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Supplementary information A new copper chloride chain by supported hydrogen bonding

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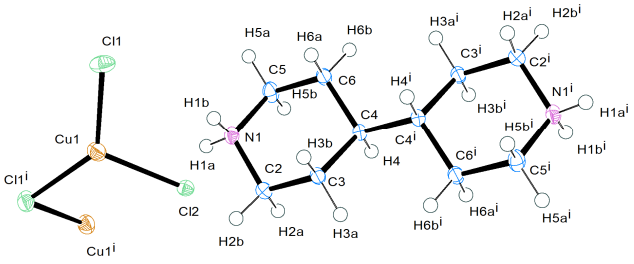

Figure 1. Showing the atomic thermal ellipsoid plot (50% probability level) and atomic numbering scheme for compound **1**.

Table 1. Crystal data and structure refinement for compound **1**.

Identification code	1	
Empirical formula	C10 H22 Cl4 Cu2 N2	
Formula weight	439.18	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 8.4958(5) Å	α= 90°.
	b = 15.7766(10) Å	β= 99.269(3)°.
	c = 5.9616(4) Å	γ = 90°.
Volume	788.63(9) Å^3	
Z	2	
Density (calculated)	1.849 Mg/m^3	
Absorption coefficient	3.358 mm^{-1}	
F(000)	444	
Crystal size	0.20 x 0.20 x 0.04 mm^3	
Theta range for data collection	2.43 to 29.60°.	
Index ranges	-11<=h<=11, -21<=k<=20, -8<=l<=8	
Reflections collected	8107	
Independent reflections	2206 [R(int) = 0.0233]	
Completeness to theta = 29.60°	99.3 %	
Absorption correction	Numerical	
Max. and min. transmission	0.8774 and 0.5532	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2206 / 0 / 90	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0208, wR2 = 0.0465	
R indices (all data)	R1 = 0.0261, wR2 = 0.0486	
Largest diff. peak and hole	0.441 and -0.479 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	6750(1)	7685(1)	2213(1)	23(1)
Cl(1)	7697(1)	6607(1)	4427(1)	26(1)
Cl(2)	4421(1)	8324(1)	2890(1)	16(1)
N(1)	3302(1)	8677(1)	7629(2)	15(1)
C(2)	1624(2)	8386(1)	7613(2)	17(1)
C(3)	496(2)	8810(1)	5714(2)	15(1)
C(4)	587(2)	9778(1)	5921(2)	12(1)
C(5)	3468(2)	9618(1)	7744(2)	18(1)
C(6)	2316(2)	10042(1)	5868(2)	15(1)

Table 3. Selected bond lengths [Å] and angles [°] for compound **1**.

Cu(1)-Cl(1)	2.2227(4)
Cu(1)-Cl(1)#1	2.2552(4)
Cu(1)-Cl(2)	2.3138(4)
Cu(1)-Cu(1)#1	3.0373(2)
Cl(1)-Cu(1)#2	2.2552(4)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z-1/2 #2 x,-y+3/2,z+1/2

Table 4. Bond lengths [Å] and angles [°] for compound **1**.

Cu(1)-Cl(1)	2.2227(4)
Cu(1)-Cl(1)#1	2.2552(4)
Cu(1)-Cl(2)	2.3138(4)
Cu(1)-Cu(1)#1	3.0373(2)
Cu(1)-Cu(1)#2	3.0373(2)
Cl(1)-Cu(1)#2	2.2552(4)
N(1)-C(5)	1.4919(19)
N(1)-C(2)	1.4961(18)
N(1)-H(1A)	0.86(2)
N(1)-H(1B)	0.895(19)
C(2)-C(3)	1.5157(18)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.5333(19)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(4)#3	1.530(2)
C(4)-C(6)	1.5314(18)
C(4)-H(4)	1.0000
C(5)-C(6)	1.5180(19)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
Cl(1)-Cu(1)-Cl(1)#1	132.75(2)
Cl(1)-Cu(1)-Cl(2)	117.905(15)
Cl(1)#1-Cu(1)-Cl(2)	109.194(16)
Cl(1)-Cu(1)-Cu(1)#1	112.253(15)
Cl(1)#1-Cu(1)-Cu(1)#1	46.843(11)
Cl(2)-Cu(1)-Cu(1)#1	112.958(10)
Cl(1)-Cu(1)-Cu(1)#2	47.742(11)
Cl(1)#1-Cu(1)-Cu(1)#2	150.964(13)
Cl(2)-Cu(1)-Cu(1)#2	77.136(10)
Cu(1)#1-Cu(1)-Cu(1)#2	157.867(15)
Cu(1)-Cl(1)-Cu(1)#2	85.416(14)
C(5)-N(1)-C(2)	112.87(11)
C(5)-N(1)-H(1A)	108.9(13)
C(2)-N(1)-H(1A)	106.6(13)
C(5)-N(1)-H(1B)	108.0(12)
C(2)-N(1)-H(1B)	110.3(12)
H(1A)-N(1)-H(1B)	110.2(18)
N(1)-C(2)-C(3)	110.90(11)
N(1)-C(2)-H(2A)	109.5
C(3)-C(2)-H(2A)	109.5
N(1)-C(2)-H(2B)	109.5
C(3)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	108.0
C(2)-C(3)-C(4)	111.19(11)
C(2)-C(3)-H(3A)	109.4
C(4)-C(3)-H(3A)	109.4
C(2)-C(3)-H(3B)	109.4
C(4)-C(3)-H(3B)	109.4
H(3A)-C(3)-H(3B)	108.0
C(4)#3-C(4)-C(6)	112.18(14)
C(4)#3-C(4)-C(3)	112.28(13)
C(6)-C(4)-C(3)	107.81(11)
C(4)#3-C(4)-H(4)	108.1
C(6)-C(4)-H(4)	108.1
C(3)-C(4)-H(4)	108.1
N(1)-C(5)-C(6)	111.08(11)
N(1)-C(5)-H(5A)	109.4
C(6)-C(5)-H(5A)	109.4
N(1)-C(5)-H(5B)	109.4
C(6)-C(5)-H(5B)	109.4
H(5A)-C(5)-H(5B)	108.0
C(5)-C(6)-C(4)	111.83(11)
C(5)-C(6)-H(6A)	109.3
C(4)-C(6)-H(6A)	109.3
C(5)-C(6)-H(6B)	109.3
C(4)-C(6)-H(6B)	109.3
H(6A)-C(6)-H(6B)	107.9

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z-1/2 #2 x,-y+3/2,z+1/2 #3 -x,-y+2,-z+1

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **1**. The anisotropic displacement factor exponent takes the form: -2p2[h2 a*2U11 + ... + 2 h k a* b* U12]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	22(1)	18(1)	27(1)	2(1)	2(1)	-1(1)
Cl(1)	31(1)	25(1)	23(1)	6(1)	13(1)	10(1)
Cl(2)	18(1)	16(1)	13(1)	0(1)	4(1)	-1(1)
N(1)	15(1)	16(1)	12(1)	2(1)	1(1)	4(1)
C(2)	16(1)	16(1)	20(1)	6(1)	4(1)	2(1)
C(3)	13(1)	12(1)	18(1)	2(1)	1(1)	1(1)
C(4)	13(1)	12(1)	12(1)	0(1)	1(1)	2(1)
C(5)	16(1)	16(1)	20(1)	-1(1)	-4(1)	1(1)
C(6)	14(1)	12(1)	19(1)	2(1)	-1(1)	0(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2 x\ 10^3$) for compound **1**.

	x	y	z	U(eq)
H(1A)	3860(20)	8460(12)	8810(30)	26(5)
H(1B)	3660(20)	8498(11)	6380(30)	19(4)
H(2A)	1295	8523	9091	21
H(2B)	1566	7764	7409	21
H(3A)	-609	8622	5769	18
H(3B)	772	8636	4231	18
H(4)	314	9940	7434	15
H(5A)	4574	9777	7598	21
H(5B)	3257	9820	9240	21
H(6A)	2605	9889	4377	18
H(6B)	2410	10665	6040	18

Table 7. Hydrogen bonds for compound **1** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Cl(2)#4	0.86(2)	2.41(2)	3.1766(12)	149.3(17)
N(1)-H(1B)...Cl(2)	0.895(19)	2.291(19)	3.1717(12)	167.8(16)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z-1/2 #2 x,-y+3/2,z+1/2 #3 -x,-y+2,-z+1

#4 x,y,z+1

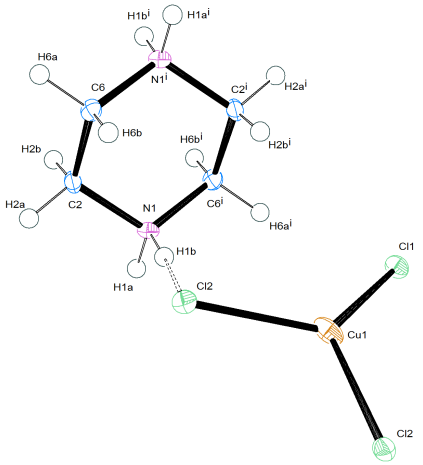

Figure 2. Showing the atomic thermal ellipsoid plot (50% probability level) and atomic numbering scheme for compound **2**.

Table 8. Crystal data and structure refinement for compound **2**.

Identification code	2	
Empirical formula	$C_4 H_{12} Cl_4 Cu N_2$	
Formula weight	293.50	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	P 43 21 2	
Unit cell dimensions	a = 7.6443(4) Å	α= 90°.
	b = 7.6443(4) Å	β= 90°.
	c = 19.1597(12) Å	γ = 90°.
Volume	1119.60(11) Å^3	
Z	4	
Density (calculated)	1.741 Mg/m^3	
Absorption coefficient	2.853 mm^{-1}	
F(000)	588	
Crystal size	0.76 x 0.60 x 0.49 mm^3	
Theta range for data collection	2.87 to 29.00°.	
Index ranges	-10<=h<=8, -10<=k<=8, -9<=l<=26	
Reflections collected	5271	
Independent reflections	1474 [R(int) = 0.0215]	
Completeness to theta = 29.00°	98.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.3378 and 0.2192	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1474 / 0 / 60	
Goodness-of-fit on F^2	1.059	
Final R indices [I>2sigma(I)]	R1 = 0.0154, wR2 = 0.0366	
R indices (all data)	R1 = 0.0163, wR2 = 0.0368	
Absolute structure parameter	0.027(10)	
Extinction coefficient	0.0034(9)	
Largest diff. peak and hole	0.288 and -0.280 e.Å^{-3}	

Table 9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for compound **2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cl(1)	3433(1)	6385(1)	5680(1)	19(1)
Cu(1)	4058(1)	4058(1)	5000	14(1)
Cl(2)	2083(1)	4501(1)	4158(1)	17(1)
N(1)	4488(2)	3145(2)	2832(1)	15(1)
C(2)	3842(2)	4765(2)	2486(1)	16(1)
C(6)	6124(2)	2470(2)	2503(1)	17(1)

Table 10. Selected bond lengths [Å] and angles [°] for compound **2**.

Cl(1)-Cu(1)	2.2559(4)
Cu(1)-Cl(2)	2.2351(4)

Table 11. Bond lengths [Å] and angles [°] for compound **2**.

Cl(1)-Cu(1)	2.2559(4)
Cu(1)-Cl(2)	2.2351(4)
Cu(1)-Cl(2)#1	2.2351(4)
Cu(1)-Cl(1)#1	2.2559(4)
N(1)-C(2)	1.4897(19)
N(1)-C(6)	1.4926(18)
N(1)-H(1A)	0.862(17)
N(1)-H(1B)	0.852(17)
C(2)-C(2)#2	1.507(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(6)-C(6)#2	1.520(3)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
Cl(2)-Cu(1)-Cl(2)#1	136.54(2)
Cl(2)-Cu(1)-Cl(1)	98.879(14)
Cl(2)#1-Cu(1)-Cl(1)	98.497(13)
Cl(2)-Cu(1)-Cl(1)#1	98.498(13)
Cl(2)#1-Cu(1)-Cl(1)#1	98.879(13)
Cl(1)-Cu(1)-Cl(1)#1	131.85(2)
C(2)-N(1)-C(6)	112.09(10)
C(2)-N(1)-H(1A)	109.8(12)
C(6)-N(1)-H(1A)	109.5(13)
C(2)-N(1)-H(1B)	106.6(12)
C(6)-N(1)-H(1B)	111.5(12)
H(1A)-N(1)-H(1B)	107.2(16)
N(1)-C(2)-C(2)#2	109.68(10)
N(1)-C(2)-H(2A)	109.7
C(2)#2-C(2)-H(2A)	109.7
N(1)-C(2)-H(2B)	109.7
C(2)#2-C(2)-H(2B)	109.7
H(2A)-C(2)-H(2B)	108.2
N(1)-C(6)-C(6)#2	110.52(9)
N(1)-C(6)-H(6A)	109.5
C(6)#2-C(6)-H(6A)	109.5
N(1)-C(6)-H(6B)	109.5
C(6)#2-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	108.1

Symmetry transformations used to generate equivalent atoms:

#1 y,x,-z+1 #2 -y+1,-x+1,-z+1/2

Table 12. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **2**. The anisotropic displacement factor exponent takes the form: -2p2[h2 a*2U11 + ... + 2 h k a* b* U12]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	30(1)	16(1)	13(1)	-2(1)	-3(1)	5(1)
Cu(1)	16(1)	16(1)	11(1)	0(1)	0(1)	3(1)
Cl(2)	17(1)	19(1)	14(1)	-2(1)	-2(1)	4(1)
N(1)	18(1)	16(1)	13(1)	2(1)	1(1)	-4(1)
C(2)	13(1)	18(1)	15(1)	3(1)	0(1)	1(1)
C(6)	21(1)	14(1)	16(1)	1(1)	3(1)	4(1)

Table 13. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2 x\ 10^3$) for compound **2**.

	x	y	z	U(eq)
H(2A)	2773	5185	2724	19
H(2B)	3543	4510	1993	19
H(6A)	5873	2097	2018	21
H(6B)	6548	1439	2765	21
H(1A)	4670(20)	3350(20)	3269(9)	28(5)
H(1B)	3660(20)	2400(20)	2808(8)	23(5)

Table 14. Hydrogen bonds for compound **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Cl(1)#1	0.862(17)	2.402(17)	3.2054(13)	155.2(17)
N(1)-H(1A)...Cl(2)	0.862(17)	2.758(18)	3.3027(13)	122.5(15)
N(1)-H(1B)...Cl(2)#3	0.852(17)	2.505(18)	3.1865(14)	137.6(14)
N(1)-H(1B)...Cl(1)#3	0.852(17)	2.598(16)	3.2497(14)	134.1(13)

Symmetry transformations used to generate equivalent atoms:

#1 y,x,-z+1 #2 -y+1,-x+1,-z+1/2 #3 -x+1/2,y-1/2,-z+3/4

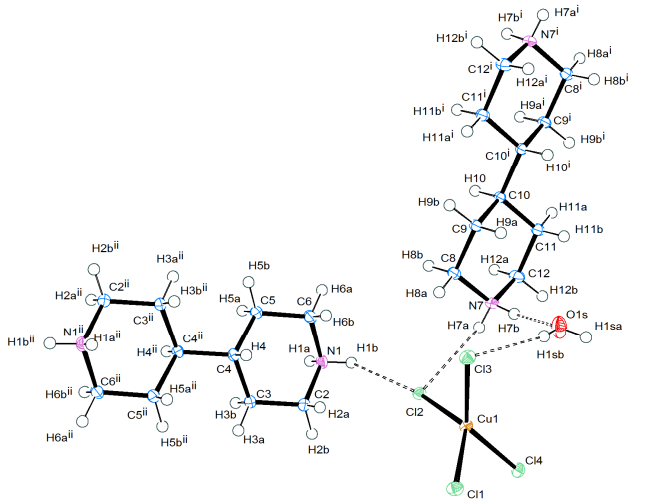

Figure 3. Showing the atomic thermal ellipsoid plot (50% probability level) and atomic numbering scheme for compound **3**.

Table 15. Crystal data and structure refinement for compound **3**.

Identification code	3	
Empirical formula	C_{10} H_{24} Cl_4 Cu N_2 O	
Formula weight	393.65	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.2245(2) Å b = 9.3525(2) Å c = 9.6145(2) Å	α= 76.7530(10)°. β= 84.9900(10)°. γ = 82.6010(10)°.
Volume	799.23(3) $Å^3$	
Z	2	
Density (calculated)	1.636 Mg/m^3	
Absorption coefficient	2.025 mm^{-1}	
F(000)	406	
Crystal size	0.48 x 0.25 x 0.18 mm^3	
Theta range for data collection	2.18 to 33.33°.	
Index ranges	-14<=h<=13, -14<=k<=13, -14<=l<=14	
Reflections collected	17070	
Independent reflections	5955 [R(int) = 0.0202]	
Completeness to theta = 33.33°	96.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7094 and 0.4450	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5955 / 0 / 187	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0185, wR2 = 0.0450	
R indices (all data)	R1 = 0.0220, wR2 = 0.0469	
Largest diff. peak and hole	0.426 and -0.408 $e.Å^{-3}$	

Table 16. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	6637(1)	7441(1)	915(1)	11(1)
Cl(1)	8542(1)	8774(1)	596(1)	16(1)
Cl(2)	6392(1)	5011(1)	1340(1)	13(1)
Cl(3)	5797(1)	7880(1)	3070(1)	16(1)
Cl(4)	6026(1)	8074(1)	-1375(1)	14(1)
O(1S)	2713(1)	8342(1)	1672(1)	28(1)
N(1)	7207(1)	1222(1)	2426(1)	14(1)
N(7)	2784(1)	5298(1)	2042(1)	14(1)
C(2)	8679(1)	1756(1)	2043(1)	16(1)
C(3)	9820(1)	737(1)	2951(1)	13(1)
C(4)	9430(1)	552(1)	4557(1)	11(1)
C(5)	7877(1)	89(1)	4894(1)	14(1)
C(6)	6756(1)	1125(1)	3971(1)	15(1)
C(8)	3237(1)	4697(1)	3540(1)	15(1)
C(9)	2092(1)	5214(1)	4607(1)	13(1)
C(10)	586(1)	4761(1)	4456(1)	11(1)
C(11)	166(1)	5409(1)	2912(1)	14(1)
C(12)	1306(1)	4918(1)	1825(1)	16(1)

Table 17. Selected bond lengths [Å] and angles [°] for compound **3**.

Cu(1)-Cl(1)	2.2432(3)
Cu(1)-Cl(4)	2.2475(3)
Cu(1)-Cl(2)	2.2521(2)
Cu(1)-Cl(3)	2.2568(3)

Table 18. Bond lengths [Å] and angles [°] for compound **3**.

Cu(1)-Cl(1)	2.2432(3)
Cu(1)-Cl(4)	2.2475(3)
Cu(1)-Cl(2)	2.2521(2)
Cu(1)-Cl(3)	2.2568(3)
O(1S)-H(1SA)	0.77(2)
O(1S)-H(1SB)	0.78(2)
N(1)-C(6)	1.4927(13)
N(1)-C(2)	1.4941(13)
N(1)-H(1A)	0.886(16)
N(1)-H(1B)	0.850(16)
N(7)-C(12)	1.4956(13)
N(7)-C(8)	1.4968(13)
N(7)-H(7A)	0.833(15)
N(7)-H(7B)	0.898(15)
C(2)-C(3)	1.5166(14)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.5304(13)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.5359(13)
C(4)-C(4)#1	1.5396(18)
C(4)-H(4)	1.0000
C(5)-C(6)	1.5177(14)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(8)-C(9)	1.5190(13)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.5319(13)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.5314(14)
C(10)-C(10)#2	1.5349(18)
C(10)-H(10)	1.0000
C(11)-C(12)	1.5204(13)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
Cl(1)-Cu(1)-Cl(4)	96.004(10)
Cl(1)-Cu(1)-Cl(2)	134.842(10)
Cl(4)-Cu(1)-Cl(2)	98.472(9)
Cl(1)-Cu(1)-Cl(3)	96.955(10)
Cl(4)-Cu(1)-Cl(3)	139.402(10)
Cl(2)-Cu(1)-Cl(3)	99.129(9)
H(1SA)-O(1S)-H(1SB)	109.7(19)
C(6)-N(1)-C(2)	111.91(8)
C(6)-N(1)-H(1A)	109.4(10)
C(2)-N(1)-H(1A)	110.1(10)
C(6)-N(1)-H(1B)	108.0(10)
C(2)-N(1)-H(1B)	111.8(11)
H(1A)-N(1)-H(1B)	105.4(14)
C(12)-N(7)-C(8)	112.57(8)
C(12)-N(7)-H(7A)	109.8(10)
C(8)-N(7)-H(7A)	108.6(10)
C(12)-N(7)-H(7B)	108.8(10)
C(8)-N(7)-H(7B)	110.4(9)
H(7A)-N(7)-H(7B)	106.5(13)
N(1)-C(2)-C(3)	110.22(8)
N(1)-C(2)-H(2A)	109.6
C(3)-C(2)-H(2A)	109.6
N(1)-C(2)-H(2B)	109.6
C(3)-C(2)-H(2B)	109.6
H(2A)-C(2)-H(2B)	108.1
C(2)-C(3)-C(4)	112.75(8)
C(2)-C(3)-H(3A)	109.0
C(4)-C(3)-H(3A)	109.0
C(2)-C(3)-H(3B)	109.0
C(4)-C(3)-H(3B)	109.0
H(3A)-C(3)-H(3B)	107.8
C(3)-C(4)-C(5)	109.22(8)
C(3)-C(4)-C(4)#1	111.29(9)
C(5)-C(4)-C(4)#1	112.13(9)
C(3)-C(4)-H(4)	108.0
C(5)-C(4)-H(4)	108.0
C(4)#1-C(4)-H(4)	108.0
C(6)-C(5)-C(4)	112.55(8)
C(6)-C(5)-H(5A)	109.1
C(4)-C(5)-H(5A)	109.1
C(6)-C(5)-H(5B)	109.1
C(4)-C(5)-H(5B)	109.1
H(5A)-C(5)-H(5B)	107.8
N(1)-C(6)-C(5)	109.88(8)
N(1)-C(6)-H(6A)	109.7
C(5)-C(6)-H(6A)	109.7
N(1)-C(6)-H(6B)	109.7
C(5)-C(6)-H(6B)	109.7
H(6A)-C(6)-H(6B)	108.2
N(7)-C(8)-C(9)	110.58(8)
N(7)-C(8)-H(8A)	109.5
C(9)-C(8)-H(8A)	109.5
N(7)-C(8)-H(8B)	109.5
C(9)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	108.1
C(8)-C(9)-C(10)	111.65(8)
C(8)-C(9)-H(9A)	109.3
C(10)-C(9)-H(9A)	109.3
C(8)-C(9)-H(9B)	109.3
C(10)-C(9)-H(9B)	109.3
H(9A)-C(9)-H(9B)	108.0
C(11)-C(10)-C(9)	107.84(7)
C(11)-C(10)-C(10)#2	111.82(9)
C(9)-C(10)-C(10)#2	112.76(9)
C(11)-C(10)-H(10)	108.1
C(9)-C(10)-H(10)	108.1
C(10)#2-C(10)-H(10)	108.1
C(12)-C(11)-C(10)	112.24(8)
C(12)-C(11)-H(11A)	109.2
C(10)-C(11)-H(11A)	109.2
C(12)-C(11)-H(11B)	109.2
C(10)-C(11)-H(11B)	109.2
H(11A)-C(11)-H(11B)	107.9
N(7)-C(12)-C(11)	110.83(8)
N(7)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12A)	109.5
N(7)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	108.1

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+1 #2 -x,-y+1,-z+1

Table 19. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **3**. The anisotropic displacement factor exponent takes the form: -2p2[h2 a*2U11 + ... + 2 h k a* b* U12]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	12(1)	11(1)	10(1)	-2(1)	-1(1)	-3(1)
Cl(1)	15(1)	18(1)	15(1)	-3(1)	-1(1)	-7(1)
Cl(2)	14(1)	11(1)	14(1)	-2(1)	1(1)	-2(1)
Cl(3)	20(1)	16(1)	12(1)	-5(1)	1(1)	-2(1)
Cl(4)	15(1)	15(1)	12(1)	-2(1)	-4(1)	-1(1)
O(1S)	21(1)	16(1)	44(1)	-2(1)	-9(1)	-2(1)
N(1)	12(1)	16(1)	15(1)	-3(1)	-3(1)	1(1)
N(7)	12(1)	16(1)	12(1)	-3(1)	3(1)	-2(1)
C(2)	13(1)	18(1)	15(1)	1(1)	-1(1)	-1(1)
C(3)	11(1)	16(1)	12(1)	-2(1)	-1(1)	0(1)
C(4)	10(1)	11(1)	12(1)	-4(1)	-2(1)	-1(1)
C(5)	11(1)	18(1)	14(1)	-2(1)	-1(1)	-2(1)
C(6)	12(1)	19(1)	14(1)	-4(1)	-1(1)	0(1)
C(8)	11(1)	18(1)	13(1)	-3(1)	1(1)	0(1)
C(9)	10(1)	17(1)	12(1)	-4(1)	1(1)	-1(1)
C(10)	11(1)	11(1)	11(1)	-2(1)	1(1)	-1(1)
C(11)	12(1)	19(1)	12(1)	-4(1)	0(1)	0(1)
C(12)	13(1)	24(1)	13(1)	-7(1)	1(1)	-4(1)

Table 20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2 x\ 10^3$) for compound **3**.

	x	y	z	U(eq)
H(1SA)	2410(20)	9050(20)	1160(20)	41(5)
H(1SB)	3430(20)	8480(20)	1970(20)	49(6)
H(2A)	8645	2770	2200	19
H(2B)	8948	1788	1017	19
H(3A)	10776	1139	2720	16
H(3B)	9926	-245	2706	16
H(4)	9430	1534	4804	13
H(5A)	7879	-924	4743	17
H(5B)	7588	67	5914	17
H(6A)	5785	755	4189	18
H(6B)	6676	2120	4185	18
H(8A)	4188	5033	3647	18
H(8B)	3365	3603	3739	18
H(9A)	2023	6303	4454	16
H(9B)	2400	4783	5591	16
H(10)	677	3659	4619	13
H(11A)	-788	5095	2781	17
H(11B)	51	6501	2739	17
H(12A)	1346	3837	1924	19
H(12B)	1022	5409	846	19
H(7A)	3409(17)	4965(16)	1482(16)	22(4)
H(7B)	2776(16)	6286(17)	1811(16)	23(4)
H(1A)	7210(17)	344(18)	2223(17)	28(4)
H(1B)	6547(18)	1783(17)	1934(17)	27(4)

Table 21. Hydrogen bonds for compound **3** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1S)-H(1SA)...Cl(1)#3	0.77(2)	2.45(2)	3.2107(10)	176.7(18)
O(1S)-H(1SB)...Cl(3)	0.78(2)	2.45(2)	3.1892(10)	158.2(19)
N(7)-H(7A)...Cl(2)#4	0.833(15)	2.699(15)	3.3428(9)	135.3(13)
N(7)-H(7A)...Cl(2)	0.833(15)	2.749(15)	3.3261(9)	127.9(12)
N(7)-H(7A)...Cl(4)#4	0.833(15)	2.847(15)	3.3874(9)	124.3(12)
N(7)-H(7B)...O(1S)	0.898(15)	1.891(15)	2.7798(12)	170.0(14)
N(1)-H(1A)...Cl(1)#5	0.886(16)	2.522(16)	3.2546(9)	140.4(13)
N(1)-H(1A)...Cl(3)#5	0.886(16)	2.720(16)	3.4443(9)	139.7(13)
N(1)-H(1B)...Cl(4)#4	0.850(16)	2.460(16)	3.1719(9)	141.8(14)
N(1)-H(1B)...Cl(2)	0.850(16)	2.928(16)	3.4592(9)	122.4(12)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+1 #2 -x,-y+1,-z+1 #3 -x+1,-y+2,-z

#4 -x+1,-y+1,-z #5 x,y-1,z

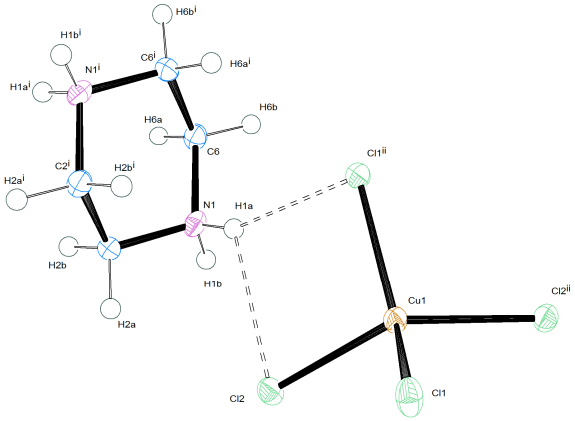

Figure 4. Showing the atomic thermal ellipsoid plot (50% probability level) and atomic numbering scheme for compound **4**.

Table 22. Crystal data and structure refinement for compound **4**.

Identification code	4	
Empirical formula	C4 H12 Cl3 Cu N2	
Formula weight	258.05	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 10.9151(9) Å	α= 90°.
	b = 6.7334(6) Å	β= 96.197(5)°.
	c = 12.1914(10) Å	γ = 90°.
Volume	890.78(13) Å^3	
Z	4	
Density (calculated)	1.924 Mg/m^3	
Absorption coefficient	3.281 mm^{-1}	
F(000)	520	
Crystal size	0.23 x 0.18 x 0.12 mm^3	
Theta range for data collection	3.36 to 33.21°.	
Index ranges	-16<=h<=16, -10<=k<=10, -18<=l<=18	
Reflections collected	5934	
Independent reflections	1706 [R(int) = 0.0520]	
Completeness to theta = 33.21°	99.6 %	
Absorption correction	Numerical	
Max. and min. transmission	0.6942 and 0.5165	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1706 / 0 / 55	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0352, wR2 = 0.0618	
R indices (all data)	R1 = 0.0527, wR2 = 0.0678	
Largest diff. peak and hole	0.575 and -0.741 e.Å^{-3}	

Table 23. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for compound **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	5000	5691(1)	2500	17(1)
Cl(1)	5000	8927(1)	2500	13(1)
Cl(2)	3943(1)	3698(1)	3583(1)	13(1)
N(1)	1938(1)	6933(3)	3930(1)	11(1)
C(2)	1507(2)	6071(3)	4951(1)	13(1)
C(6)	2554(2)	6033(3)	5873(1)	12(1)

Table 24. Selected bond lengths [Å] and angles [°] for compound **4**.

Cu(1)-Cl(1)	2.1792(9)
Cu(1)-Cl(2)	2.2816(5)

Table 25. Bond lengths [Å] and angles [°] for compound **4**.

Cu(1)-Cl(1)	2.1792(9)		
Cu(1)-Cl(2)	2.2816(5)		
Cu(1)-Cl(2)#1	2.2816(5)		
N(1)-C(6)#2	1.487(3)		
N(1)-C(2)	1.495(2)		
N(1)-H(1A)	0.89(2)		
N(1)-H(1B)	0.82(3)		
C(2)-C(6)	1.515(2)		
C(2)-H(2A)	0.9900		
C(2)-H(2B)	0.9900		
C(6)-N(1)#2	1.487(3)		
C(6)-H(6A)	0.9900		
C(6)-H(6B)	0.9900		
Cl(1)-Cu(1)-Cl(2)	126.036(15)		
Cl(1)-Cu(1)-Cl(2)#1	126.035(15)		
Cl(2)-Cu(1)-Cl(2)#1	107.93(3)		
C(6)#2-N(1)-C(2)	111.61(14)		
C(6)#2-N(1)-H(1A)	110.4(17)		
C(2)-N(1)-H(1A)	109.7(14)		
C(6)#2-N(1)-H(1B)	111.4(17)		
C(2)-N(1)-H(1B)	112.0(17)		
H(1A)-N(1)-H(1B)	101(2)		
N(1)-C(2)-C(6)	110.15(14)		
N(1)-C(2)-H(2A)	109.6		
C(6)-C(2)-H(2A)	109.6		
N(1)-C(2)-H(2B)	109.6		
C(6)-C(2)-H(2B)	109.6		
H(2A)-C(2)-H(2B)	108.1		
N(1)#2-C(6)-C(2)	110.03(16)		
N(1)#2-C(6)-H(6A)	109.7		
C(2)-C(6)-H(6A)	109.7		
N(1)#2-C(6)-H(6B)	109.7		
C(2)-C(6)-H(6B)	109.7		
H(6A)-C(6)-H(6B)	108.2		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2 #2 -x+1/2,-y+3/2,-z+1

Table 26. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **4**. The anisotropic displacement factor exponent takes the form: -2p2[h2 a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cu(1)	17(1)	10(1)	21(1)	0	-6(1)	0
Cl(1)	15(1)	9(1)	15(1)	0	0(1)	0
Cl(2)	14(1)	11(1)	13(1)	0(1)	1(1)	2(1)
N(1)	12(1)	10(1)	9(1)	-1(1)	-1(1)	2(1)
C(2)	12(1)	14(1)	13(1)	2(1)	0(1)	-5(1)
C(6)	13(1)	12(1)	11(1)	3(1)	0(1)	0(1)

Table 27. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2 x\ 10^3$) for compound **4.**

	x	y	z	U(eq)
H(1A)	1322(19)	6950(40)	3393(17)	15(5)
H(1B)	2430(20)	6210(40)	3666(18)	21(6)
H(2A)	1200	4704	4800	15
H(2B)	819	6879	5178	15
H(6A)	2251	5523	6556	14
H(6B)	3212	5133	5673	14

Table 28. Hydrogen bonds for compound **4** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Cl(1)#3	0.89(2)	2.66(2)	3.2882(17)	129(2)
N(1)-H(1A)...Cl(2)#4	0.89(2)	2.67(2)	3.3293(15)	132.1(18)
N(1)-H(1A)...Cl(2)#5	0.89(2)	2.88(2)	3.4616(16)	124.2(16)
N(1)-H(1B)...Cl(2)	0.82(3)	2.37(3)	3.1483(18)	159(2)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,y,-z+1/2 #2 -x+1/2,-y+3/2,-z+1 #3 x-1/2,y-1/2,z #4 -x+1/2,y+1/2,-z+1/2 #5 x-1/2,y+1/2,z

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