Supplementary Information

Novel Linear Trinuclear Cu^{II} Compound with Trapped Chiral Hemiaminal Ligand: Magnetostructural Study

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1. Synthetical procedure and supplementary analysis

The trinuclear complex is very soluble in methanol and acetonitrile. Several attempts were made to accelerate the crystallization using layering and vapor diffusion with tetrahydrofuran, chloroform, and diethyl ether as antisolvent without success.

The infrared spectra of **1** show broadband between 1130 and 948 cm^{-1} and 995 cm^{-1} characteristics of the ClO_4^- ion (Figure S1b).

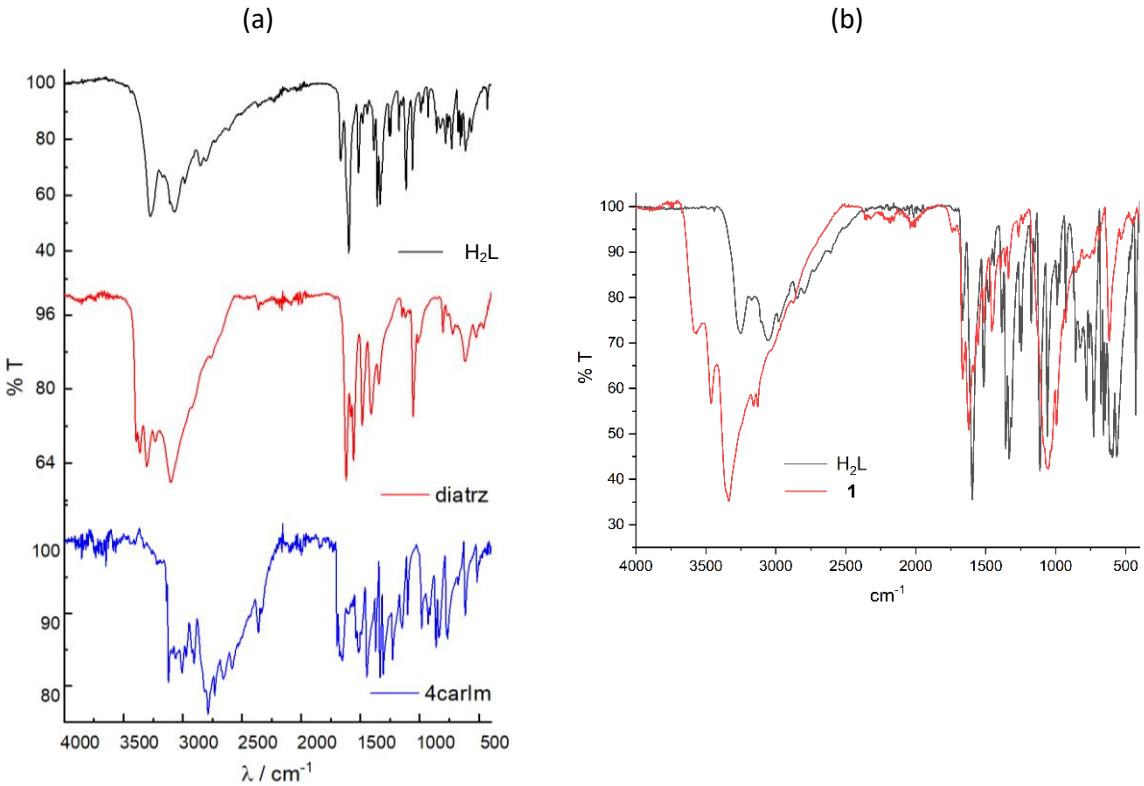


Figure S1. (a) Spectra of H_2L ligand (black) diatrz (red) and 4carIm (blue). (b) Spectra of H_2L (black) and of **1** (red).

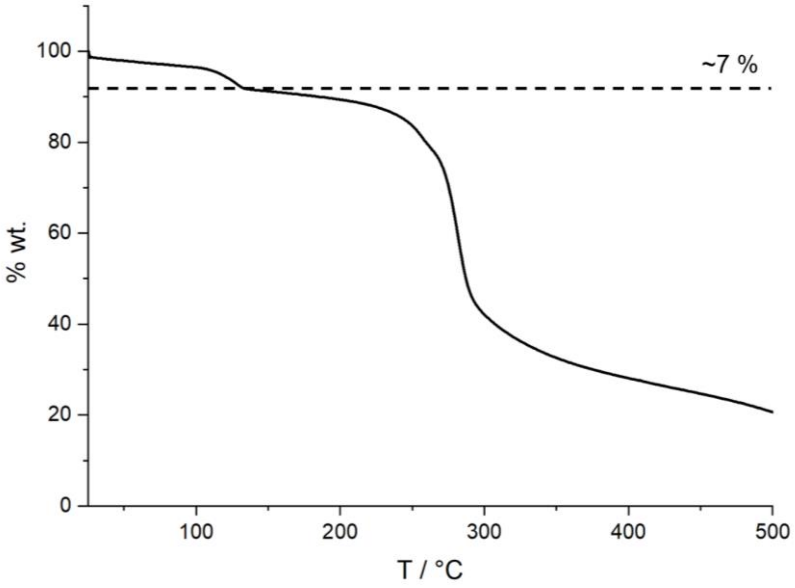
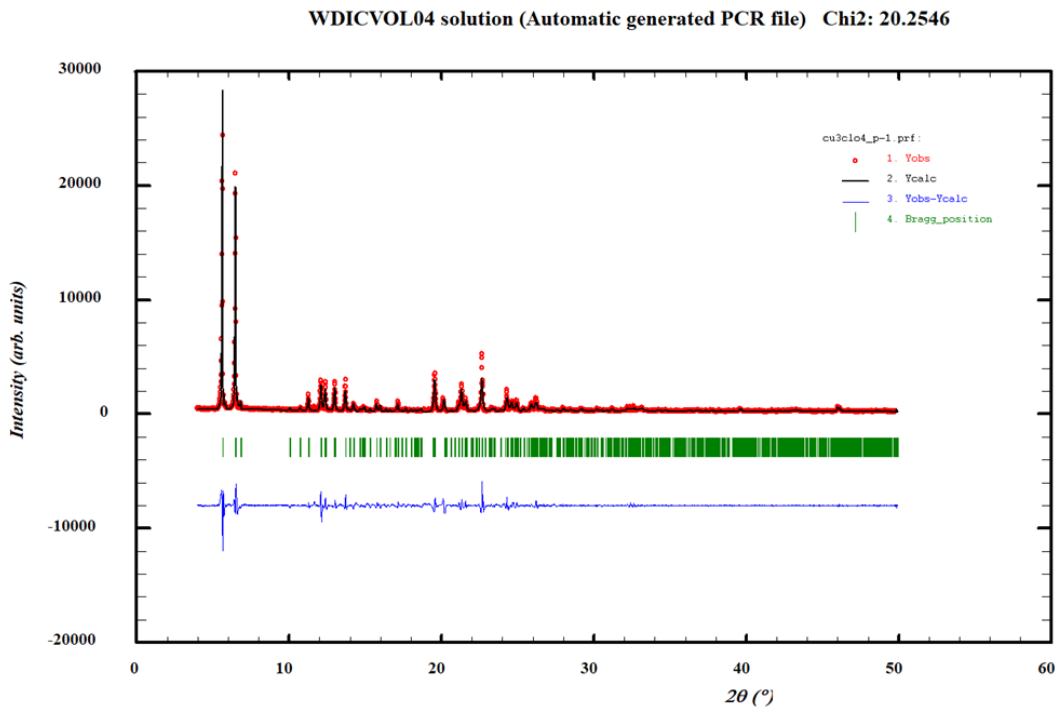


Figure S2. Thermogram in N_2 atmosphere of compound **1**.



Refined unit-cell in P-1:
a = 7.38553 (0.00036)
b = 14.71983 (0.00073)
c = 17.13576 (0.00127)
α = 110.25927 (0.00595)
β = 99.78921 (0.00918)
γ = 95.57783 (0.00880)

Rp: 13.5
Rwp: 20.8
Rexp: 4.63
Chi2: 20.3

Figure S3. Le Bail fit of the X-ray powder diffraction patterns of powder sample of **1**. The powder pattern fittings by pattern-matching with the Le Bail fit is possible to determine that the experimental XRPD of **1** agree with the calculated pattern generated by the SC-XRD data.

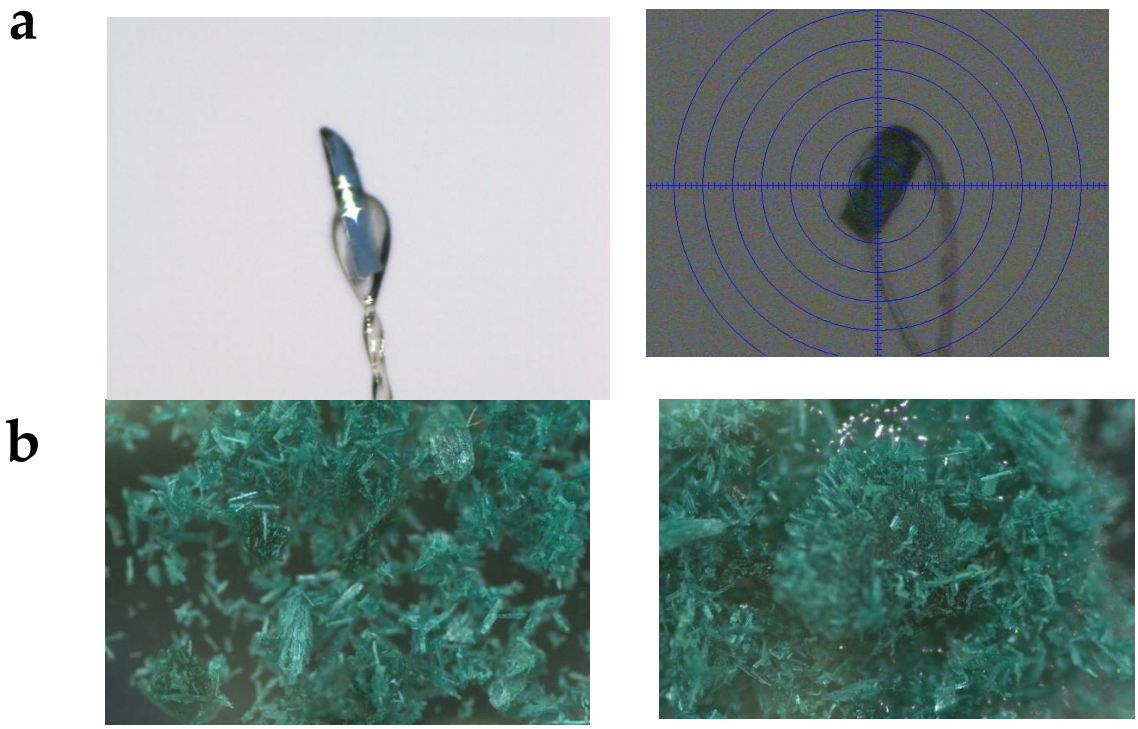


Figure S4. (a) Crystal of **1** used for X-ray Crystal Structure Analysis and (b) bulk crystalline sample used for characterization.

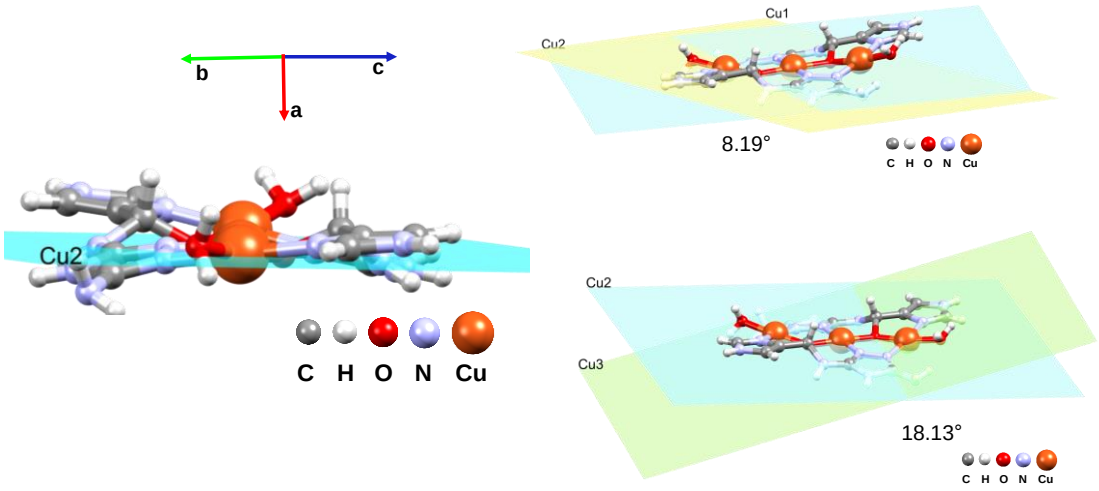


Figure S5. view of Cu1-Cu2-Cu3 linear core in compound **1**; Cu1/Cu2 and Cu2/Cu3 planes.

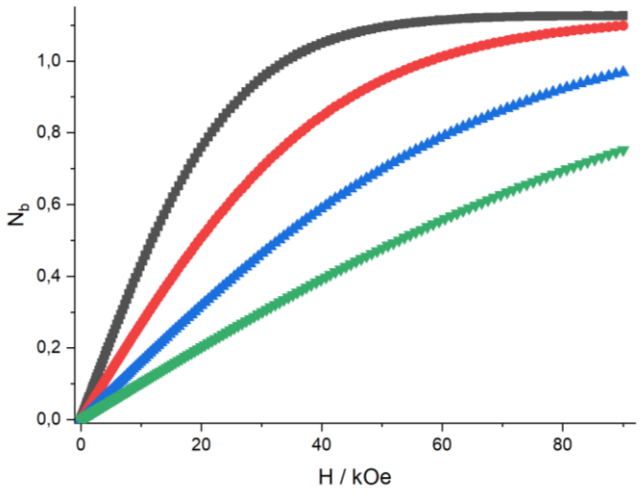
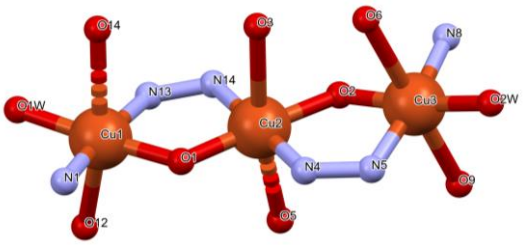
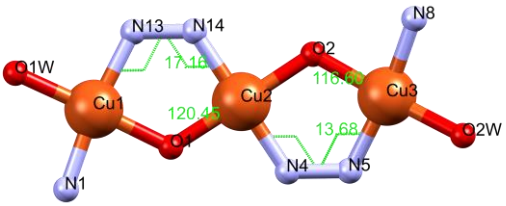


Figure S6. Isothermal magnetization at 1.8 (■), 3 (●), 5 (Δ) and 8 K (Δ) for **1**.





Cu-NN-Cu torsion angle (°)		Cu-O-Cu bite angle (°)	
Cu1 N13 N14 Cu2	17.2(8)	Cu2 O1 Cu1	120.5(3)
Cu2 N4 N5 Cu3	13.7(8)	Cu2 O2 Cu3	116.6(3)

Figure S7. Atom label in Cu_3 central core; Cu-NN-Cu torsion angles in Cu_3 central core in **1**.

2. Additional crystallographic data

Table S1. Complete Data of refinement of 1.

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cu1	2251.5(16)	6405.9(7)	2675.8(7)	31.1(3)
Cu2	2601.5(15)	7579.9(7)	4777.9(6)	25.0(3)
Cu3	2487.6(15)	8694.4(7)	6817.9(6)	28.0(3)
O1W	1766(10)	6373(5)	1485(4)	45.0(17)
O1	2493(8)	6392(4)	3829(4)	30.5(14)
O2	2830(8)	8807(4)	5748(3)	24.2(12)
O2W	1867(10)	8630(5)	7888(4)	42.0(16)
N1	1834(11)	4994(5)	2350(4)	32.7(17)
N2	1553(15)	3420(6)	1887(6)	56(3)
N3	2771(12)	5296(5)	4568(5)	36.2(19)
N4	2716(10)	6864(5)	5529(4)	27.7(16)
N5	2914(10)	7322(5)	6417(4)	29.2(16)
N6	3610(14)	6750(6)	7560(5)	52(2)
N7	3283(11)	5782(5)	6097(4)	30.4(17)
N8	2024(11)	10040(5)	7069(4)	32.4(17)
N9	1750(11)	11582(5)	7492(5)	37.9(19)
N10	2785(11)	9903(5)	5006(4)	31.2(17)
N11	3171(11)	9446(5)	3543(4)	31.0(17)
N12	3475(13)	8464(6)	2146(5)	49(2)
N13	2663(10)	7856(5)	3169(4)	27.8(16)
N14	2510(10)	8297(5)	4016(4)	27.3(16)
C1	1692(17)	4175(7)	1685(7)	51(3)
C2	1557(17)	3716(7)	2733(6)	51(3)
C3	1720(13)	4706(6)	3016(5)	31(2)
C4	1687(13)	5498(6)	3854(6)	31(2)
C5	2880(12)	5944(6)	5356(6)	29.5(19)
C6	3265(13)	6656(6)	6741(6)	32(2)
C7	1894(14)	10816(6)	7711(6)	36(2)
C8	1787(12)	11299(6)	6636(6)	31.0(19)
C9	1924(11)	10332(6)	6374(5)	27.2(18)
C10	1927(12)	9519(5)	5550(5)	25.8(18)
C11	2811(11)	9238(6)	4229(5)	23.9(17)
C12	3087(13)	8551(6)	2910(6)	35(2)
Cl1	-2196(3)	7543.9(16)	5282.6(16)	38.3(6)
O3	-1063(10)	7402(6)	4656(5)	54.8(19)
O4	-3035(12)	6609(6)	5216(7)	77(3)
O5	-3613(11)	8098(6)	5121(6)	62(2)
O6	-1036(12)	8048(8)	6112(5)	86(3)
Cl2	6843(4)	5893.4(17)	2375.0(16)	41.1(6)
O11	6924(16)	5421(8)	2948(7)	100(4)

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O12	5573(12)	6559(7)	2536(8)	93(4)
O13	6310(20)	5178(10)	1582(7)	148(6)
O14	8619(11)	6438(6)	2515(6)	71(3)
Cl3	7119(4)	9219.0(17)	8171.8(16)	42.9(6)
O7	8330(18)	10051(8)	8653(10)	140(6)
O8	5952(16)	8966(11)	8666(7)	119(4)
O9	5868(13)	9336(7)	7472(6)	81(3)
O10	8035(15)	8418(6)	7883(7)	91(3)
Cl4	4078(6)	7458(3)	9912(2)	85.4(11)
O15	5120(40)	6850(20)	9360(16)	103(8)
O17	4940(50)	8280(20)	10590(20)	133(10)
O19	2910(40)	7910(20)	9340(19)	135(9)
O22	4740(30)	7118(16)	10606(14)	99(7)
O16	5500(40)	7400(20)	9432(16)	108(8)
O18	3850(40)	8500(20)	10343(18)	120(9)
O20	2470(50)	6790(20)	9330(20)	150(11)
O21	2680(60)	6930(30)	10040(30)	186(15)
O3W	3000(20)	5040(10)	196(9)	141(5)
O4W	−1250(14)	7006(7)	833(6)	84(3)
O5W	9380(18)	8142(8)	9848(7)	113(4)
O6W	2875(17)	10122(8)	9451(6)	102(4)

Anisotropic Displacement Parameters (Å^2×10^3) for 1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu1	41.0(7)	26.4(5)	28.9(6)	11.6(4)	11.5(5)	7.2(5)
Cu2	32.7(6)	19.2(5)	28.0(6)	12.6(4)	10.3(4)	6.7(4)
Cu3	33.0(6)	25.9(5)	29.6(6)	13.3(4)	10.7(4)	7.1(4)
O1W	59(5)	49(4)	34(4)	20(3)	19(3)	12(3)
O1	41(4)	13(3)	41(4)	9(2)	18(3)	5(2)
O2	35(3)	25(3)	21(3)	15(2)	11(2)	10(2)
O2W	51(4)	46(4)	43(4)	23(3)	28(3)	14(3)
N1	44(5)	20(3)	31(4)	8(3)	4(3)	3(3)
N2	88(8)	28(4)	52(6)	11(4)	22(5)	13(5)
N3	58(6)	21(3)	37(4)	18(3)	11(4)	11(3)
N4	36(4)	20(3)	25(4)	2(3)	10(3)	8(3)
N5	39(4)	28(4)	25(4)	13(3)	10(3)	10(3)
N6	89(8)	42(5)	32(5)	25(4)	8(4)	14(5)
N7	46(5)	22(3)	28(4)	15(3)	7(3)	10(3)
N8	42(5)	31(4)	28(4)	14(3)	7(3)	8(3)
N9	45(5)	25(4)	41(5)	6(3)	13(4)	10(3)
N10	40(5)	20(3)	35(4)	12(3)	11(3)	−2(3)

Anisotropic Displacement Parameters ($Å^2×10^3$) for 1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N11	42(5)	26(4)	35(4)	18(3)	16(3)	3(3)
N12	74(7)	51(5)	32(4)	21(4)	20(4)	17(5)
N13	38(4)	24(3)	29(4)	17(3)	9(3)	9(3)
N14	25(4)	34(4)	26(4)	16(3)	4(3)	3(3)
C1	73(8)	36(5)	47(6)	13(5)	18(5)	17(5)
C2	83(9)	31(5)	35(6)	10(4)	10(5)	1(5)
C3	37(5)	24(4)	32(5)	10(4)	4(4)	4(4)
C4	28(5)	30(4)	41(5)	18(4)	13(4)	-1(4)
C5	27(5)	26(4)	40(5)	16(4)	10(4)	5(4)
C6	33(5)	22(4)	40(5)	13(4)	6(4)	1(4)
C7	50(6)	30(5)	35(5)	13(4)	20(4)	11(4)
C8	27(5)	30(4)	34(5)	12(4)	4(4)	0(4)
C9	16(4)	31(4)	34(5)	11(4)	6(3)	4(3)
C10	31(5)	19(4)	30(5)	11(3)	8(4)	7(3)
C11	17(4)	29(4)	35(5)	21(4)	10(3)	6(3)
C12	40(6)	32(5)	33(5)	14(4)	10(4)	1(4)
Cl1	26.2(12)	39.1(12)	56.2(15)	26.4(11)	8.4(10)	2.7(9)
O3	40(4)	74(5)	59(5)	31(4)	16(4)	14(4)
O4	55(5)	54(5)	150(9)	73(6)	21(5)	5(4)
O5	45(5)	58(5)	108(7)	53(5)	25(4)	24(4)
O6	50(5)	141(9)	50(5)	23(5)	10(4)	-17(6)
Cl2	42.7(15)	33.0(12)	51.3(15)	18.9(11)	12.8(11)	5.5(10)
O11	113(9)	106(8)	111(8)	89(7)	12(7)	-3(7)
O12	35(5)	66(6)	197(11)	67(7)	31(6)	12(4)
O13	182(14)	130(10)	67(7)	-33(7)	29(8)	-31(10)
O14	40(5)	51(5)	139(8)	45(5)	41(5)	11(4)
Cl3	40.6(14)	38.2(12)	51.9(15)	18.0(11)	10.6(11)	10.1(11)
O7	104(10)	68(7)	198(14)	40(8)	-56(9)	-19(6)
O8	88(8)	209(14)	95(8)	85(9)	41(7)	31(9)
O9	70(6)	83(6)	95(7)	59(6)	-13(5)	-7(5)
O10	107(8)	53(5)	122(8)	31(5)	39(7)	38(5)
Cl4	98(3)	98(3)	52(2)	15.6(19)	25.2(19)	0(2)
O3W	175(14)	115(10)	146(12)	28(9)	102(11)	23(9)
O4W	98(8)	83(6)	71(6)	26(5)	17(5)	38(6)
O5W	118(10)	93(8)	102(8)	12(7)	1(7)	26(7)
O6W	126(10)	121(9)	43(5)	13(5)	6(5)	30(7)

Bond Lengths for 1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	$Cu1^1$	7.4052(9)	N9	C7	1.312(11)
Cu1	Cu2	3.3635(14)	N9	C8	1.384(11)
Cu1	O1W	1.991(6)	N10	C10	1.456(11)

Bond Lengths for 1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	O1	1.960(6)	N10	C11	1.356(10)
Cu1	N1	1.939(7)	N11	C11	1.377(10)
Cu1	N13	1.979(7)	N11	C12	1.375(11)
Cu1	O12	2.514(9)	N12	C12	1.356(12)
Cu2	Cu2[1]	7.4052(9)	N13	N14	1.400(9)
Cu2	Cu3[1]	7.3084(17)	N13	C12	1.287(11)
Cu2	Cu3	3.3284(14)	N14	C11	1.293(10)
Cu2	O1	1.915(5)	C2	C3	1.354(12)
Cu2	O2	1.955(5)	C3	C4	1.509(12)
Cu2	N4	1.921(7)	C8	C9	1.354(11)
Cu2	N14	1.939(7)	C9	C10	1.502(11)
Cu2	O3	2.669(7)	Cl1	O3	1.449(8)
Cu2	O5[1]	2.747(8)	Cl1	O4	1.423(7)
Cu3	O2	1.957(5)	Cl1	O5	1.424(7)
Cu3	O2W	2.002(6)	Cl1	O6	1.427(9)
Cu3	N5	1.966(7)	Cl2	O11	1.382(8)
Cu3	N8	1.946(7)	Cl2	O12	1.403(9)
Cu3	O6	2.617(9)	Cl2	O13	1.364(10)
Cu3	O9	2.510(9)	Cl2	O14	1.421(8)
O1	C4	1.419(10)	O14	Cu1[1]	2.660(8)
O2	C10	1.390(9)	Cl3	O7	1.359(10)
N1	C1	1.321(12)	Cl3	O8	1.427(11)
N1	C3	1.363(11)	Cl3	O9	1.446(8)
N2	C1	1.274(13)	Cl3	O10	1.391(9)
N2	C2	1.363(13)	Cl4	O15	1.44(3)
N3	C4	1.473(11)	Cl4	O17	1.36(3)
N3	C5	1.341(11)	Cl4	O19	1.55(3)
N4	N5	1.409(9)	Cl4	O22	1.46(2)
N4	C5	1.303(10)	Cl4	O16	1.44(3)
N5	C6	1.305(10)	Cl4	O18	1.49(3)
N6	C6	1.336(12)	Cl4	O20	1.45(3)
N7	C5	1.357(11)	Cl4	O21	1.34(4)
N7	C6	1.377(10)	O17	O22	1.71(4)
N8	C7	1.308(11)	O20	O21	1.15(4)
N8	C9	1.394(11)			

[1]1+X,+Y,+Z

Bond Angles for 1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cu2	Cu1	Cu1[1]	99.01(3)	C10	O2	Cu3	113.7(5)
O1W	Cu1	Cu1[1]	89.6(2)	C1	N1	Cu1	141.3(7)
O1W	Cu1	Cu2	151.3(2)	C1	N1	C3	105.4(8)

Bond Angles for 1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1W	Cu1	O12	82.4(4)	C3	N1	Cu1	113.2(5)
O1	Cu1	Cu1[1]	95.19(18)	C1	N2	C2	108.7(9)
O1	Cu1	Cu2	29.39(15)	C5	N3	C4	117.1(7)
O1	Cu1	O1W	174.9(3)	N5	N4	Cu2	122.9(5)
O1	Cu1	N13	89.1(2)	C5	N4	Cu2	128.2(6)
O1	Cu1	O12	102.5(3)	C5	N4	N5	108.3(7)
N1	Cu1	Cu1[1]	91.4(2)	N4	N5	Cu3	115.5(5)
N1	Cu1	Cu2	112.0(2)	C6	N5	Cu3	137.8(6)
N1	Cu1	O1W	95.0(3)	C6	N5	N4	106.5(6)
N1	Cu1	O1	83.0(3)	C5	N7	C6	106.5(7)
N1	Cu1	N13	172.1(3)	C7	N8	Cu3	140.5(6)
N1	Cu1	O12	96.9(3)	C7	N8	C9	105.9(7)
N13	Cu1	Cu1[1]	90.4(2)	C9	N8	Cu3	113.3(5)
N13	Cu1	Cu2	60.12(19)	C7	N9	C8	108.1(7)
N13	Cu1	O1W	92.7(3)	C11	N10	C10	115.5(6)
N13	Cu1	O12	85.8(3)	C12	N11	C11	105.4(7)
O12	Cu1	Cu1[1]	8.7(2)	N14	N13	Cu1	116.9(5)
O12	Cu1	Cu2	103.0(3)	C12	N13	Cu1	135.9(6)
Cu1	Cu2	Cu2[1]	80.99(3)	C12	N13	N14	107.2(7)
Cu1	Cu2	Cu3[1]	107.13(3)	N13	N14	Cu2	122.0(5)
Cu3	Cu2	Cu1	174.28(4)	C11	N14	Cu2	127.0(6)
Cu3	Cu2	Cu2[1]	104.69(3)	C11	N14	N13	108.4(6)
Cu3[1]	Cu2	Cu2[1]	26.137(12)	N2	C1	N1	111.9(10)
Cu3	Cu2	Cu3[1]	78.55(3)	C3	C2	N2	105.5(9)
O1	Cu2	Cu1	30.15(17)	N1	C3	C4	116.9(7)
O1	Cu2	Cu2[1]	79.49(19)	C2	C3	N1	108.4(8)
O1	Cu2	Cu3	149.28(17)	C2	C3	C4	134.5(9)
O1	Cu2	Cu3[1]	101.92(19)	O1	C4	N3	110.2(7)
O1	Cu2	O2	177.4(3)	O1	C4	C3	106.6(7)
O1	Cu2	N4	90.4(3)	N3	C4	C3	110.2(7)
O1	Cu2	N14	89.3(3)	N3	C5	N7	126.9(7)
O1	Cu2	O3	94.8(2)	N4	C5	N3	123.9(8)
O1	Cu2	O5[1]	95.6(3)	N4	C5	N7	109.0(7)
O2	Cu2	Cu1	149.31(15)	N5	C6	N6	128.5(8)
O2	Cu2	Cu2[1]	97.99(17)	N5	C6	N7	109.5(8)
O2	Cu2	Cu3	31.73(15)	N6	C6	N7	122.0(8)
O2	Cu2	Cu3[1]	75.73(17)	N8	C7	N9	111.8(8)
O2	Cu2	O3	87.7(2)	C9	C8	N9	105.6(8)
O2	Cu2	O5[1]	81.9(2)	N8	C9	C10	114.2(7)
N4	Cu2	Cu1	120.54(19)	C8	C9	N8	108.6(7)
N4	Cu2	Cu2[1]	92.0(2)	C8	C9	C10	137.2(8)
N4	Cu2	Cu3	59.30(18)	O2	C10	N10	113.1(7)
N4	Cu2	Cu3[1]	78.6(2)	O2	C10	C9	107.7(7)
N4	Cu2	O2	90.1(2)	N10	C10	C9	110.2(7)

Bond Angles for 1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N4	Cu2	N14	179.4(3)	N10	C11	N11	126.1(7)
N4	Cu2	O3	87.4(3)	N14	C11	N10	125.0(7)
N4	Cu2	O5[1]	94.0(3)	N14	C11	N11	108.9(7)
N14	Cu2	Cu1	59.2(2)	N12	C12	N11	122.3(8)
N14	Cu2	Cu2[1]	87.5(2)	N13	C12	N11	110.1(8)
N14	Cu2	Cu3[1]	101.0(2)	N13	C12	N12	127.6(8)
N14	Cu2	Cu3	121.1(2)	O4	Cl1	O3	108.6(6)
N14	Cu2	O2	90.2(3)	O4	Cl1	O5	109.2(5)
N14	Cu2	O3	93.1(3)	O4	Cl1	O6	110.2(6)
N14	Cu2	O5[1]	85.5(3)	O5	Cl1	O3	109.9(5)
O3	Cu2	Cu1	94.42(16)	O5	Cl1	O6	110.2(6)
O3	Cu2	Cu2[1]	174.27(17)	O6	Cl1	O3	108.8(5)
O3	Cu2	Cu3	79.87(16)	Cl1	O3	Cu2	132.9(4)
O3	Cu2	Cu3[1]	158.14(16)	Cl1	O6	Cu3	138.9(5)
O3	Cu2	O5[1]	169.5(2)	O11	Cl2	O12	108.8(7)
O5[1]	Cu2	Cu1	93.80(19)	O11	Cl2	O14	108.6(6)
O5[1]	Cu2	Cu2[1]	16.22(17)	O12	Cl2	O14	107.8(5)
O5[1]	Cu2	Cu3	91.90(19)	O13	Cl2	O11	106.3(9)
O5[1]	Cu2	Cu3[1]	16.71(18)	O13	Cl2	O12	112.4(9)
O2	Cu3	Cu2	31.68(15)	O13	Cl2	O14	112.8(8)
O2	Cu3	O2W	173.7(3)	Cl2	O12	Cu1	133.6(5)
O2	Cu3	N5	91.0(2)	Cl2	O14	Cu1[1]	146.4(5)
O2	Cu3	O6	88.8(3)	O7	Cl3	O8	110.7(9)
O2	Cu3	O9	90.0(3)	O7	Cl3	O9	112.2(7)
O2W	Cu3	Cu2	149.7(2)	O7	Cl3	O10	111.7(8)
O2W	Cu3	O6	86.2(3)	O8	Cl3	O9	105.3(7)
O2W	Cu3	O9	94.9(3)	O10	Cl3	O8	105.4(7)
N5	Cu3	Cu2	61.1(2)	O10	Cl3	O9	111.2(7)
N5	Cu3	O2W	92.7(3)	Cl3	O9	Cu3	131.6(5)
N5	Cu3	O6	87.6(3)	O15	Cl4	O19	103.9(15)
N5	Cu3	O9	93.0(3)	O15	Cl4	O22	93.1(14)
N8	Cu3	Cu2	111.9(2)	O17	Cl4	O15	120.8(18)
N8	Cu3	O2	82.2(3)	O17	Cl4	O19	100.8(18)
N8	Cu3	O2W	93.9(3)	O17	Cl4	O22	74.7(15)
N8	Cu3	N5	173.0(3)	O22	Cl4	O19	162.0(15)
N8	Cu3	O6	90.4(4)	O16	Cl4	O18	110.6(16)
N8	Cu3	O9	88.9(3)	O16	Cl4	O20	105.7(18)
O6	Cu3	Cu2	78.25(19)	O20	Cl4	O18	117.7(18)
O9	Cu3	Cu2	101.0(2)	O21	Cl4	O16	144(2)
O9	Cu3	O6	178.7(3)	O21	Cl4	O18	105(2)
Cu2	O1	Cu1	120.5(3)	O21	Cl4	O20	48.4(18)
C4	O1	Cu1	114.1(5)	Cl4	O17	O22	55.5(14)
C4	O1	Cu2	118.5(5)	Cl4	O22	O17	49.8(13)
Cu2	O2	Cu3	116.6(3)	O21	O20	Cl4	61(3)

Bond Angles for 1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C10	O2	Cu2	114.2(5)	O20	O21	Cl4	71(3)

[1]1+X,+Y,+Z

Hydrogen Bonds for 1.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N7	H7	O11[1]	0.86	2.14	2.811(11)	134.0

[1]1-X,1-Y,1-Z

Torsion Angles for 1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Cu1	O1	C4	N3	146.2(5)	C4	N3	C5	N7	158.4(8)
Cu1	O1	C4	C3	26.6(8)	C5	N3	C4	O1	62.1(10)
Cu1	N1	C1	N2	174.4(8)	C5	N3	C4	C3	179.5(8)
Cu1	N1	C3	C2	-175.9(7)	C5	N4	N5	Cu3	-174.6(6)
Cu1	N1	C3	C4	7.5(10)	C5	N4	N5	C6	2.5(10)
Cu1	N13	N14	Cu2	17.2(8)	C5	N7	C6	N5	-1.4(10)
Cu1	N13	N14	C11	-179.7(5)	C5	N7	C6	N6	179.9(9)
Cu1	N13	C12	N11	179.4(6)	C6	N7	C5	N3	179.2(9)
Cu1	N13	C12	N12	-2.8(17)	C6	N7	C5	N4	3.0(10)
Cu2	O1	C4	N3	-62.7(8)	C7	N8	C9	C8	1.7(10)
Cu2	O1	C4	C3	177.7(5)	C7	N8	C9	C10	-176.3(8)
Cu2	O2	C10	N10	-68.4(8)	C7	N9	C8	C9	1.1(10)
Cu2	O2	C10	C9	169.7(5)	C8	N9	C7	N8	0.0(12)
Cu2	N4	N5	Cu3	13.7(8)	C8	C9	C10	O2	156.7(10)
Cu2	N4	N5	C6	-169.2(6)	C8	C9	C10	N10	32.9(14)
Cu2	N4	C5	N3	-8.6(13)	C9	N8	C7	N9	-1.0(11)
Cu2	N4	C5	N7	167.7(6)	C10	N10	C11	N11	165.2(8)
Cu2	N14	C11	N10	-17.7(12)	C10	N10	C11	N14	-15.3(12)
Cu2	N14	C11	N11	161.9(6)	C11	N10	C10	O2	61.5(10)
Cu3	O2	C10	N10	154.5(5)	C11	N10	C10	C9	-177.9(7)
Cu3	O2	C10	C9	32.5(8)	C11	N11	C12	N12	-176.2(9)
Cu3	N5	C6	N6	-5.9(17)	C11	N11	C12	N13	1.7(10)
Cu3	N5	C6	N7	175.5(7)	C12	N11	C11	N10	178.6(8)
Cu3	N8	C7	N9	172.7(8)	C12	N11	C11	N14	-0.9(10)
Cu3	N8	C9	C8	-174.0(6)	C12	N13	N14	Cu2	-161.9(6)
Cu3	N8	C9	C10	8.1(9)	C12	N13	N14	C11	1.2(10)
N1	C3	C4	O1	-22.1(11)	O3	Cl1	O6	Cu3	-4.0(12)
N1	C3	C4	N3	-141.8(8)	O4	Cl1	O3	Cu2	-106.6(7)
N2	C2	C3	N1	-0.7(13)	O4	Cl1	O6	Cu3	114.9(10)

Torsion Angles for 1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N2	C2	C3	C4	175.1(10)	O5	Cl1	O3	Cu2	134.1(6)
N4	N5	C6	N6	178.0(10)	O5	Cl1	O6	Cu3	-124.5(9)
N4	N5	C6	N7	-0.6(10)	O6	Cl1	O3	Cu2	13.3(8)
N5	N4	C5	N3	-179.7(8)	O11	Cl2	O12	Cu1	-52.4(11)
N5	N4	C5	N7	-3.4(10)	O11	Cl2	O14	Cu1[1]	51.9(13)
N8	C9	C10	O2	-26.1(10)	O12	Cl2	O14	Cu1[1]	169.6(10)
N8	C9	C10	N10	-149.8(7)	O13	Cl2	O12	Cu1	65.1(12)
N9	C8	C9	N8	-1.7(10)	O13	Cl2	O14	Cu1[1]	-65.7(14)
N9	C8	C9	C10	175.6(10)	O14	Cl2	O12	Cu1	-170.0(8)
N13	N14	C11	N10	-179.7(8)	O7	Cl3	O9	Cu3	-142.2(10)
N13	N14	C11	N11	-0.1(9)	O8	Cl3	O9	Cu3	-21.8(10)
N14	N13	C12	N11	-1.8(10)	O10	Cl3	O9	Cu3	91.9(9)
N14	N13	C12	N12	176.0(10)	O15	Cl4	O17	O22	-84.4(18)
C1	N1	C3	C2	1.5(12)	O15	Cl4	O22	O17	121.2(19)
C1	N1	C3	C4	-175.2(9)	O19	Cl4	O17	O22	162.1(15)
C1	N2	C2	C3	-0.3(14)	O19	Cl4	O22	O17	-78(5)
C2	N2	C1	N1	1.3(15)	O16	Cl4	O20	O21	151(3)
C2	C3	C4	O1	162.3(12)	O16	Cl4	O21	O20	-53(5)
C2	C3	C4	N3	42.7(15)	O18	Cl4	O20	O21	-85(3)
C3	N1	C1	N2	-1.7(13)	O18	Cl4	O21	O20	114(3)
C4	N3	C5	N4	-25.9(13)					

[1]1+X,+Y,+Z

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 1.

Atom	*x*	*y*	*z*	U(eq)
H2	1471	2824	1545	67
H3	3311	4784	4483	43
H6A	3846	6180	7716	62
H6B	3627	7389	8008	62
H7	3506	5240	6152	36
H9	1649	12160	7822	45
H10	3245	10511	5166	37
H11	3399	10016	3517	37
H12A	3295	7850	1819	59
H12B	2746	8769	1904	59
H1	1694	4152	1136	62
H2A	1468	3320	3050	62
H4	402	5535	3916	38
H7A	1902	10825	8257	43
H8	1730	11691	6311	37
H10A	637	9230	5255	31

Atomic Occupancy for 1.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
O15	0.5	O17	0.5	O19	0.5
O22	0.5	O16	0.5	O18	0.5
O20	0.5	O21	0.5		