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Supporting information for article:

A new photoluminescent coordination polymer constructed with an N-donor ligand with extended coordination capabilities derived from quinoline and pyridine

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Supplementary files:

TGA

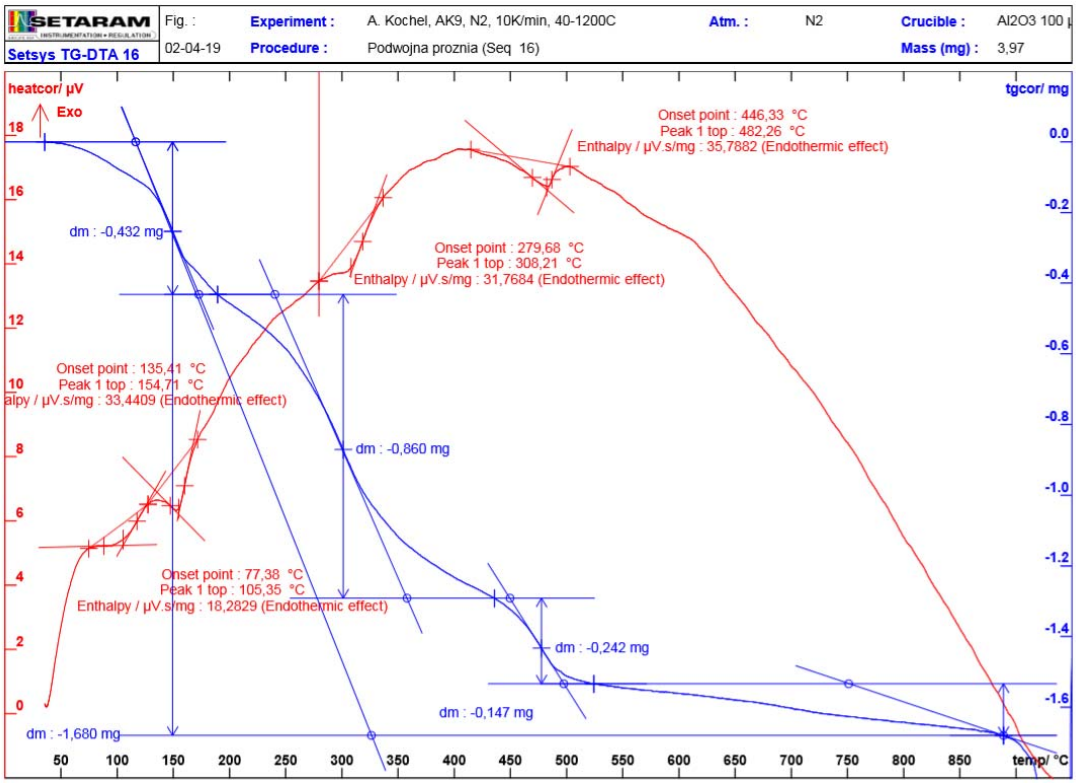

Figure S1 TGA diagram for **1**.

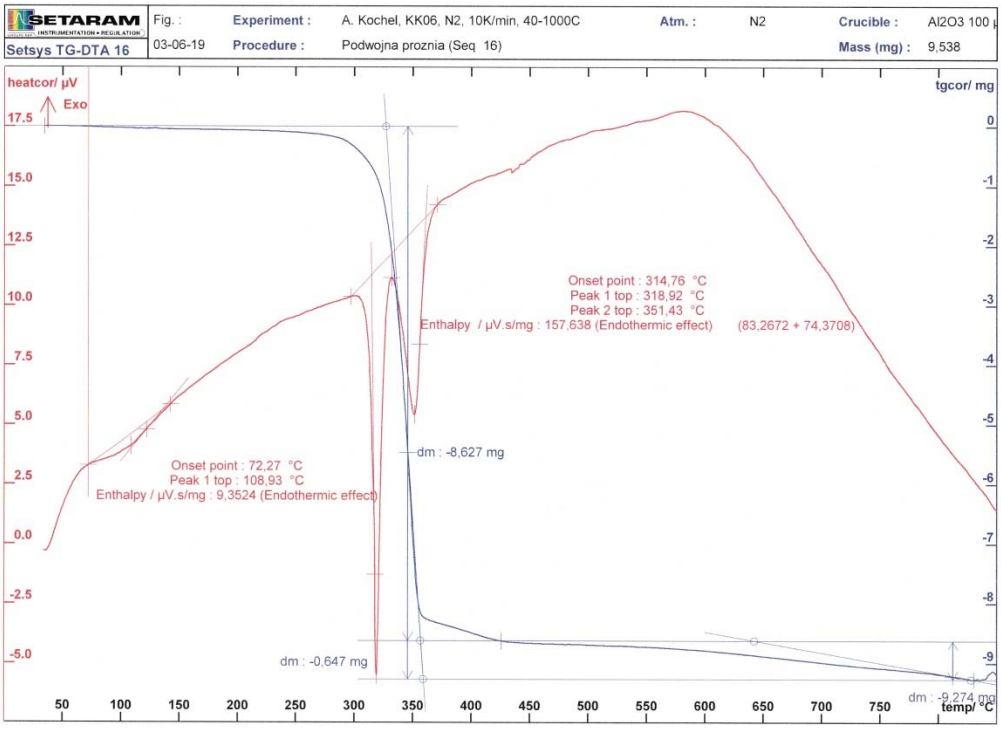

Figure S2 TGA diagram for the organic ligand.

NMR spectroscopy

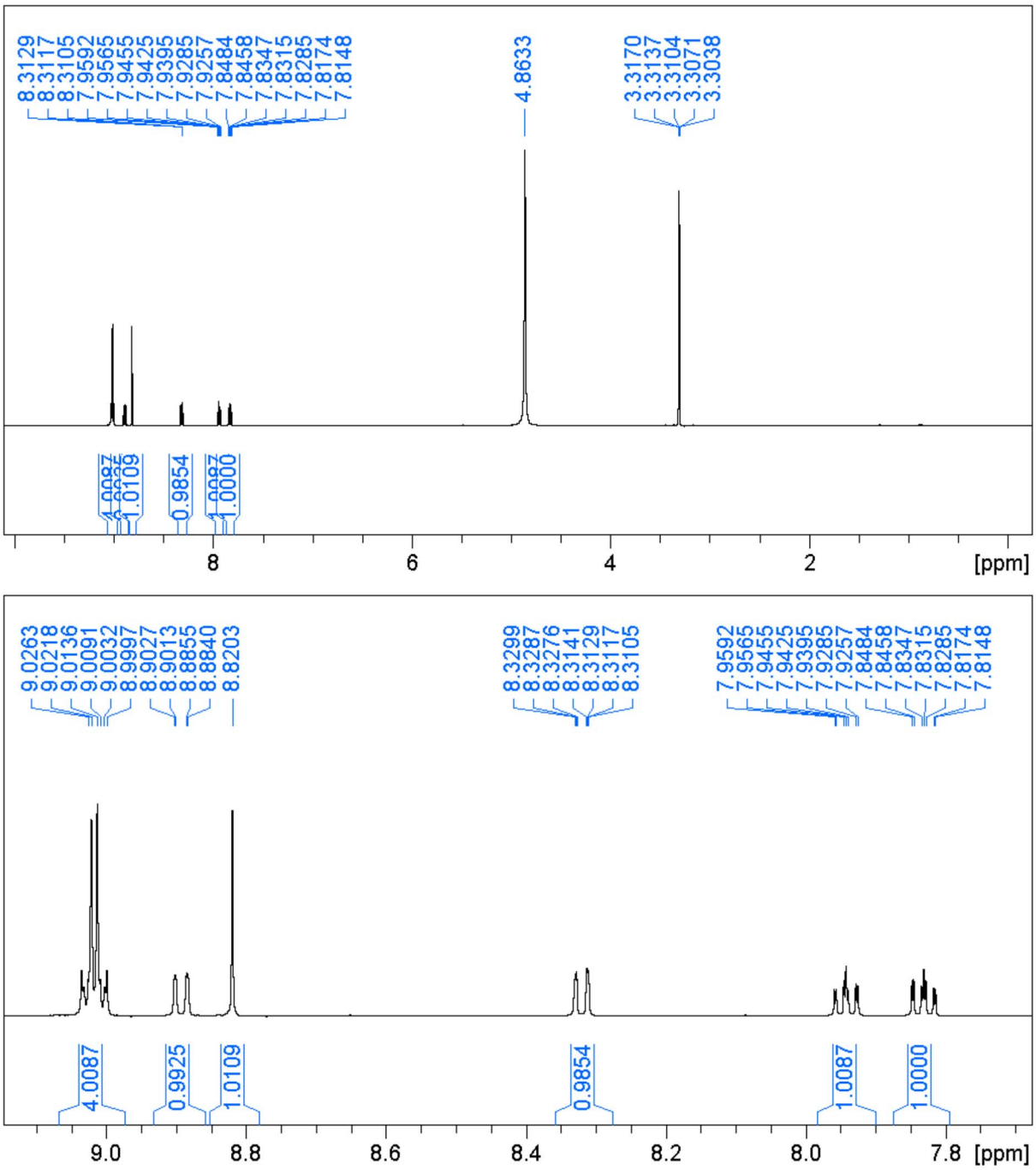

Figure S3 ^{1}H NMR spectrum of the ligand 2-pyridin-4-yl-quinoline-4-carboxylic acid (500 MHz, methanol-d_4, 300 K).

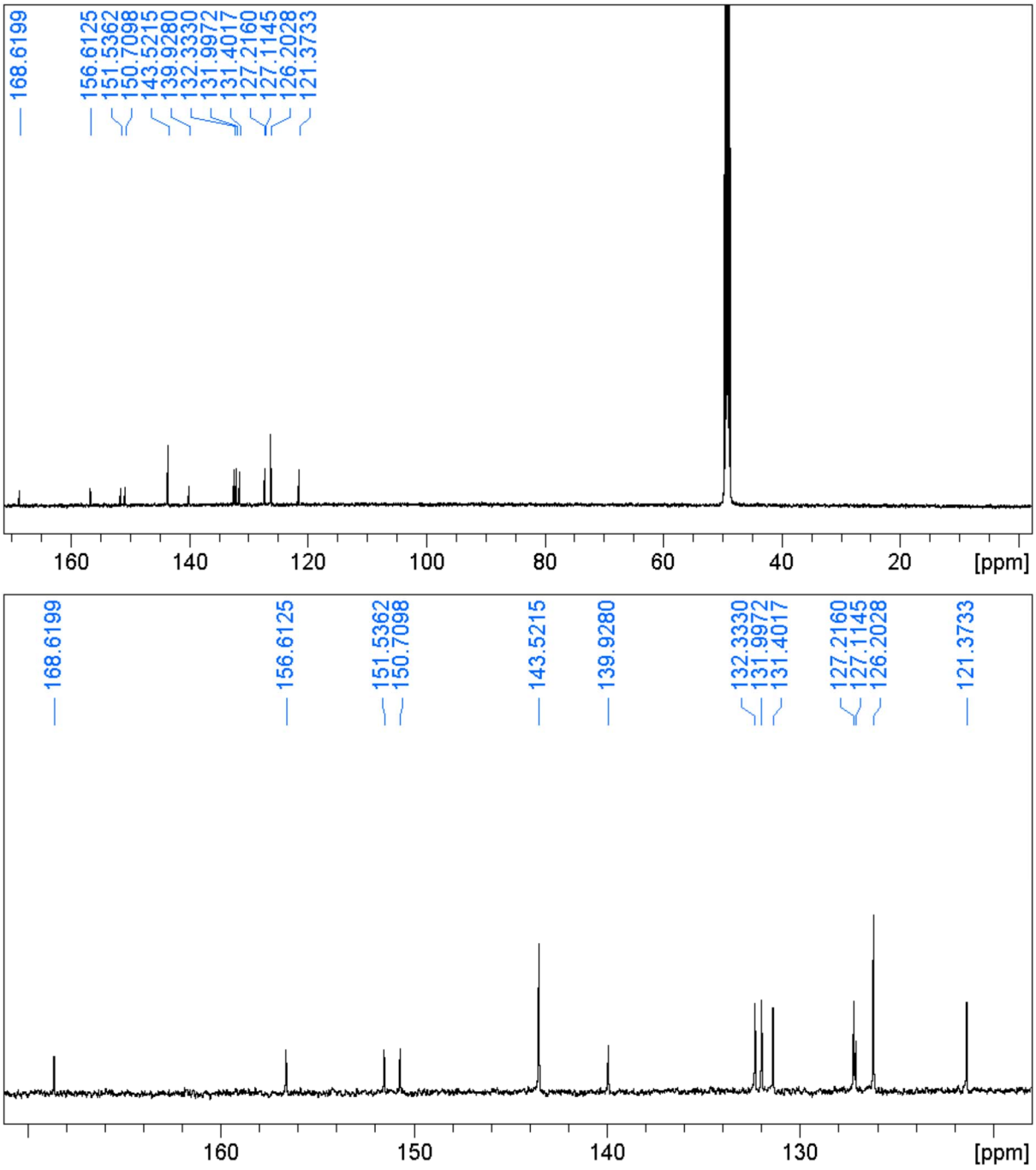

Figure S4 ^{13}C NMR spectrum for the ligand 2-pyridin-4-yl-quinoline-4-carboxylic acid (125 MHz, methanol-d_4, 300 K)

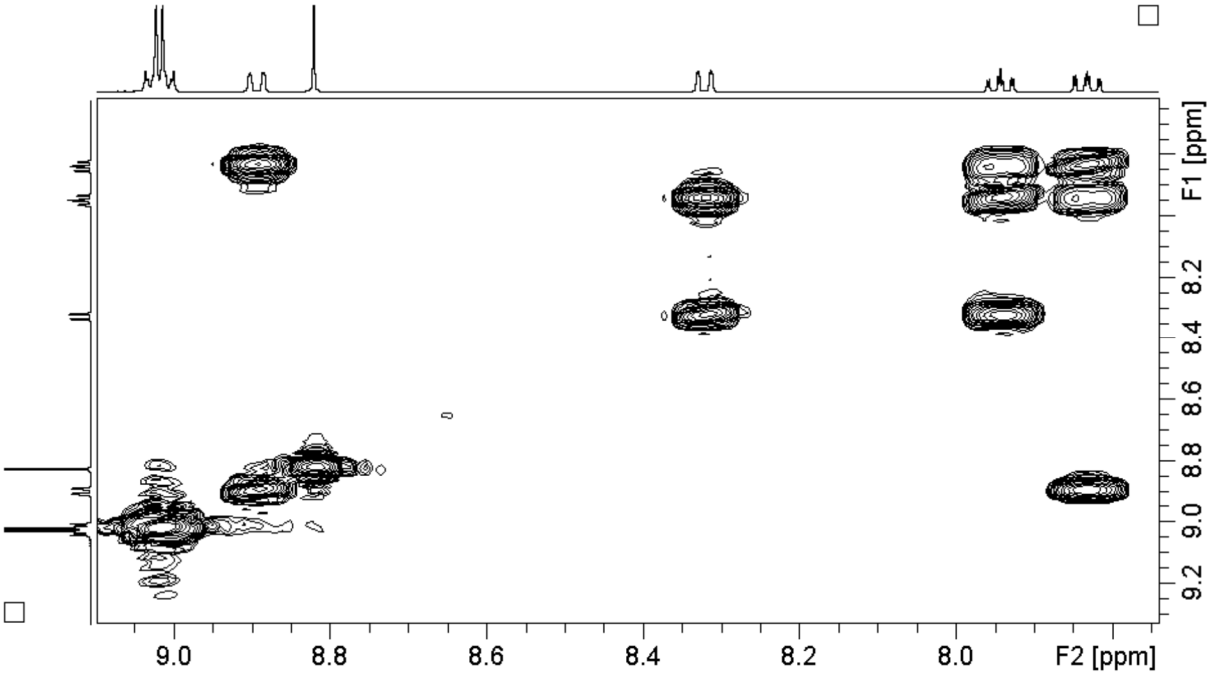

Figure S5 ^{1}H-^{1}H COSY spectrum of compound 2-pyridin-4-yl-quinoline-4-carboxylic acid (fragment).

Tables S1-S7

Table S1. Crystal data and structure refinement for $[Cu(C_{15}H_{20}N_2O_4)_2(H_2O)_2]\cdot 2H_2O$.

Crystal data

$[Cu(C_{15}H_{20}N_2O_4)_2(H_2O)_2]\cdot 2H_2O$	$F(000) = 327$
$M_r = 634.09$	$D_x = 1.503$ Mg m^{-3}
Triclinic, P-1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

a = 8.647(3) Å	Cell parameters from 3142 reflections
b = 8.819(3) Å	θ = 2.145 to 28.764
c = 10.125(2) Å α = 70.58(2)°.	μ = 0.840 mm^{-1}
β = 79.61(3)° γ = 75.26(3)°	T = 100 K
V = 700.3(4) Å^3	Block, blue/green
Z = 1	0.20 × 0.18 × 0.15 mm

Data collection

XCalibur Ruby area detector diffractometer	2397 reflections with $I > 2\sigma(I)$
phi and ω scans	R_{int} = 0.053
Absorption correction: empirical (using intensity measurements) (Rigaku; CrysAlis 2017)	θ_{max} = 28.764°, θ_{min} = 2.145°
T_{min} = 0.867, T_{max} = 0.940	h = −10→11
4791 measured reflections	k = −11→10
	l = −13→11
3141 independent reflections	

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)]$ = 0.040	H-atom parameters constrained
	$w = 2/[\sigma^2(F_o^2) + (0.0448P)^2]$
$wR(F^2)$ = 0.098	where $P = (F_o^2 + 2F_c^2)/3$
S = 0.997	$(\Delta/\sigma)_{max} < 0.001$
3141 reflections	$\Delta\rho_{max}$ = 0.918 e Å^{-3}
196 parameters	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for $[Cu(C_{15}H_{20}N_2O_4)_2(H_2O)_2]\cdot 2H_2O$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	5000	10000	0	16(1)
O(1)	3010(2)	9513(2)	1250(2)	18(1)
O(2)	2854(3)	7167(3)	924(2)	32(1)
O(1W)	2261(3)	4050(2)	1788(2)	32(1)
O(2W)	5056(2)	8188(2)	-1296(2)	23(1)
N(1)	33(3)	6870(3)	5775(2)	16(1)
N(2)	3666(3)	1777(3)	8565(2)	17(1)
C(1)	1575(3)	7750(3)	3026(3)	16(1)
C(2)	135(3)	8792(3)	3388(3)	15(1)
C(3)	-599(3)	10275(3)	2441(3)	19(1)
C(4)	-1986(4)	11217(4)	2876(3)	22(1)
C(5)	-2697(4)	10718(4)	4268(3)	22(1)
C(6)	-2034(3)	9299(3)	5214(3)	18(1)
C(7)	-592(3)	8285(3)	4800(3)	16(1)
C(8)	1395(3)	5940(3)	5397(3)	16(1)
C(9)	2181(3)	6343(3)	4019(3)	18(1)
C(10)	2543(3)	8177(4)	1587(3)	18(1)
C(11)	2129(3)	4456(3)	6501(3)	16(1)
C(12)	3270(3)	3172(3)	6151(3)	18(1)
C(13)	3997(3)	1878(3)	7199(3)	18(1)
C(14)	2525(3)	2975(3)	8913(3)	19(1)
C(15)	1750(3)	4312(3)	7933(3)	19(1)

Table S3. Bond lengths [Å] and angles [°] for $[Cu(C_{15}H_{20}N_2O_4)_2(H_2O)_2]\cdot 2H_2O$.

Cu(1)-O(1)^{i}	1.994(2)	O(1)-Cu(1)-N(2)^{iii}	90.47(9)
Cu(1)-O(1)	1.994(2)	N(2)#2-Cu(1)-N(2)^{iii}	180.0
Cu(1)-N(2)^{ii}	2.017(2)	O(1)#1-Cu(1)-O(2W)	84.76(8)
Cu(1)-N(2)^{iii}	2.017(2)	O(1)-Cu(1)-O(2W)	95.24(8)
Cu(1)-O(2W)	2.368(2)	N(2)#2-Cu(1)-O(2W)	92.18(9)
Cu(1)-O(2W)^{i}	2.368(2)	N(2)#3-Cu(1)-O(2W)	87.82(9)
O(1)-C(10)	1.262(3)	O(1)#1-Cu(1)-O(2W)^{i}	95.24(8)
O(2)-C(10)	1.235(3)	O(1)-Cu(1)-O(2W)^{i}	84.76(8)
O(1W)-H(1WA)	0.85	N(2)#2-Cu(1)-O(2W)^{i}	87.82(9)
O(1W)-H(1WB)	0.85	N(2)#3-Cu(1)-O(2W)^{i}	92.18(9)
O(2W)-H(2WA)	0.85	O(2W)-Cu(1)-O(2W)^{i}	180.0
O(2W)-H(2WB)	0.85	C(10)-O(1)-Cu(1)	125.15(19)
N(1)-C(8)	1.327(4)	H(1WA)-O(1W)-H(1WB)	104.1
N(1)-C(7)	1.362(3)	Cu(1)-O(2W)-H(2WA)	91.1
N(2)-C(13)	1.339(4)	Cu(1)-O(2W)-H(2WB)	128.4
N(2)-C(14)	1.344(4)	H(2WA)-O(2W)-H(2WB)	108.3
C(1)-C(9)	1.362(4)	C(8)-N(1)-C(7)	118.3(2)
C(1)-C(2)	1.417(4)	C(13)-N(2)-C(14)	117.5(2)
C(1)-C(10)	1.524(4)	C(13)-N(2)-Cu(1)^{iv}	120.15(19)
C(2)-C(3)	1.413(4)	C(14)-N(2)-Cu(1)^{iv}	122.07(19)
C(2)-C(7)	1.426(4)	C(9)-C(1)-C(2)	119.3(3)
C(3)-C(4)	1.367(4)	C(9)-C(1)-C(10)	117.8(3)
C(3)-H(3)	0.95	C(2)-C(1)-C(10)	122.9(2)
C(4)-C(5)	1.403(4)	C(3)-C(2)-C(1)	123.9(3)
C(4)-H(4)	0.95	C(3)-C(2)-C(7)	119.2(3)
C(5)-C(6)	1.359(4)	C(1)-C(2)-C(7)	116.8(2)
C(5)-H(5)	0.95	C(4)-C(3)-C(2)	120.3(3)
C(6)-C(7)	1.422(4)	C(4)-C(3)-H(3)	119.8
C(6)-H(6)	0.95	C(2)-C(3)-H(3)	119.8
C(8)-C(9)	1.410(4)	C(3)-C(4)-C(5)	120.3(3)
C(8)-C(11)	1.492(4)	C(3)-C(4)-H(4)	119.8
C(9)-H(9)	0.95	C(5)-C(4)-H(4)	119.8
C(11)-C(15)	1.397(4)	C(6)-C(5)-C(4)	121.3(3)
C(11)-C(12)	1.398(4)	C(6)-C(5)-H(5)	119.3
C(12)-C(13)	1.376(4)	C(4)-C(5)-H(5)	119.3
C(12)-H(12)	0.95	C(5)-C(6)-C(7)	120.0(3)
C(13)-H(13)	0.95	C(5)-C(6)-H(6)	120.0
C(14)-C(15)	1.372(4)	C(7)-C(6)-H(6)	120.0
C(14)-H(14)	0.95	N(1)-C(7)-C(6)	118.3(2)
C(15)-H(15)	0.95	N(1)-C(7)-C(2)	122.9(3)
O(1)#1-Cu(1)-O(1)	180.00(7)	C(6)-C(7)-C(2)	118.8(2)
O(1)#1-Cu(1)-N(2)^{ii}	90.47(9)	N(1)-C(8)-C(9)	122.3(2)

O(1)-Cu(1)-N(2)^{ii}	89.53(9)	N(1)-C(8)-C(11)	117.8(2)
O(1)#1-Cu(1)-N(2)^{iii}	89.53(9)	C(9)-C(8)-C(11)	119.8(3)
C(9)-H(9)	0.95	C(5)-C(4)-H(4)	119.8
C(1)-C(9)-C(8)	120.3(3)	N(2)-C(13)-C(12)	123.0(3)
C(1)-C(9)-H(9)	119.8	N(2)-C(13)-H(13)	118.5
C(8)-C(9)-H(9)	119.8	C(12)-C(13)-H(13)	118.5
O(2)-C(10)-O(1)	127.6(3)	N(2)-C(14)-C(15)	123.0(3)
O(1)-C(10)-C(1)	114.5(3)	C(15)-C(14)-H(14)	118.5
C(15)-C(11)-C(12)	116.9(3)	C(14)-C(15)-C(11)	119.8(3)
C(15)-C(11)-C(8)	121.5(3)	C(14)-C(15)-H(15)	120.1
C(12)-C(11)-C(8)	121.6(3)	C(11)-C(15)-H(15)	120.1
C(13)-C(12)-C(11)	119.7(3)		
C(13)-C(12)-H(12)	120.2		
C(11)-C(12)-H(12)	120.2		

Symmetry codes: (i) -x+1,-y+2,-z: (ii) -x+1,-y+1,-z+1: (iii) x,y+1,z-1: (iv) x,y-1,z+1

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Cu(C_{15}H_{20}N_2O_4)_2(H_2O)_2]\cdot 2H_2O$. The anisotropicdisplacement 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(1)	16(1)	14(1)	11(1)	4(1)	1(1)	-1(1)
O(1)	18(1)	13(1)	17(1)	1(1)	2(1)	-3(1)
O(2)	47(2)	27(1)	24(1)	-11(1)	14(1)	-18(1)
O(1W)	35(1)	22(1)	31(1)	-7(1)	15(1)	-8(1)
O(2W)	22(1)	22(1)	20(1)	-2(1)	3(1)	-4(1)
N(1)	16(1)	15(1)	14(1)	-1(1)	-2(1)	-2(1)
N(2)	16(1)	16(1)	12(1)	-1(1)	1(1)	-1(1)
C(1)	17(2)	16(2)	12(1)	-2(1)	-2(1)	-5(1)
C(2)	16(2)	15(1)	14(1)	-1(1)	-2(1)	-5(1)
C(3)	21(2)	19(2)	15(1)	0(1)	-3(1)	-3(1)
C(4)	23(2)	17(2)	24(2)	-1(1)	-9(1)	-1(1)
C(5)	17(2)	20(2)	27(2)	-8(1)	-3(1)	1(1)
C(6)	17(2)	18(2)	17(2)	-4(1)	1(1)	-3(1)
C(7)	17(2)	14(1)	14(1)	-3(1)	-1(1)	-2(1)
C(8)	19(2)	14(1)	12(1)	0(1)	0(1)	-6(1)
C(9)	18(2)	15(2)	15(1)	-2(1)	0(1)	0(1)
C(10)	16(2)	18(2)	14(1)	0(1)	-2(1)	0(1)
C(11)	18(2)	16(2)	13(1)	0(1)	-4(1)	-5(1)
C(12)	21(2)	18(2)	11(1)	-2(1)	1(1)	-3(1)
C(13)	20(2)	16(2)	14(1)	-2(1)	1(1)	-1(1)
C(14)	22(2)	20(2)	12(1)	-2(1)	1(1)	-3(1)
C(15)	20(2)	18(2)	14(1)	-3(1)	1(1)	0(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for $[Cu(C_{15}H_{20}N_2O_4)_2(H_2O)_2]\cdot 2H_2O$.

	x	y	z	U(eq)
H(1WA)	2392	5016	1650	47
H(1WB)	1539	3869	2478	47
H(2WA)	4442	7668	-646	35
H(2WB)	5851	7493	-1521	35
H(3)	-126	10620	1497	23
H(4)	-2472	12213	2234	27
H(5)	-3660	11386	4555	26
H(6)	-2534	8984	6151	22
H(9)	3138	5630	3781	21
H(12)	3543	3193	5194	22
H(13)	4768	1016	6941	22
H(14)	2240	2893	9881	23
H(15)	960	5136	8227	23

Table S6. Torsion angles [°] for $[Cu(C_{15}H_{20}N_2O_4)_2(H_2O)_2]\cdot 2H_2O$.

C(9)-C(1)-C(2)-C(3)	-179.9(3)
C(10)-C(1)-C(2)-C(3)	3.8(4)
C(9)-C(1)-C(2)-C(7)	0.2(4)
C(10)-C(1)-C(2)-C(7)	-176.2(3)
C(1)-C(2)-C(3)-C(4)	-179.7(3)
C(7)-C(2)-C(3)-C(4)	0.3(4)
C(2)-C(3)-C(4)-C(5)	-0.1(5)
C(3)-C(4)-C(5)-C(6)	-0.1(5)
C(4)-C(5)-C(6)-C(7)	0.0(4)
C(8)-N(1)-C(7)-C(6)	-178.7(3)
C(8)-N(1)-C(7)-C(2)	1.3(4)
C(5)-C(6)-C(7)-N(1)	-179.8(3)
C(5)-C(6)-C(7)-C(2)	0.3(4)
C(3)-C(2)-C(7)-N(1)	179.7(3)
C(1)-C(2)-C(7)-N(1)	-0.4(4)
C(3)-C(2)-C(7)-C(6)	-0.4(4)
C(1)-C(2)-C(7)-C(6)	179.6(3)
C(7)-N(1)-C(8)-C(9)	-2.0(4)
C(7)-N(1)-C(8)-C(11)	175.7(2)
C(2)-C(1)-C(9)-C(8)	-0.8(4)
C(10)-C(1)-C(9)-C(8)	175.7(3)
N(1)-C(8)-C(9)-C(1)	1.8(4)
C(11)-C(8)-C(9)-C(1)	-175.9(2)
Cu(1)-O(1)-C(10)-O(2)	-25.3(4)
Cu(1)-O(1)-C(10)-C(1)	150.54(18)
C(9)-C(1)-C(10)-O(2)	58.0(4)
C(2)-C(1)-C(10)-O(2)	-125.6(3)
C(9)-C(1)-C(10)-O(1)	-118.3(3)
C(2)-C(1)-C(10)-O(1)	58.1(4)
N(1)-C(8)-C(11)-C(15)	-20.8(4)
C(9)-C(8)-C(11)-C(15)	156.9(3)
N(1)-C(8)-C(11)-C(12)	161.5(3)
C(9)-C(8)-C(11)-C(12)	-20.7(4)
C(15)-C(11)-C(12)-C(13)	-2.1(4)
C(8)-C(11)-C(12)-C(13)	175.6(2)
C(14)-N(2)-C(13)-C(12)	2.7(4)

Cu(1)^{i}-N(2)-C(13)-C(12)	-171.7(2)
C(11)-C(12)-C(13)-N(2)	-0.1(4)
C(13)-N(2)-C(14)-C(15)	-3.0(4)
Cu(1)^{i}-N(2)-C(14)-C(15)	171.2(2)
N(2)-C(14)-C(15)-C(11)	0.8(5)
C(12)-C(11)-C(15)-C(14)	1.8(4)
C(8)-C(11)-C(15)-C(14)	-176.0(3)

Symmetry transformations used to generate equivalent atoms:
(i) x,y-1,z+1

Table S7. Hydrogen bonds for $[Cu(C_{15}H_{20}N_2O_4)_2(H_2O)_2]\cdot 2H_2O$ [Å and °].

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*W*—H2*WA*···O3	0.85	1.91	2.733 (3)	162
O2*W*—H2*WA*···O1*W*^{i}	0.85	1.88	2.726 (3)	172
O1*W*—H1*WA*···O3	0.85	1.91	2.747 (3)	167
O1*W*—H1*WB*···N2^{ii}	0.85	2.05	2.899 (3)	173
C3—H3*A*···O2*W*^{iii}	0.93	2.53	3.073 (3)	118
C10—H10*A*···O1*W*^{iv}	0.93	2.49	3.304 (4)	147

Symmetry codes: (i) 1-x,1-y,-z; (ii) -x,1-y,1-z; (iii) x,-1+y,1+z; (iv) x,y,1+z;

Tables S8-S16

Table S8. Crystal data and structure refinement for $C_{15}H_{11}N_2O_2 \cdot Cl \cdot H_2O$.

Crystal data

$C_{15}H_{11}N_2O_2 \cdot Cl \cdot H_2O$	*F*(000) = 1264

M_r = 304.72	D_x = 1.496 Mg m^{-3}
Monoclinic, P1(1)/n	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 8.402(3) Å	Cell parameters from 5974 reflections
b = 13.243(3) Å	θ = 2.87 to 28.84
c = 24.421(3) Å	μ = 0.294 mm^{-1}
β = 95.08(3)°	T = 100 K
V = 2706,6(12) Å^3	Block, colorless
Z = 8	0.20 × 0.19 × 0.18 mm

Data collection

KM4CCD Sapphire area detector diffractometer	3590 reflections with $I > 2\sigma(I)$
phi and ω scans	R_{int} = 0.087
Absorption correction: empirical (using intensity measurements) (Rigaku; CrysAlis 2017)	θ_{max} = 28.84°, θ_{min} = 2.87°
T_{min} = 0.789, T_{max} = 0.879	h = −8→11
24472 measured reflections	k = −17→17
	l = −32→32
6671 independent reflections	

Refinement

Refinement on F^2	4 restraints
Least-squares matrix: full	Hydrogen site location: diff maps and than constreind
$R[F^2 > 2\sigma(F^2)]$ = 0.0569	H-atom parameters constrained
$wR(F^2)$ = 0.1109	$w = 2/[\sigma^2(F_o^2) + (0.0448P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max} < 0.001$
6671 reflections	$\Delta\rho_{max}$ = 0.46 e Å^{-3}
379 parameters	$\Delta\rho_{min}$ = -0.48 e Å^{-3}

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for $C_{15}H_{11}N_2O_2 \cdot Cl \cdot H_2O$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	9154(1)	2418(1)	7156(1)	24(1)
Cl(2)	4205(1)	12172(1)	7304(1)	25(1)
O(1)	5546(3)	5008(1)	6021(1)	31(1)
O(2)	5066(2)	5603(1)	6838(1)	29(1)
C(1)	4911(3)	6744(2)	6086(1)	17(1)
C(2)	4145(3)	7443(2)	6389(1)	15(1)
C(3)	3802(3)	8418(2)	6176(1)	15(1)
N(1)	4195(3)	8715(2)	5691(1)	18(1)
C(4)	4982(3)	8052(2)	5386(1)	18(1)
C(5)	5443(3)	8400(2)	4872(1)	20(1)
C(6)	6231(3)	7785(2)	4544(1)	24(1)
C(7)	6600(3)	6794(2)	4710(1)	24(1)
C(8)	6192(3)	6424(2)	5199(1)	21(1)
C(9)	5369(3)	7039(2)	5559(1)	17(1)
C(10)	5190(3)	5733(2)	6355(1)	19(1)
C(11)	2945(3)	9160(2)	6491(1)	17(1)
C(12)	2209(3)	10004(2)	6223(1)	20(1)
C(13)	1381(3)	10676(2)	6516(1)	21(1)
N(2)	1257(3)	10533(2)	7051(1)	18(1)
C(14)	1958(3)	9762(2)	7323(1)	22(1)
C(15)	2825(3)	9065(2)	7054(1)	21(1)
C(20)	9949(3)	6649(2)	6029(1)	16(1)
C(21)	9134(3)	7334(2)	6322(1)	17(1)
C(22)	8871(3)	8320(2)	6119(1)	16(1)
N(21)	9329(3)	8629(2)	5643(1)	18(1)
C(23)	10097(3)	7954(2)	5336(1)	18(1)
C(24)	10549(3)	8287(2)	4822(1)	23(1)
C(25)	11265(3)	7656(2)	4483(1)	25(1)
C(26)	11589(3)	6651(2)	4645(1)	24(1)
C(27)	11202(3)	6302(2)	5145(1)	23(1)
C(28)	10457(3)	6937(2)	5508(1)	17(1)
C(29)	10198(3)	5617(2)	6280(1)	19(1)

O(20)	11530(2)	5182(1)	6164(1)	29(1)
O(21)	9256(3)	5252(2)	6567(1)	37(1)
C(30)	8033(3)	9078(2)	6436(1)	17(1)
C(31)	7371(3)	9937(2)	6170(1)	20(1)
C(32)	6582(3)	10634(2)	6465(1)	22(1)
N(22)	6447(3)	10489(2)	7001(1)	21(1)
C(33)	7059(3)	9683(2)	7273(1)	22(1)
C(34)	7879(3)	8965(2)	6997(1)	19(1)
O(1W)	11739(2)	3346(1)	6514(1)	27(1)
O(2W)	6212(2)	3284(1)	6481(1)	28(1)

Table S10. Bond lengths [Å] and angles [°] for $C_{15}H_{11}N_2O_2 \cdot Cl \cdot H_2O$.

O(1)-C(10)	1.311(3)	C(31)-C(32)	1.378(4)
O(1)-H(1O)	0.85	C(31)-H(31)	0.95
O(2)-C(10)	1.206(3)	C(32)-N(22)	1.338(3)
C(1)-C(2)	1.379(4)	C(32)-H(32)	0.95
C(1)-C(9)	1.430(4)	N(22)-C(33)	1.335(3)
C(1)-C(10)	1.499(4)	N(22)-H(22N)	0.86
C(2)-C(3)	1.412(3)	C(33)-C(34)	1.384(4)
C(2)-H(2)	0.95	C(33)-H(33)	0.95
C(3)-N(1)	1.317(3)	C(34)-H(34)	0.95
C(3)-C(11)	1.475(4)	O(1W)-H(1W)	0.85
N(1)-C(4)	1.360(3)	O(1W)-H(2W)	0.85
C(4)-C(5)	1.422(4)	O(2W)-H(3W)	0.85
C(4)-C(9)	1.436(4)	O(2W)-H(4W)	0.85
C(5)-C(6)	1.355(4)	C(10)-O(1)-H(1O)	107.5
C(5)-H(5)	0.95	C(2)-C(1)-C(9)	118.3(2)
C(6)-C(7)	1.400(4)	C(2)-C(1)-C(10)	115.3(2)
C(6)-H(6)	0.9500	C(9)-C(1)-C(10)	126.4(2)
C(7)-C(8)	1.362(4)	C(1)-C(2)-C(3)	120.4(2)
C(7)-H(7)	0.95	C(1)-C(2)-H(2)	119.8
C(8)-C(9)	1.423(4)	C(3)-C(2)-H(2)	119.8
C(8)-H(8)	0.95	N(1)-C(3)-C(2)	123.1(2)
C(11)-C(15)	1.395(4)	N(1)-C(3)-C(11)	116.3(2)
C(11)-C(12)	1.410(4)	C(2)-C(3)-C(11)	120.6(2)
C(12)-C(13)	1.370(4)	C(3)-N(1)-C(4)	118.2(2)
C(12)-H(12)	0.95	N(1)-C(4)-C(5)	117.3(2)
C(13)-N(2)	1.334(3)	N(1)-C(4)-C(9)	123.4(3)
C(13)-H(13)	0.95	C(5)-C(4)-C(9)	119.4(3)
N(2)-C(14)	1.327(3)	C(6)-C(5)-C(4)	120.8(3)
N(2)-H(2N)	0.86	C(6)-C(5)-H(5)	119.6
C(14)-C(15)	1.378(4)	C(4)-C(5)-H(5)	119.6
C(14)-H(14)	0.95	C(5)-C(6)-C(7)	120.0(3)

C(15)-H(15)	0.95	C(5)-C(6)-H(6)	120.0
C(20)-C(21)	1.374(4)	C(7)-C(6)-H(6)	120.0
C(20)-C(28)	1.431(4)	C(8)-C(7)-C(6)	121.6(3)
C(20)-C(29)	1.505(4)	C(8)-C(7)-H(7)	119.2
C(21)-C(22)	1.407(4)	C(6)-C(7)-H(7)	119.2
C(21)-H(21)	0.95	C(7)-C(8)-C(9)	120.7(3)
C(22)-N(21)	1.322(3)	C(7)-C(8)-H(8)	119.6
C(22)-C(30)	1.484(4)	C(9)-C(8)-H(8)	119.6
N(21)-C(23)	1.365(3)	C(8)-C(9)-C(1)	125.8(3)
C(23)-C(24)	1.413(4)	C(8)-C(9)-C(4)	117.5(3)
C(23)-C(28)	1.435(4)	C(1)-C(9)-C(4)	116.7(2)
C(24)-C(25)	1.354(4)	O(2)-C(10)-O(1)	123.2(3)
C(24)-H(24)	0.95	O(2)-C(10)-C(1)	122.1(3)
C(25)-C(26)	1.407(4)	O(1)-C(10)-C(1)	114.6(2)
C(25)-H(25)	0.95	C(15)-C(11)-C(12)	117.5(3)
C(26)-C(27)	1.372(4)	C(15)-C(11)-C(3)	122.4(2)
C(26)-H(26)	0.95	C(12)-C(11)-C(3)	120.1(2)
C(27)-C(28)	1.408(4)	C(13)-C(12)-C(11)	119.7(3)
C(27)-H(27)	0.95	C(13)-C(12)-H(12)	120.2
C(29)-O(21)	1.203(3)	C(11)-C(12)-H(12)	120.2
C(29)-O(20)	1.312(3)	N(2)-C(13)-C(12)	120.5(3)
O(20)-H(2O)	0.85	N(2)-C(13)-H(13)	119.8
C(30)-C(34)	1.394(4)	C(12)-C(13)-H(13)	119.8
C(30)-C(31)	1.400(4)	C(14)-N(2)-C(13)	122.0(2)
C(20)-C(29)	1.505(4)	C(14)-N(2)-H(2N)	123.0
C(13)-N(2)-H(2N)	114.9	C(24)-C(25)-C(26)	119.8(3)
N(2)-C(14)-C(15)	120.4(3)	C(24)-C(25)-H(25)	120.1
N(2)-C(14)-H(14)	119.8	C(26)-C(25)-H(25)	120.1
C(15)-C(14)-H(14)	119.8	C(27)-C(26)-C(25)	120.9(3)
C(14)-C(15)-C(11)	119.9(3)	C(27)-C(26)-H(26)	119.5
C(14)-C(15)-H(15)	120.1	C(25)-C(26)-H(26)	119.5
C(11)-C(15)-H(15)	120.1	C(26)-C(27)-C(28)	120.8(3)
C(21)-C(20)-C(28)	119.3(2)	C(26)-C(27)-H(27)	119.6

C(21)-C(20)-C(29)	116.5(2)	C(28)-C(27)-H(27)	119.6
C(28)-C(20)-C(29)	124.2(2)	C(27)-C(28)-C(20)	125.8(2)
C(20)-C(21)-C(22)	119.9(2)	C(27)-C(28)-C(23)	118.0(3)
C(20)-C(21)-H(21)	120.0	C(20)-C(28)-C(23)	116.1(2)
C(22)-C(21)-H(21)	120.0	O(21)-C(29)-O(20)	124.6(3)
N(21)-C(22)-C(21)	123.2(2)	O(21)-C(29)-C(20)	121.7(3)
N(21)-C(22)-C(30)	116.0(2)	O(20)-C(29)-C(20)	113.6(2)
C(21)-C(22)-C(30)	120.7(2)	C(29)-O(20)-H(2O)	113.8
C(22)-N(21)-C(23)	118.0(2)	C(34)-C(30)-C(31)	118.5(3)
N(21)-C(23)-C(24)	117.4(3)	C(31)-C(30)-C(22)	119.6(2)
N(21)-C(23)-C(28)	123.4(2)	C(32)-C(31)-C(30)	119.3(3)
C(24)-C(23)-C(28)	119.2(3)	C(32)-C(31)-H(31)	120.3
C(25)-C(24)-C(23)	121.2(3)	C(30)-C(31)-H(31)	120.3
C(31)-C(32)-H(32)	119.9	N(22)-C(32)-C(31)	120.2(3)
C(33)-N(22)-C(32)	122.6(2)	N(22)-C(32)-H(32)	119.9
C(33)-N(22)-H(22N)	118.4	C(33)-C(34)-C(30)	119.8(3)
C(32)-N(22)-H(22N)	119.1	C(33)-C(34)-H(34)	120.1
N(22)-C(33)-C(34)	119.6(3)	C(30)-C(34)-H(34)	120.1
N(22)-C(33)-H(33)	120.2	H(1W)-O(1W)-H(2W)	105.2
C(34)-C(33)-H(33)	120.2	H(3W)-O(2W)-H(4W)	105.2

Table S11. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $C_{15}H_{11}N_2O_2 \cdot Cl \cdot H_2O$. The anisotropicdisplacement 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}
Cl(1)	25(1)	19(1)	27(1)	-3(1)	2(1)	3(1)
Cl(2)	24(1)	19(1)	30(1)	-3(1)	-1(1)	2(1)
O(1)	59(2)	14(1)	20(1)	4(1)	6(1)	11(1)
O(2)	47(1)	21(1)	21(1)	4(1)	10(1)	5(1)
C(1)	21(2)	17(1)	13(2)	1(1)	-1(1)	-2(1)
C(2)	18(1)	15(1)	13(1)	1(1)	3(1)	-2(1)
C(3)	16(1)	15(1)	14(2)	0(1)	0(1)	-2(1)
N(1)	23(1)	16(1)	14(1)	0(1)	2(1)	0(1)
C(4)	20(2)	18(2)	14(2)	2(1)	-2(1)	-4(1)
C(5)	24(2)	15(1)	21(2)	2(1)	0(1)	-1(1)
C(6)	30(2)	26(2)	16(2)	1(1)	4(1)	-4(1)
C(7)	29(2)	23(2)	21(2)	-2(1)	7(1)	2(1)
C(8)	26(2)	15(1)	21(2)	-1(1)	3(1)	2(1)
C(9)	18(2)	18(1)	15(2)	-2(1)	-1(1)	-2(1)
C(10)	22(2)	16(2)	18(2)	-1(1)	1(1)	3(1)
C(11)	18(2)	14(1)	18(2)	-1(1)	1(1)	-3(1)
C(12)	29(2)	15(1)	16(2)	0(1)	-1(1)	-4(1)
C(13)	28(2)	13(1)	22(2)	0(1)	0(1)	2(1)
N(2)	22(1)	14(1)	20(1)	-3(1)	3(1)	1(1)
C(14)	32(2)	15(2)	18(2)	1(1)	6(1)	-1(1)
C(15)	27(2)	19(2)	16(2)	2(1)	1(1)	0(1)
C(20)	21(2)	15(1)	13(2)	-2(1)	-1(1)	-3(1)
C(21)	17(1)	19(2)	14(1)	4(1)	1(1)	-1(1)
C(22)	19(2)	15(1)	15(2)	-1(1)	-1(1)	-2(1)
N(21)	23(1)	18(1)	12(1)	1(1)	1(1)	-2(1)
C(23)	18(2)	21(2)	13(2)	-1(1)	-2(1)	-3(1)
C(24)	27(2)	19(2)	22(2)	3(1)	1(1)	-1(1)
C(25)	32(2)	31(2)	12(2)	1(1)	4(1)	0(1)
C(26)	29(2)	23(2)	22(2)	-1(1)	7(1)	7(1)
C(27)	26(2)	21(2)	22(2)	2(1)	5(1)	5(1)
C(28)	19(2)	18(2)	14(2)	-2(1)	1(1)	-2(1)
C(29)	21(2)	19(2)	18(2)	1(1)	2(1)	1(1)
O(20)	34(1)	22(1)	31(1)	10(1)	7(1)	10(1)

O(21)	45(1)	26(1)	43(2)	13(1)	25(1)	10(1)
C(30)	19(2)	13(1)	18(2)	-1(1)	0(1)	-5(1)
C(31)	26(2)	19(2)	16(2)	1(1)	0(1)	-2(1)
C(32)	27(2)	17(1)	22(2)	6(1)	0(1)	1(1)
N(22)	25(1)	13(1)	25(1)	-5(1)	4(1)	2(1)
C(33)	27(2)	22(2)	16(2)	1(1)	3(1)	-2(1)
C(34)	24(2)	16(1)	18(2)	1(1)	3(1)	1(1)
O(1W)	32(1)	23(1)	25(1)	7(1)	4(1)	7(1)
O(2W)	33(1)	22(1)	28(1)	6(1)	3(1)	9(1)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for $C_{15}H_{11}N_2O_2 \cdot Cl \cdot H_2O$.

	x	y	z	U(eq)
H(1O)	5679	4471	6210	46
H(2)	3846	7268	6743	18
H(5)	5197	9072	4758	24
H(6)	6531	8026	4202	29
H(7)	7149	6369	4476	29
H(8)	6460	5749	5300	25
H(12)	2287	10106	5841	24
H(13)	892	11248	6337	25
H(2N)	721	10988	7207	28
H(14)	1861	9690	7706	26
H(15)	3341	8522	7252	25
H(21)	8748	7142	6661	20
H(24)	10347	8967	4712	28
H(25)	11548	7890	4137	30
H(26)	12083	6209	4405	29
H(27)	11438	5623	5248	28
H(2O)	11702	4616	6322	43
H(31)	7466	10037	5789	24
H(32)	6131	11219	6288	26
H(22N)	5932	10925	7178	31
H(33)	6932	9603	7653	26
H(34)	8337	8397	7189	23
H(1W)	10947	3162	6683	40
H(2W)	12544	3054	6680	40
H(3W)	7124	3132	6638	42
H(4W)	5546	3098	6703	42

Table S15. Torsion angles [°] for $C_{15}H_{11}N_2O_2 \cdot Cl \cdot H_2O$.

C(9)-C(1)-C(2)-C(3)	1.1(4)
C(10)-C(1)-C(2)-C(3)	-179.3(2)
C(1)-C(2)-C(3)-N(1)	-0.7(4)
C(1)-C(2)-C(3)-C(11)	178.4(2)
C(2)-C(3)-N(1)-C(4)	-0.7(4)
C(11)-C(3)-N(1)-C(4)	-179.8(2)
C(3)-N(1)-C(4)-C(5)	-177.9(2)
C(3)-N(1)-C(4)-C(9)	1.6(4)
N(1)-C(4)-C(5)-C(6)	-179.9(2)
C(9)-C(4)-C(5)-C(6)	0.5(4)
C(4)-C(5)-C(6)-C(7)	-0.1(4)
C(5)-C(6)-C(7)-C(8)	-0.2(4)
C(6)-C(7)-C(8)-C(9)	0.0(4)
C(7)-C(8)-C(9)-C(1)	-178.5(3)
C(7)-C(8)-C(9)-C(4)	0.4(4)
C(2)-C(1)-C(9)-C(8)	178.7(3)
C(10)-C(1)-C(9)-C(8)	-0.8(4)
C(2)-C(1)-C(9)-C(4)	-0.3(4)
C(10)-C(1)-C(9)-C(4)	-179.8(2)
N(1)-C(4)-C(9)-C(8)	179.8(2)
C(5)-C(4)-C(9)-C(8)	-0.7(4)
N(1)-C(4)-C(9)-C(1)	-1.1(4)
C(5)-C(4)-C(9)-C(1)	178.4(2)
C(2)-C(1)-C(10)-O(2)	-14.9(4)
C(9)-C(1)-C(10)-O(2)	164.6(3)
C(2)-C(1)-C(10)-O(1)	163.9(2)
C(9)-C(1)-C(10)-O(1)	-16.5(4)
N(1)-C(3)-C(11)-C(15)	-162.7(3)
C(2)-C(3)-C(11)-C(15)	18.2(4)
N(1)-C(3)-C(11)-C(12)	17.3(4)
C(2)-C(3)-C(11)-C(12)	-161.8(2)
C(15)-C(11)-C(12)-C(13)	-1.7(4)
C(3)-C(11)-C(12)-C(13)	178.3(2)
C(11)-C(12)-C(13)-N(2)	-0.5(4)
C(12)-C(13)-N(2)-C(14)	2.0(4)
C(13)-N(2)-C(14)-C(15)	-1.1(4)

N(2)-C(14)-C(15)-C(11)	-1.1(4)
C(12)-C(11)-C(15)-C(14)	2.5(4)
C(3)-C(11)-C(15)-C(14)	-177.5(3)
C(28)-C(20)-C(21)-C(22)	-2.8(4)
C(29)-C(20)-C(21)-C(22)	179.1(2)
C(20)-C(21)-C(22)-N(21)	2.2(4)
C(20)-C(21)-C(22)-C(30)	-178.3(2)
C(21)-C(22)-N(21)-C(23)	-0.1(4)
C(30)-C(22)-N(21)-C(23)	-179.6(2)
C(22)-N(21)-C(23)-C(24)	178.6(2)
C(22)-N(21)-C(23)-C(28)	-1.3(4)
N(21)-C(23)-C(24)-C(25)	-177.7(2)
C(28)-C(23)-C(24)-C(25)	2.2(4)
C(23)-C(24)-C(25)-C(26)	-0.8(4)
C(24)-C(25)-C(26)-C(27)	-0.6(4)
C(25)-C(26)-C(27)-C(28)	0.5(4)
C(26)-C(27)-C(28)-C(20)	177.7(3)
C(26)-C(27)-C(28)-C(23)	0.9(4)
C(21)-C(20)-C(28)-C(27)	-175.4(3)
C(29)-C(20)-C(28)-C(27)	2.5(4)
C(21)-C(20)-C(28)-C(23)	1.5(4)
C(29)-C(20)-C(28)-C(23)	179.4(2)
N(21)-C(23)-C(28)-C(27)	177.7(2)
C(24)-C(23)-C(28)-C(27)	-2.2(4)
N(21)-C(23)-C(28)-C(20)	0.5(4)
C(24)-C(23)-C(28)-C(20)	-179.3(2)
C(21)-C(20)-C(29)-O(21)	30.5(4)
C(28)-C(20)-C(29)-O(21)	-147.4(3)
C(21)-C(20)-C(29)-O(20)	-148.3(2)
C(28)-C(20)-C(29)-O(20)	33.8(4)
N(21)-C(22)-C(30)-C(34)	-161.8(3)
C(21)-C(22)-C(30)-C(34)	18.7(4)
N(21)-C(22)-C(30)-C(31)	18.2(4)
C(21)-C(22)-C(30)-C(31)	-161.3(2)
C(34)-C(30)-C(31)-C(32)	-0.6(4)
C(22)-C(30)-C(31)-C(32)	179.4(2)
C(30)-C(31)-C(32)-N(22)	-0.1(4)
C(31)-C(32)-N(22)-C(33)	0.2(4)

C(32)-N(22)-C(33)-C(34)	0.5(4)
N(22)-C(33)-C(34)-C(30)	-1.3(4)
C(31)-C(30)-C(34)-C(33)	1.3(4)
C(22)-C(30)-C(34)-C(33)	-178.7(2)

Table S16. Hydrogen bonds for $C_{15}H_{11}N_2O_2 \cdot Cl \cdot H_2O$ [Å and °].

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H10···O2*W*	0.85	1.75	2.584 (3)	167
O1*W*—H1*W*···Cl1^{i}	0.85	2.21	3.047 (2)	169
N2—H2*N*···Cl1^{i}	0.86	2.30	2.082 (3)	151
N2—H2*N*···O2^{ii}	0.86	2.53	3.022 (3)	117
O1*W*—H2*W*···Cl2^{iii}	0.85	2.29	3.119 (2)	164
O2*W*—H3*W*···Cl1	0.85	2.24	3.069 (2)	165
O2*W*—H4*W*···Cl2^{iv}	0.85	2.28	3.107 (2)	163
N22—H22*N*···Cl2	0.86	2.24	3.051 (2)	158
C8—H8···O1	0.95	2.21	2.834 (3)	122
C14—H14···O2^{ii}	0.92	2.37	2.990 (3)	122
C27—H27···O20	0.95	2.31	2.888 (4)	119
C33—H33···O21^{v}	0.95	2.39	3.222 (4)	146
C34—H34···Cl2^{vi}	0.95	2.39	3.222 (4)	146

Symmetry codes: (i) -1+x,1+y,z; (ii) 1/2-x,1/2+y,3/2-z (iii) 1+x,-1+y,z; (iv) x,-1+y,z; (v) 3/2-x,1/2+y,3/2-z; (vi) 3/2-x,-1/2+y,3/2-z,