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catena-Poly[[[aquacopper(II)]-bis-[μ-bis(3,5-dimethyl-1*H*-pyrazol-4-yl) selenide-κ^2N^2:$N^{2'}$]] dichloride monohydrate]

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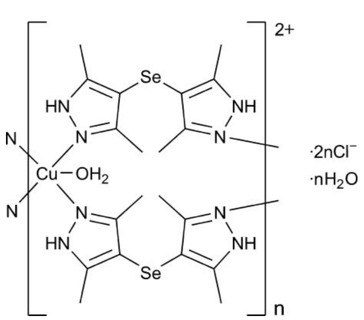
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.026; wR factor = 0.072; data-to-parameter ratio = 14.5.

In the title compound, {[Cu($C_{10}H_{14}N_4Se$)$_2$(H_2O)]Cl_2·H_2O}$_n$, the Cu^{II} ion, lying on a twofold rotation axis, has a square-pyramidal geometry constituted by four N atoms of pyrazolyl groups in the basal plane and an apical O atom of a water molecule. A pair of bis(3,5-dimethyl-1*H*-pyrazol-4-yl) selenide ligands bridge the Cu centers into a polymeric double-chain extending along [001]. The chloride anions are involved in intermolecular N—H···Cl and O—H···Cl hydrogen bonds, which link the chains into a three-dimensional network.

Related literature

For general background to the applications of coordination polymers, see: Farha *et al.* (2009); Shibahara *et al.* (2007); Zhang *et al.* (2009). For our studies of similar complexes, see: Seredyuk *et al.* (2007, 2009).



Experimental

Crystal data

[Cu($C_{10}H_{14}N_4Se$)$_2$(H_2O)]Cl_2·H_2O
M_r = 708.90
Monoclinic, $C2/c$
a = 11.332 (1) Å
b = 13.229 (2) Å
c = 18.786 (1) Å
β = 92.45 (3)°
V = 2813.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.59 mm^{-1}
T = 100 K
0.10 × 0.05 × 0.01 mm

Data collection

Kuma KM-4 CCD diffractometer
6625 measured reflections
2377 independent reflections
2217 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.072
S = 1.10
2377 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···Cl1	0.93	2.43	3.354 (2)	169
O1—H1O1···Cl1	0.88	2.25	3.0702 (10)	156
N2—H2N···Cl1^{i}	0.88	2.33	3.117 (2)	148
N4—H4N···Cl1^{ii}	0.88	2.27	3.144 (2)	176

Symmetry codes: (i) $-x-\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, y, -z+\frac{1}{2}$.

Data collection: *KM-4 CCD Software.* (Kuma Diffraction, 1998); cell refinement: *KM-4 CCD Software.*; data reduction: *KM-4 CCD Software.*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2286).

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supporting information

Acta Cryst. (2010). E**66**, m363 [doi:10.1107/S1600536810007403]

catena-Poly[[[aquacopper(II)]-bis[μ-bis(3,5-dimethyl-1*H*-pyrazol-4-yl) selenide-$\kappa^2N^2:N^{2\prime}$]] dichloride monohydrate]

Maksym Seredyuk, Yurii S. Moroz, Kateryna O. Znovjyak, Vadim A. Pavlenko and Igor O. Fritsky

S1. Comment

Study of metal-organic polymers is a well elaborated research area in coordination chemistry. Infinite molecular polymeric arrays are potentially applicable as specifically ordered crystalline substances with reversible selective sorption (Farha *et al.*, 2009; Zhang *et al.*, 2009), electrical conductivity (Zhang *et al.*, 2009) and molecular magnetism functionality (Shibahara *et al.*, 2007).

The title compound was prepared in a water–methanolic medium by mixing solutions of $CuCl_2.2H_2O$ and the bis(3,5-dimethyl-1*H*-pyrazolyl)selenide (*L*) ligand. It is similar to the copper compounds reported recently (Seredyuk *et al.*, 2007, 2009). A square pyramidal environment of the Cu^{II} ion is constituted by four non-coplanar N atoms of pyrazolyl rings [the Cu—N distances are 1.988 (2) and 2.017 (2) Å, the Cu—O distance is 2.208 (3) Å]. Adjacent Cu^{II} ions are linked by symmetrically equivalent ligands in a double-stranded bridge fashion (Fig. 1). Formed one-dimensional linear chain is running along the *c* axis, where the Cu atom deviates from the average basal plane by a value of 0.392 (1) Å (Fig. 2). The NH group of a pyrazole ring is involved in hydrogen bonding with chloride anion (Table 1), which further forms hydrogen bonds with both free and coordinated water molecules and additionally with a pyrazole ring of a neighbouring polymeric chain (Table 1). As a result, a dense network of hydrogen bonds is formed.

S2. Experimental

The ligand *L* was prepared according to a previously reported method (Seredyuk *et al.*, 2007). Copper(II) chloride dihydrate (0.034 g, 0.19 mmol) in water (5 ml) was added to 5 ml of hot methanol solution of *L* (0.100 g, 0.37 mmol). The solution was left for slow cooling at room temperature. After several days plate-like blue-violet crystals of the title compound suitable for X-ray analysis were isolated. Analysis, calculated for $C_{20}H_{32}Cl_2CuN_8O_2Se_2$: C 33.89, H 4.55, N 15.81%; found: C 33.67, H 4.51, N 15.60%.

S3. Refinement

C- and N-bound H atoms were placed at calculated positions and treated as riding on their parent atoms [C—H = 0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$; N—H = 0.88 Å and $U_{iso}(H) = 1.2U_{eq}(N)$]. The H atoms of water molecules were located from a difference Fourier map and were refined as riding, with $U_{iso}(H) = 1.5U_{eq}(O)$.

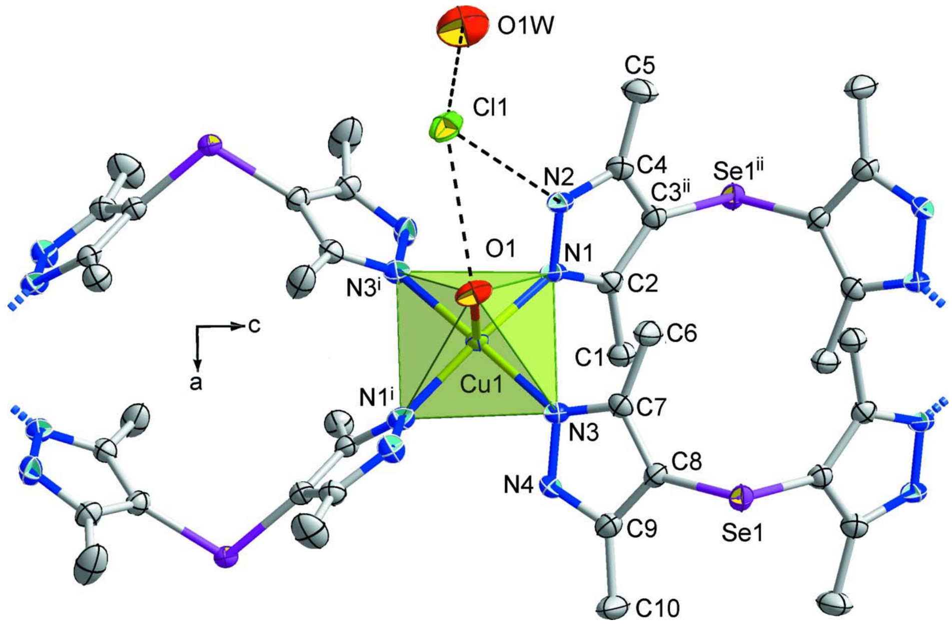

Figure 1

A portion of the double-chain structure of the title compound, showing the 50% probability displacement ellipsoids. H atoms are omitted for clarity. Dashed lines denote hydrogen bonds. [Symmetry codes: (i) -x, y, 1/2-z; (ii) -x, -y, 1-z.]

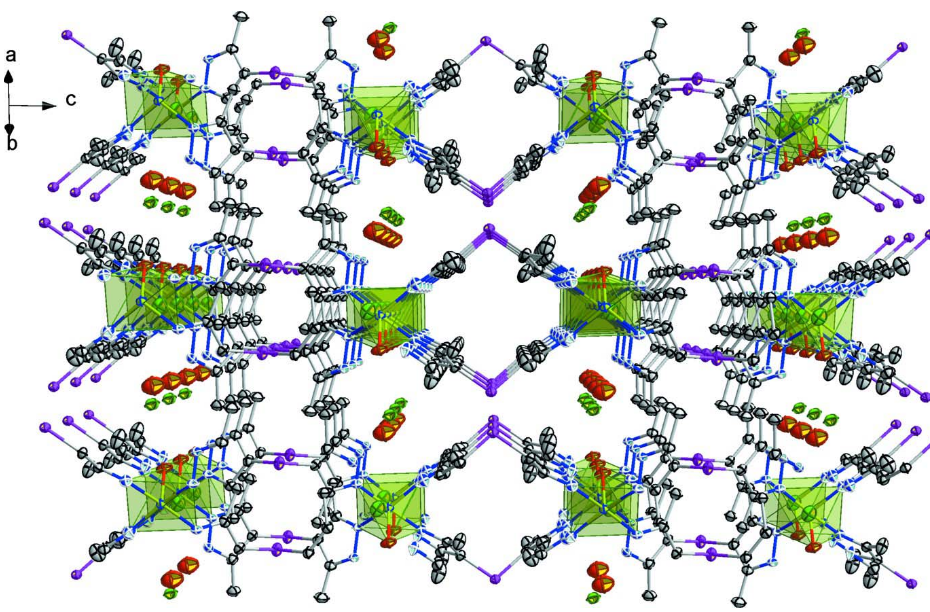

Figure 2

A packing diagram of the title compound. H atoms are omitted for clarity.

catena-Poly[[[aquacopper(II)]-bis[μ-bis(3,5-dimethyl-1H- pyrazol-4-yl) selenide-κ^2N^2:$N^{2'}$]] dichloride monohydrate]

Crystal data

$[Cu(C_{10}H_{14}N_4Se)_2(H_2O)]Cl_2 \cdot H_2O$
$M_r = 708.90$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 11.332$ (1) Å
$b = 13.229$ (2) Å
$c = 18.786$ (1) Å
$\beta = 92.45$ (3)°
$V = 2813.7$ (5) Å^3
$Z = 4$
$F(000) = 1420$
$D_x = 1.673$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6625 reflections
$\theta = 3.2$–28.4°
$\mu = 3.59$ mm^{-1}
$T = 100$ K
Plates, blue
0.10 × 0.05 × 0.01 mm

Data collection

Kuma KM-4 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
6625 measured reflections
2377 independent reflections
2217 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.2°$
$h = -13 \rightarrow 7$
$k = -15 \rightarrow 15$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.072$
$S = 1.10$
2377 reflections
164 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0419P)^2 + 1.7165P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.57$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	−0.0470 (2)	−0.1461 (2)	0.41623 (14)	0.0171 (6)
H22A	0.0111	−0.1105	0.4471	0.026*
H22B	−0.0068	−0.1790	0.3773	0.026*
H22C	−0.0873	−0.1974	0.4440	0.026*
C2	−0.1350 (2)	−0.07273 (19)	0.38631 (13)	0.0112 (5)
C3	0.2414 (2)	0.04235 (18)	0.58358 (13)	0.0106 (5)
C4	−0.2939 (2)	0.02624 (19)	0.36872 (14)	0.0137 (5)
C5	−0.4086 (2)	0.0822 (2)	0.36926 (16)	0.0232 (7)
H9A	−0.4637	0.0538	0.3330	0.035*
H9B	−0.3950	0.1538	0.3589	0.035*
H9C	−0.4421	0.0758	0.4163	0.035*
C6	0.0587 (2)	0.14112 (19)	0.38756 (14)	0.0124 (5)
H5A	0.0236	0.1593	0.3407	0.019*

H5B	0.1033	0.1988	0.4074	0.019*
H5C	−0.0040	0.1230	0.4196	0.019*
C7	0.1401 (2)	0.05297 (19)	0.37995 (13)	0.0106 (5)
C8	0.2365 (2)	0.02232 (19)	0.42508 (13)	0.0115 (5)
C9	0.2796 (2)	−0.0650 (2)	0.39493 (13)	0.0129 (5)
C10	0.3787 (2)	−0.1344 (2)	0.41780 (15)	0.0205 (6)
H14A	0.3463	−0.1955	0.4392	0.031*
H14B	0.4311	−0.1001	0.4529	0.031*
H14C	0.4234	−0.1532	0.3763	0.031*
N1	−0.12324 (17)	−0.02426 (15)	0.32427 (11)	0.0112 (4)
N2	−0.22165 (18)	0.03492 (15)	0.31502 (11)	0.0128 (4)
H2N	−0.2356	0.0742	0.2778	0.015*
N3	0.12555 (17)	−0.01244 (16)	0.32624 (11)	0.0113 (4)
N4	0.21226 (19)	−0.08360 (16)	0.33652 (12)	0.0123 (5)
H4N	0.2223	−0.1354	0.3080	0.015*
O1	0.0000	−0.19654 (18)	0.2500	0.0154 (5)
H1O1	−0.0625	−0.2317	0.2606	0.023*
O1W	−0.5000	−0.1193 (3)	0.2500	0.0387 (8)
H1W	−0.4338	−0.1589	0.2619	0.058*
Cl1	−0.25642 (5)	−0.26253 (5)	0.26925 (3)	0.01824 (17)
Cu1	0.0000	−0.02962 (3)	0.2500	0.00888 (13)
Se1	0.30884 (2)	0.097275 (18)	0.501388 (12)	0.01122 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0139 (12)	0.0217 (15)	0.0161 (14)	0.0071 (11)	0.0043 (11)	0.0059 (10)
C2	0.0097 (11)	0.0122 (12)	0.0116 (13)	−0.0016 (10)	−0.0015 (10)	−0.0020 (10)
C3	0.0099 (11)	0.0106 (12)	0.0114 (13)	−0.0014 (9)	0.0035 (10)	−0.0007 (9)
C4	0.0112 (12)	0.0169 (14)	0.0134 (14)	0.0001 (10)	0.0038 (11)	−0.0019 (10)
C5	0.0174 (14)	0.0321 (17)	0.0204 (15)	0.0133 (12)	0.0048 (12)	0.0067 (12)
C6	0.0120 (12)	0.0111 (13)	0.0139 (13)	0.0018 (10)	0.0005 (10)	−0.0001 (9)
C7	0.0087 (11)	0.0117 (12)	0.0113 (13)	−0.0023 (10)	0.0020 (10)	0.0011 (9)
C8	0.0077 (11)	0.0162 (13)	0.0105 (13)	−0.0012 (10)	0.0007 (10)	−0.0004 (9)
C9	0.0091 (12)	0.0158 (13)	0.0138 (14)	0.0009 (10)	0.0004 (11)	−0.0009 (10)
C10	0.0153 (13)	0.0217 (15)	0.0242 (15)	0.0091 (11)	−0.0030 (12)	−0.0013 (11)
N1	0.0090 (10)	0.0106 (11)	0.0139 (11)	0.0019 (8)	−0.0005 (9)	−0.0001 (8)
N2	0.0118 (10)	0.0162 (11)	0.0103 (11)	0.0042 (9)	−0.0009 (9)	0.0022 (8)
N3	0.0069 (10)	0.0116 (11)	0.0154 (11)	0.0024 (8)	0.0013 (9)	0.0009 (8)
N4	0.0108 (10)	0.0126 (11)	0.0134 (11)	0.0041 (8)	0.0004 (9)	−0.0020 (8)
O1	0.0122 (12)	0.0104 (13)	0.0241 (14)	0.000	0.0053 (11)	0.000
O1W	0.0318 (17)	0.0365 (19)	0.048 (2)	0.000	0.0058 (16)	0.000
Cl1	0.0215 (3)	0.0131 (3)	0.0206 (4)	−0.0055 (2)	0.0061 (3)	−0.0008 (2)
Cu1	0.0069 (2)	0.0108 (2)	0.0089 (2)	0.000	0.00069 (17)	0.000
Se1	0.00924 (16)	0.01421 (17)	0.01027 (17)	−0.00342 (9)	0.00104 (11)	−0.00041 (8)

Geometric parameters (Å, º)

C1—C2	1.485 (3)	C7—N3	1.334 (3)
C1—H22A	0.9800	C7—C8	1.413 (4)
C1—H22B	0.9800	C8—C9	1.385 (4)
C1—H22C	0.9800	C8—Se1	1.900 (2)
C2—N1	1.342 (3)	C9—N4	1.332 (3)
C2—C3^{i}	1.412 (3)	C9—C10	1.499 (3)
C3—C4^{i}	1.391 (4)	C10—H14A	0.9800
C3—C2^{i}	1.412 (3)	C10—H14B	0.9800
C3—Se1	1.896 (2)	C10—H14C	0.9800
C4—N2	1.331 (3)	N1—N2	1.368 (3)
C4—C3^{i}	1.391 (4)	N2—H2N	0.8800
C4—C5	1.496 (4)	N3—N4	1.368 (3)
C5—H9A	0.9800	N4—H4N	0.8800
C5—H9B	0.9800	O1—H1O1	0.8771
C5—H9C	0.9800	O1W—H1W	0.9337
C6—C7	1.497 (3)	Cu1—N1^{ii}	2.017 (2)
C6—H5A	0.9800	Cu1—N3^{ii}	1.988 (2)
C6—H5B	0.9800	Cu1—O1	2.208 (3)
C6—H5C	0.9800		
C2—C1—H22A	109.5	N4—C9—C8	106.9 (2)
C2—C1—H22B	109.5	N4—C9—C10	121.2 (2)
H22A—C1—H22B	109.5	C8—C9—C10	131.8 (2)
C2—C1—H22C	109.5	C9—C10—H14A	109.5
H22A—C1—H22C	109.5	C9—C10—H14B	109.5
H22B—C1—H22C	109.5	H14A—C10—H14B	109.5
N1—C2—C3^{i}	109.3 (2)	C9—C10—H14C	109.5
N1—C2—C1	123.4 (2)	H14A—C10—H14C	109.5
C3^{i}—C2—C1	127.3 (2)	H14B—C10—H14C	109.5
C4^{i}—C3—C2^{i}	106.1 (2)	C2—N1—N2	105.85 (19)
C4^{i}—C3—Se1	126.76 (19)	C2—N1—Cu1	132.97 (17)
C2^{i}—C3—Se1	126.70 (19)	N2—N1—Cu1	121.14 (15)
N2—C4—C3^{i}	106.5 (2)	C4—N2—N1	112.3 (2)
N2—C4—C5	121.7 (2)	C4—N2—H2N	123.9
C3^{i}—C4—C5	131.8 (2)	N1—N2—H2N	123.9
C4—C5—H9A	109.5	C7—N3—N4	105.95 (19)
C4—C5—H9B	109.5	C7—N3—Cu1	132.87 (17)
H9A—C5—H9B	109.5	N4—N3—Cu1	120.69 (16)
C4—C5—H9C	109.5	C9—N4—N3	111.8 (2)
H9A—C5—H9C	109.5	C9—N4—H4N	124.1
H9B—C5—H9C	109.5	N3—N4—H4N	124.1
C7—C6—H5A	109.5	Cu1—O1—H1O1	122.0
C7—C6—H5B	109.5	N3^{ii}—Cu1—N3	166.88 (12)
H5A—C6—H5B	109.5	N3^{ii}—Cu1—N1^{ii}	89.60 (8)
C7—C6—H5C	109.5	N3—Cu1—N1^{ii}	89.94 (8)
H5A—C6—H5C	109.5	N3^{ii}—Cu1—N1	89.94 (8)

H5B—C6—H5C	109.5	N3—Cu1—N1	89.60 (8)
N3—C7—C8	109.6 (2)	N1^{ii}—Cu1—N1	175.97 (11)
N3—C7—C6	121.4 (2)	N3^{ii}—Cu1—O1	96.56 (6)
C8—C7—C6	129.0 (2)	N3—Cu1—O1	96.56 (6)
C9—C8—C7	105.7 (2)	N1^{ii}—Cu1—O1	92.01 (6)
C9—C8—Se1	126.54 (19)	N1—Cu1—O1	92.01 (6)
C7—C8—Se1	126.90 (19)	C3—Se1—C8	103.80 (10)
N3—C7—C8—C9	0.5 (3)	C10—C9—N4—N3	178.6 (2)
C6—C7—C8—C9	178.4 (2)	C7—N3—N4—C9	0.4 (3)
N3—C7—C8—Se1	170.61 (17)	Cu1—N3—N4—C9	−172.60 (17)
C6—C7—C8—Se1	−11.5 (4)	C7—N3—Cu1—N3^{ii}	38.4 (2)
C7—C8—C9—N4	−0.2 (3)	N4—N3—Cu1—N3^{ii}	−150.87 (17)
Se1—C8—C9—N4	−170.41 (18)	C7—N3—Cu1—N1^{ii}	126.3 (2)
C7—C8—C9—C10	−178.7 (3)	N4—N3—Cu1—N1^{ii}	−62.89 (17)
Se1—C8—C9—C10	11.1 (4)	C7—N3—Cu1—N1	−49.7 (2)
C3^{i}—C2—N1—N2	−0.7 (3)	N4—N3—Cu1—N1	121.11 (17)
C1—C2—N1—N2	179.3 (2)	C7—N3—Cu1—O1	−141.6 (2)
C3^{i}—C2—N1—Cu1	−178.10 (17)	N4—N3—Cu1—O1	29.13 (17)
C1—C2—N1—Cu1	2.0 (4)	C2—N1—Cu1—N3^{ii}	143.2 (2)
C3^{i}—C4—N2—N1	−0.1 (3)	N2—N1—Cu1—N3^{ii}	−33.83 (17)
C5—C4—N2—N1	−178.6 (2)	C2—N1—Cu1—N3	−49.9 (2)
C2—N1—N2—C4	0.5 (3)	N2—N1—Cu1—N3	133.06 (17)
Cu1—N1—N2—C4	178.26 (17)	C2—N1—Cu1—O1	46.7 (2)
C8—C7—N3—N4	−0.5 (3)	N2—N1—Cu1—O1	−130.39 (16)
C6—C7—N3—N4	−178.6 (2)	C4^{i}—C3—Se1—C8	102.0 (2)
C8—C7—N3—Cu1	171.23 (17)	C2^{i}—C3—Se1—C8	−87.0 (2)
C6—C7—N3—Cu1	−6.9 (4)	C9—C8—Se1—C3	−92.4 (2)
C8—C9—N4—N3	−0.1 (3)	C7—C8—Se1—C3	99.4 (2)

Symmetry codes: (i) −*x*, −*y*, −*z*+1; (ii) −*x*, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···Cl1	0.93	2.43	3.354 (2)	169
O1—H1*O*1···Cl1	0.88	2.25	3.0702 (10)	156
N2—H2*N*···Cl1^{iii}	0.88	2.33	3.117 (2)	148
N4—H4*N*···Cl1^{ii}	0.88	2.27	3.144 (2)	176

Symmetry codes: (ii) −*x*, *y*, −*z*+1/2; (iii) −*x*−1/2, *y*+1/2, −*z*+1/2.