126.4(5)
O(11A)-Cl(1)-O(12)	107.2(6)
O(14A)-Cl(1)-O(12)	93.0(5)
O(11)-Cl(1)-O(12)	108.89(7)
O(12A)-Cl(1)-O(12)	19.4(5)

C(11A)-O(1)-Cu	108.47(10)
H(1W1)-O(1W)-H(1W2)	104(3)
C(1)-N(1)-C(5)	119.38(14)
C(1)-N(1)-Cu	122.99(11)
C(5)-N(1)-Cu	117.58(11)
C(10)-N(2)-C(6)	118.56(14)
C(10)-N(2)-Cu	129.68(12)
C(6)-N(2)-Cu	111.73(10)
C(11)-N(3)-C(15)	118.58(14)
C(11)-N(3)-Cu	128.08(11)
C(15)-N(3)-Cu	113.33(10)
C(20)-N(4)-C(16)	119.89(14)
C(20)-N(4)-Cu	124.14(11)
C(16)-N(4)-Cu	115.65(11)
N(1)-C(1)-C(2)	122.50(15)
N(1)-C(1)-H(1A)	118.7
C(2)-C(1)-H(1A)	118.7
C(1)-C(2)-C(3)	118.26(16)
C(1)-C(2)-H(2A)	120.9
C(3)-C(2)-H(2A)	120.9
C(4)-C(3)-C(2)	119.69(16)
C(4)-C(3)-H(3A)	120.2
C(2)-C(3)-H(3A)	120.2
C(3)-C(4)-C(5)	119.12(15)
C(3)-C(4)-H(4A)	120.4
C(5)-C(4)-H(4A)	120.4
N(1)-C(5)-C(4)	120.99(15)
N(1)-C(5)-C(6)	115.88(14)
C(4)-C(5)-C(6)	123.14(14)
N(2)-C(6)-C(7)	121.88(15)
N(2)-C(6)-C(5)	115.60(14)
C(7)-C(6)-C(5)	122.52(15)
C(8)-C(7)-C(6)	118.81(16)
C(8)-C(7)-H(7A)	120.6
C(6)-C(7)-H(7A)	120.6
C(9)-C(8)-C(7)	119.55(16)

C(9)-C(8)-H(8A)	120.2
C(7)-C(8)-H(8A)	120.2
C(8)-C(9)-C(10)	118.28(16)
C(8)-C(9)-H(9A)	120.9
C(10)-C(9)-H(9A)	120.9
N(2)-C(10)-C(9)	122.90(16)
N(2)-C(10)-H(10A)	118.6
C(9)-C(10)-H(10A)	118.6
N(3)-C(11)-C(12)	122.60(16)
N(3)-C(11)-H(11A)	118.7
C(12)-C(11)-H(11A)	118.7
C(11)-C(12)-C(13)	118.76(16)
C(11)-C(12)-H(12A)	120.6
C(13)-C(12)-H(12A)	120.6
C(12)-C(13)-C(14)	119.31(15)
C(12)-C(13)-H(13A)	120.3
C(14)-C(13)-H(13A)	120.3
C(15)-C(14)-C(13)	118.80(16)
C(15)-C(14)-H(14A)	120.6
C(13)-C(14)-H(14A)	120.6
N(3)-C(15)-C(14)	121.94(15)
N(3)-C(15)-C(16)	114.66(13)
C(14)-C(15)-C(16)	123.40(14)
N(4)-C(16)-C(17)	121.39(15)
N(4)-C(16)-C(15)	114.87(14)
C(17)-C(16)-C(15)	123.74(14)
C(18)-C(17)-C(16)	118.68(15)
C(18)-C(17)-H(17A)	120.7
C(16)-C(17)-H(17A)	120.7
C(19)-C(18)-C(17)	119.57(16)
C(19)-C(18)-H(18A)	120.2
C(17)-C(18)-H(18A)	120.2
C(20)-C(19)-C(18)	118.79(16)
C(20)-C(19)-H(19A)	120.6
C(18)-C(19)-H(19A)	120.6
N(4)-C(20)-C(19)	121.67(16)

N(4)-C(20)-H(20A)	119.2
C(19)-C(20)-H(20A)	119.2
O(2)-C(11A)-O(1)	122.79(16)
O(2)-C(11A)-C(12A)	120.44(16)
O(1)-C(11A)-C(12A)	116.76(15)
C(11A)-C(12A)-H(12B)	109.5
C(11A)-C(12A)-H(12C)	109.5
H(12B)-C(12A)-H(12C)	109.5
C(11A)-C(12A)-H(12D)	109.5
H(12B)-C(12A)-H(12D)	109.5
H(12C)-C(12A)-H(12D)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S11. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Cu(bipy)_2(CH_3COO)](ClO_4)H_2O$ **(2)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	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)
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 S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $Cu(bipy)_2(CH_3COO)](ClO_4)H_2O$ **(2)**.

	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
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

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241 Table S13. Torsion angles [°] for $Cu(bipy)_2(CH_3COO)](ClO_4)H_2O$ **(2)**.

N(4)-Cu-O(1)-C(11A)	-80.21(11)
N(1)-Cu-O(1)-C(11A)	103.66(11)
N(3)-Cu-O(1)-C(11A)	-0.64(17)
N(2)-Cu-O(1)-C(11A)	-177.38(11)
N(4)-Cu-N(1)-C(1)	146.8(5)
O(1)-Cu-N(1)-C(1)	-77.67(13)
N(3)-Cu-N(1)-C(1)	72.18(13)
N(2)-Cu-N(1)-C(1)	-178.07(14)
N(4)-Cu-N(1)-C(5)	-35.8(6)
O(1)-Cu-N(1)-C(5)	99.69(12)
N(3)-Cu-N(1)-C(5)	-110.45(12)
N(2)-Cu-N(1)-C(5)	-0.71(11)
N(4)-Cu-N(2)-C(10)	-3.57(15)
O(1)-Cu-N(2)-C(10)	91.79(14)
N(1)-Cu-N(2)-C(10)	179.62(15)
N(3)-Cu-N(2)-C(10)	-86.42(15)
N(4)-Cu-N(2)-C(6)	178.41(11)
O(1)-Cu-N(2)-C(6)	-86.23(11)
N(1)-Cu-N(2)-C(6)	1.60(11)
N(3)-Cu-N(2)-C(6)	95.56(11)
N(4)-Cu-N(3)-C(11)	177.52(15)
O(1)-Cu-N(3)-C(11)	94.37(16)
N(1)-Cu-N(3)-C(11)	-7.87(14)
N(2)-Cu-N(3)-C(11)	-89.06(14)
N(4)-Cu-N(3)-C(15)	-1.45(11)
O(1)-Cu-N(3)-C(15)	-84.60(14)
N(1)-Cu-N(3)-C(15)	173.16(11)
N(2)-Cu-N(3)-C(15)	91.97(11)
O(1)-Cu-N(4)-C(20)	-32.56(14)
N(1)-Cu-N(4)-C(20)	102.8(6)

N(3)-Cu-N(4)-C(20)	178.20(14)
N(2)-Cu-N(4)-C(20)	68.17(14)
O(1)-Cu-N(4)-C(16)	153.98(11)
N(1)-Cu-N(4)-C(16)	-70.7(6)
N(3)-Cu-N(4)-C(16)	4.74(11)
N(2)-Cu-N(4)-C(16)	-105.29(12)
C(5)-N(1)-C(1)-C(2)	2.3(2)
Cu-N(1)-C(1)-C(2)	179.64(13)
N(1)-C(1)-C(2)-C(3)	-0.3(3)
C(1)-C(2)-C(3)-C(4)	-1.5(3)
C(2)-C(3)-C(4)-C(5)	1.4(3)
C(1)-N(1)-C(5)-C(4)	-2.5(2)
Cu-N(1)-C(5)-C(4)	-179.92(12)
C(1)-N(1)-C(5)-C(6)	177.23(14)
Cu-N(1)-C(5)-C(6)	-0.23(18)
C(3)-C(4)-C(5)-N(1)	0.6(2)
C(3)-C(4)-C(5)-C(6)	-179.03(15)
C(10)-N(2)-C(6)-C(7)	-0.7(2)
Cu-N(2)-C(6)-C(7)	177.53(13)
C(10)-N(2)-C(6)-C(5)	179.57(14)
Cu-N(2)-C(6)-C(5)	-2.16(17)
N(1)-C(5)-C(6)-N(2)	1.7(2)
C(4)-C(5)-C(6)-N(2)	-178.62(15)
N(1)-C(5)-C(6)-C(7)	-177.99(15)
C(4)-C(5)-C(6)-C(7)	1.7(2)
N(2)-C(6)-C(7)-C(8)	1.5(3)
C(5)-C(6)-C(7)-C(8)	-178.83(16)
C(6)-C(7)-C(8)-C(9)	-1.2(3)
C(7)-C(8)-C(9)-C(10)	0.1(3)
C(6)-N(2)-C(10)-C(9)	-0.4(2)
Cu-N(2)-C(10)-C(9)	-178.28(12)
C(8)-C(9)-C(10)-N(2)	0.7(3)
C(15)-N(3)-C(11)-C(12)	0.5(2)
Cu-N(3)-C(11)-C(12)	-178.40(12)
N(3)-C(11)-C(12)-C(13)	-0.5(3)
C(11)-C(12)-C(13)-C(14)	0.2(3)

C(12)-C(13)-C(14)-C(15)	-0.1(3)
C(11)-N(3)-C(15)-C(14)	-0.4(2)
Cu-N(3)-C(15)-C(14)	178.70(12)
C(11)-N(3)-C(15)-C(16)	179.18(14)
Cu-N(3)-C(15)-C(16)	-1.74(16)
C(13)-C(14)-C(15)-N(3)	0.2(2)
C(13)-C(14)-C(15)-C(16)	-179.35(15)
C(20)-N(4)-C(16)-C(17)	-1.4(2)
Cu-N(4)-C(16)-C(17)	172.32(12)
C(20)-N(4)-C(16)-C(15)	179.25(14)
Cu-N(4)-C(16)-C(15)	-6.99(17)
N(3)-C(15)-C(16)-N(4)	5.7(2)
C(14)-C(15)-C(16)-N(4)	-174.74(15)
N(3)-C(15)-C(16)-C(17)	-173.58(15)
C(14)-C(15)-C(16)-C(17)	6.0(2)
N(4)-C(16)-C(17)-C(18)	0.3(2)
C(15)-C(16)-C(17)-C(18)	179.59(15)
C(16)-C(17)-C(18)-C(19)	0.9(3)
C(17)-C(18)-C(19)-C(20)	-1.0(3)
C(16)-N(4)-C(20)-C(19)	1.3(2)
Cu-N(4)-C(20)-C(19)	-171.91(13)
C(18)-C(19)-C(20)-N(4)	0.0(3)
Cu-O(1)-C(11A)-O(2)	2.4(2)
Cu-O(1)-C(11A)-C(12A)	-176.70(14)

Symmetry transformations used to generate equivalent atoms:

Table S14. Hydrogen bonds for $Cu(bipy)_2(CH_3COO)](ClO_4)H_2O$ **(2)** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(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)

Symmetry transformations used to generate equivalent atoms: