

Diaqua(1,4,8,11-tetraazacyclotetradecane- $\kappa^4 N^1, N^4, N^8, N^{11}$)copper(II) bis(2,3,4,5,6-pentafluorobenzoate) dihydrate

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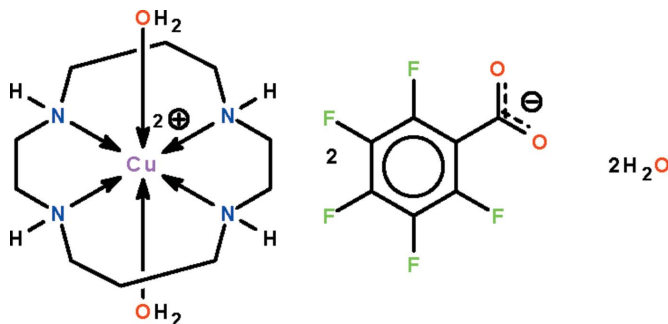
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.037; wR factor = 0.111; data-to-parameter ratio = 13.9.

The Cu^{II} atom in the title salt, $[\text{Cu}(\text{C}_{10}\text{H}_{24}\text{N}_4)(\text{H}_2\text{O})_2](\text{C}_6\text{F}_5\text{CO}_2)_2 \cdot 2\text{H}_2\text{O}$, is chelated by the four N atoms of the 1,4,8,11-tetraazacyclotetradecane (cyclam) ligand and is coordinated by two water molecules in a Jahn–Teller-type tetragonally distorted octahedral geometry. The Cu^{II} atom lies on a center of inversion. The cations, anions and uncoordinated water molecules are linked by $\text{N}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds, forming a layer structure parallel to (001).

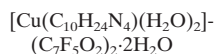
Related literature

For related (1,4,8,11-tetraazacyclotetradecane)copper carboxylates, see: Lindoy *et al.* (2003); Hunter *et al.* (2005).



Experimental

Crystal data



$M_r = 758.08$
Triclinic, $P\bar{1}$

$a = 7.1976$ (6) Å
 $b = 8.7632$ (7) Å
 $c = 12.1574$ (10) Å
 $\alpha = 79.378$ (1)°
 $\beta = 75.408$ (1)°
 $\gamma = 80.606$ (1)°

$V = 723.85$ (10) Å³
 $Z = 1$
Mo $K\alpha$ radiation
 $\mu = 0.87$ mm⁻¹
 $T = 100$ K
 $0.35 \times 0.15 \times 0.05$ mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.750$, $T_{\text{max}} = 0.958$

6996 measured reflections
3306 independent reflections
3028 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.111$
 $S = 1.06$
3306 reflections
238 parameters
6 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.49$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.75$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{N1}-\text{H1} \cdots \text{O2w}^{\text{i}}$	0.86 (1)	2.17 (2)	2.997 (2)	157 (3)
$\text{N2}-\text{H2} \cdots \text{O1w}$	0.86 (1)	2.70 (3)	3.123 (2)	112 (2)
$\text{O1w}-\text{H11} \cdots \text{O2}^{\text{i}}$	0.83 (1)	1.98 (1)	2.785 (2)	162 (3)
$\text{O1w}-\text{H12} \cdots \text{O2w}$	0.83 (1)	2.10 (2)	2.898 (2)	160 (3)
$\text{O2w}-\text{H21} \cdots \text{O1}$	0.83 (1)	1.90 (1)	2.723 (2)	169 (3)
$\text{O2w}-\text{H22} \cdots \text{O1}^{\text{ii}}$	0.83 (1)	2.08 (2)	2.842 (2)	152 (4)

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

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: publCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5287).

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supporting information

Acta Cryst. (2010). E66, m889 [https://doi.org/10.1107/S1600536810025705]

Diaqua(1,4,8,11-tetraazacyclotetradecane- $\kappa^4N^1,N^4,N^8,N^{11}$)copper(II) bis-(2,3,4,5,6-pentafluorobenzoate) dihydrate

Nur Syamimi Ahmad Tajidi, Norbani Abdullah, Zainudin Arifin, Kong Wai Tan and Seik Weng Ng

S1. Comment

The copper(II) ion forms a number of complexes with 1,4,8,11-tetraazacyclotetradecane in which the metal atom is coordinated by the four amino donor-atoms of the cyclic ligand. Among the carboxylate derivatives, neither the acetate nor the benzoate ions bind directly with the copper atom. The copper atom is coordinated instead by water molecules so that the carboxylate group interacts indirectly with the metal atom through the coordinated water molecules (Hunter *et al.*, 2005; Lindoy *et al.*, 2003). The copper(II) atom in the salt, $[\text{Cu}(\text{H}_2\text{O})_2(\text{C}_{10}\text{H}_{24}\text{N}_4)]^{2+} 2(\text{C}_6\text{F}_5\text{CO}_2)^-\cdot 2\text{H}_2\text{O}$ (Scheme I), is chelated by the four nitrogen atoms of the cyclam ligand and is coordinated by two water molecules in a Jahn-Teller type of tetragonally distorted octahedral geometry. The copper atom lies on a center of inversion (Fig. 1). The cations, anions and lattice water molecules are linked by N–H \cdots O and O–H \cdots O hydrogen bonds to form a layer structure.

S2. Experimental

1,4,8,11-Tetraazacyclotetradecane (0.50 g, 2.50 mmol) dissolved in ethanol (25 ml) was mixed with a suspension of copper pentafluorobenzoate (1.22 g, 2.5 mmol) in ethanol (50 ml) to give a purple solution. The solution was heated for an hour and then filtered. Prismatic crystals separated from the solution when it was left to cool slowly.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.95 to 0.98 Å) and were included in the refinement in the riding model approximation, with $U(\text{H})$ set to 1.2 to 1.5 $U(\text{C})$.

The water H-atoms were located in a difference Fourier map, and were refined with a distance restraint of O–H 0.84±0.01 Å; their displacement parameters were freely refined.

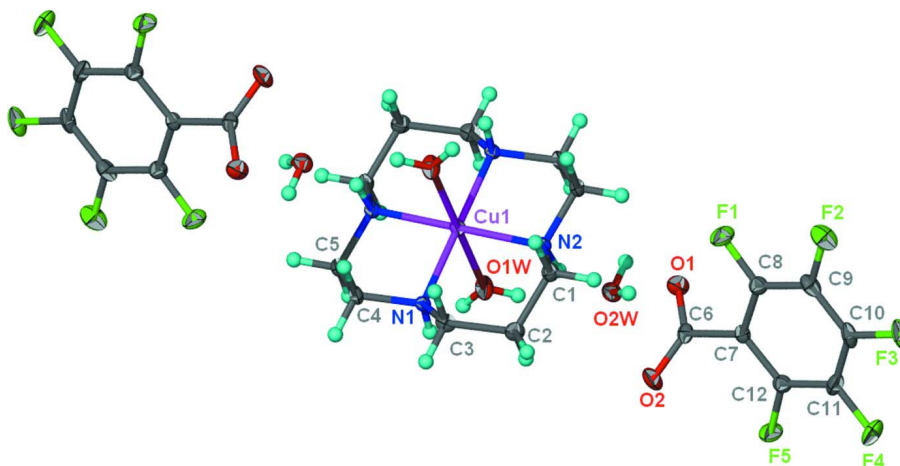


Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $[\text{Cu}(\text{H}_2\text{O})_2(\text{C}_{10}\text{H}_{24}\text{N}_4)]^{2+} 2(\text{C}_6\text{F}_5\text{CO}_2)\cdot 2\text{H}_2\text{O}$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Diaqua(1,4,8,11-tetraazacyclotetradecane- $\kappa^4\text{N}^1, \text{N}^4, \text{N}^8, \text{N}^{11}$)copper(II) bis(2,3,4,5,6-pentafluorobenzoate) dihydrate

Crystal data

$[\text{Cu}(\text{C}_{10}\text{H}_{24}\text{N}_4)(\text{H}_2\text{O})_2](\text{C}_7\text{F}_5\text{O}_2)_2\cdot 2\text{H}_2\text{O}$

$M_r = 758.08$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.1976$ (6) Å

$b = 8.7632$ (7) Å

$c = 12.1574$ (10) Å

$\alpha = 79.378$ (1)°

$\beta = 75.408$ (1)°

$\gamma = 80.606$ (1)°

$V = 723.85$ (10) Å³

$Z = 1$

$F(000) = 387$

$D_x = 1.739$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3327 reflections

$\theta = 2.4\text{--}28.3^\circ$

$\mu = 0.87$ mm⁻¹

$T = 100$ K

Plate, purple

$0.35 \times 0.15 \times 0.05$ mm

Data collection

Bruker SMART APEX

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.750$, $T_{\max} = 0.958$

6996 measured reflections

3306 independent reflections

3028 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 1.8^\circ$

$h = -9 \rightarrow 9$

$k = -11 \rightarrow 11$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.111$

$S = 1.06$

3306 reflections

238 parameters

6 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H atoms treated by a mixture of independent
and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0585P)^2 + 0.8764P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 0.49 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.75 \text{ e } \text{\AA}^{-3}$$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.5000	0.5000	0.5000	0.01239 (13)
F1	0.30292 (19)	1.10724 (17)	0.18468 (12)	0.0207 (3)
F2	0.2995 (2)	1.34413 (17)	0.01066 (13)	0.0238 (3)
F3	-0.0014 (2)	1.41338 (16)	-0.09309 (12)	0.0232 (3)
F4	-0.3014 (2)	1.23540 (18)	-0.02310 (13)	0.0257 (3)
F5	-0.29974 (19)	0.99746 (17)	0.14925 (13)	0.0201 (3)
O1	0.0371 (2)	0.94440 (19)	0.36194 (14)	0.0171 (3)
O2	-0.0383 (3)	0.78296 (19)	0.26114 (14)	0.0185 (4)
O1W	0.1535 (2)	0.4892 (2)	0.59710 (15)	0.0184 (4)
H11	0.095 (4)	0.418 (3)	0.641 (2)	0.027 (8)*
H12	0.059 (3)	0.558 (3)	0.598 (3)	0.030 (9)*
O2W	-0.1025 (2)	0.77849 (19)	0.57103 (14)	0.0149 (3)
H21	-0.057 (4)	0.818 (4)	0.5037 (13)	0.025 (8)*
H22	-0.101 (5)	0.843 (3)	0.613 (3)	0.038 (10)*
N1	0.4818 (3)	0.3368 (2)	0.40734 (15)	0.0101 (3)
H1	0.3625 (19)	0.321 (3)	0.428 (2)	0.018 (7)*
N2	0.4084 (3)	0.6798 (2)	0.38696 (16)	0.0112 (4)
H2	0.2840 (15)	0.687 (3)	0.404 (2)	0.015 (7)*
C1	0.4771 (3)	0.6699 (3)	0.26255 (19)	0.0136 (4)
H1A	0.6192	0.6702	0.2399	0.016*
H1B	0.4176	0.7627	0.2179	0.016*
C2	0.4258 (3)	0.5219 (3)	0.23401 (19)	0.0142 (4)
H2A	0.2861	0.5155	0.2660	0.017*
H2B	0.4499	0.5295	0.1494	0.017*
C3	0.5400 (3)	0.3721 (3)	0.28057 (18)	0.0133 (4)
H3A	0.5188	0.2837	0.2467	0.016*
H3B	0.6798	0.3832	0.2572	0.016*
C4	0.5931 (3)	0.1921 (2)	0.45282 (19)	0.0129 (4)
H4A	0.7335	0.1972	0.4225	0.016*
H4B	0.5591	0.1002	0.4289	0.016*
C5	0.5434 (3)	0.1775 (3)	0.58302 (19)	0.0139 (4)
H5A	0.4041	0.1679	0.6137	0.017*
H5B	0.6190	0.0835	0.6163	0.017*
C6	0.0001 (3)	0.9099 (3)	0.27439 (18)	0.0120 (4)
C7	0.0021 (3)	1.0433 (2)	0.17373 (18)	0.0109 (4)
C8	0.1511 (3)	1.1355 (3)	0.13503 (19)	0.0134 (4)

C9	0.1521 (3)	1.2583 (3)	0.04536 (19)	0.0155 (4)
C10	-0.0004 (4)	1.2919 (3)	-0.00841 (19)	0.0160 (5)
C11	-0.1512 (3)	1.2027 (3)	0.0274 (2)	0.0160 (4)
C12	-0.1483 (3)	1.0797 (3)	0.11656 (19)	0.0133 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0154 (2)	0.0093 (2)	0.0126 (2)	-0.00158 (14)	-0.00413 (14)	-0.00071 (14)
F1	0.0142 (6)	0.0252 (8)	0.0237 (7)	-0.0079 (6)	-0.0080 (6)	0.0036 (6)
F2	0.0242 (7)	0.0200 (7)	0.0245 (8)	-0.0133 (6)	0.0020 (6)	0.0023 (6)
F3	0.0431 (9)	0.0114 (7)	0.0126 (7)	-0.0011 (6)	-0.0065 (6)	0.0031 (5)
F4	0.0268 (8)	0.0269 (8)	0.0255 (8)	0.0027 (6)	-0.0174 (6)	0.0015 (6)
F5	0.0137 (6)	0.0226 (7)	0.0254 (7)	-0.0070 (5)	-0.0070 (5)	0.0008 (6)
O1	0.0234 (8)	0.0172 (8)	0.0119 (7)	-0.0064 (7)	-0.0057 (6)	0.0003 (6)
O2	0.0269 (9)	0.0103 (8)	0.0185 (8)	-0.0056 (6)	-0.0049 (7)	-0.0001 (6)
O1W	0.0117 (8)	0.0138 (8)	0.0253 (9)	-0.0024 (6)	-0.0008 (7)	0.0039 (7)
O2W	0.0165 (8)	0.0135 (8)	0.0143 (8)	-0.0046 (6)	-0.0025 (6)	-0.0002 (6)
N1	0.0088 (8)	0.0090 (8)	0.0124 (9)	-0.0023 (7)	-0.0021 (7)	-0.0011 (7)
N2	0.0096 (8)	0.0100 (8)	0.0136 (9)	-0.0022 (7)	-0.0027 (7)	-0.0001 (7)
C1	0.0153 (10)	0.0117 (10)	0.0132 (10)	-0.0033 (8)	-0.0043 (8)	0.0024 (8)
C2	0.0164 (10)	0.0154 (11)	0.0112 (10)	-0.0042 (8)	-0.0042 (8)	0.0000 (8)
C3	0.0134 (10)	0.0147 (10)	0.0113 (10)	-0.0029 (8)	-0.0005 (8)	-0.0032 (8)
C4	0.0139 (10)	0.0074 (9)	0.0172 (11)	0.0000 (8)	-0.0041 (8)	-0.0014 (8)
C5	0.0161 (10)	0.0089 (10)	0.0174 (11)	-0.0024 (8)	-0.0068 (8)	0.0009 (8)
C6	0.0097 (9)	0.0120 (10)	0.0121 (10)	0.0006 (8)	-0.0009 (8)	-0.0002 (8)
C7	0.0121 (10)	0.0094 (9)	0.0103 (9)	-0.0005 (8)	-0.0013 (8)	-0.0017 (8)
C8	0.0129 (10)	0.0135 (10)	0.0140 (10)	-0.0016 (8)	-0.0031 (8)	-0.0024 (8)
C9	0.0181 (11)	0.0118 (10)	0.0142 (10)	-0.0054 (8)	0.0027 (8)	-0.0013 (8)
C10	0.0266 (12)	0.0089 (10)	0.0093 (10)	0.0007 (9)	-0.0017 (9)	0.0005 (8)
C11	0.0172 (11)	0.0164 (11)	0.0145 (10)	0.0041 (9)	-0.0074 (8)	-0.0031 (8)
C12	0.0133 (10)	0.0129 (10)	0.0143 (10)	-0.0015 (8)	-0.0030 (8)	-0.0037 (8)

Geometric parameters (Å, °)

Cu1—N1	2.0149 (18)	C1—C2	1.525 (3)
Cu1—N1 ⁱ	2.0149 (18)	C1—H1A	0.9900
Cu1—N2	2.0313 (18)	C1—H1B	0.9900
Cu1—N2 ⁱ	2.0313 (18)	C2—C3	1.526 (3)
Cu1—O1W	2.4849 (17)	C2—H2A	0.9900
F1—C8	1.345 (3)	C2—H2B	0.9900
F2—C9	1.337 (3)	C3—H3A	0.9900
F3—C10	1.338 (3)	C3—H3B	0.9900
F4—C11	1.340 (3)	C4—C5	1.518 (3)
F5—C12	1.341 (3)	C4—H4A	0.9900
O1—C6	1.258 (3)	C4—H4B	0.9900
O2—C6	1.236 (3)	C5—N2 ⁱ	1.479 (3)
O1W—H11	0.834 (10)	C5—H5A	0.9900

O1W—H12	0.832 (10)	C5—H5B	0.9900
O2W—H21	0.833 (10)	C6—C7	1.528 (3)
O2W—H22	0.830 (10)	C7—C8	1.383 (3)
N1—C3	1.479 (3)	C7—C12	1.393 (3)
N1—C4	1.480 (3)	C8—C9	1.383 (3)
N1—H1	0.859 (10)	C9—C10	1.380 (3)
N2—C5 ⁱ	1.479 (3)	C10—C11	1.376 (3)
N2—C1	1.482 (3)	C11—C12	1.382 (3)
N2—H2	0.861 (10)		
N1—Cu1—N1 ⁱ	180.00 (9)	N1—C3—H3A	109.3
N1—Cu1—N2	93.24 (7)	C2—C3—H3A	109.3
N1 ⁱ —Cu1—N2	86.76 (7)	N1—C3—H3B	109.3
N1—Cu1—N2 ⁱ	86.76 (7)	C2—C3—H3B	109.3
N1 ⁱ —Cu1—N2 ⁱ	93.24 (7)	H3A—C3—H3B	107.9
N2—Cu1—N2 ⁱ	180.0	N1—C4—C5	108.02 (17)
N1—Cu1—O1W	88.91 (7)	N1—C4—H4A	110.1
N1 ⁱ —Cu1—O1W	91.09 (7)	C5—C4—H4A	110.1
N2—Cu1—O1W	86.87 (6)	N1—C4—H4B	110.1
N2 ⁱ —Cu1—O1W	93.13 (6)	C5—C4—H4B	110.1
Cu1—O1W—H11	132 (2)	H4A—C4—H4B	108.4
Cu1—O1W—H12	131 (2)	N2 ⁱ —C5—C4	107.48 (17)
H11—O1W—H12	97 (3)	N2 ⁱ —C5—H5A	110.2
H21—O2W—H22	107 (3)	C4—C5—H5A	110.2
C3—N1—C4	111.85 (17)	N2 ⁱ —C5—H5B	110.2
C3—N1—Cu1	118.22 (13)	C4—C5—H5B	110.2
C4—N1—Cu1	105.50 (13)	H5A—C5—H5B	108.5
C3—N1—H1	110 (2)	O2—C6—O1	127.9 (2)
C4—N1—H1	106 (2)	O2—C6—C7	117.14 (19)
Cu1—N1—H1	104 (2)	O1—C6—C7	114.94 (19)
C5 ⁱ —N2—C1	112.36 (17)	C8—C7—C12	116.3 (2)
C5 ⁱ —N2—Cu1	105.50 (13)	C8—C7—C6	122.22 (19)
C1—N2—Cu1	118.01 (14)	C12—C7—C6	121.49 (19)
C5 ⁱ —N2—H2	106 (2)	F1—C8—C9	117.3 (2)
C1—N2—H2	108.4 (19)	F1—C8—C7	120.12 (19)
Cu1—N2—H2	105.8 (19)	C9—C8—C7	122.6 (2)
N2—C1—C2	111.28 (17)	F2—C9—C10	120.0 (2)
N2—C1—H1A	109.4	F2—C9—C8	120.5 (2)
C2—C1—H1A	109.4	C10—C9—C8	119.5 (2)
N2—C1—H1B	109.4	F3—C10—C9	119.3 (2)
C2—C1—H1B	109.4	F3—C10—C11	120.9 (2)
H1A—C1—H1B	108.0	C9—C10—C11	119.7 (2)
C3—C2—C1	113.62 (18)	F4—C11—C10	120.3 (2)
C3—C2—H2A	108.8	F4—C11—C12	120.0 (2)
C1—C2—H2A	108.8	C10—C11—C12	119.7 (2)
C3—C2—H2B	108.8	F5—C12—C11	117.48 (19)
C1—C2—H2B	108.8	F5—C12—C7	120.30 (19)
H2A—C2—H2B	107.7	C11—C12—C7	122.2 (2)

N1—C3—C2	111.72 (18)		
N2—Cu1—N1—C3	38.53 (15)	C12—C7—C8—F1	-179.30 (19)
N2 ⁱ —Cu1—N1—C3	-141.47 (15)	C6—C7—C8—F1	1.4 (3)
O1W—Cu1—N1—C3	125.34 (15)	C12—C7—C8—C9	0.5 (3)
N2—Cu1—N1—C4	164.50 (13)	C6—C7—C8—C9	-178.8 (2)
N2 ⁱ —Cu1—N1—C4	-15.50 (13)	F1—C8—C9—F2	0.0 (3)
O1W—Cu1—N1—C4	-108.70 (13)	C7—C8—C9—F2	-179.9 (2)
N1—Cu1—N2—C5 ⁱ	-165.17 (14)	F1—C8—C9—C10	180.0 (2)
N1 ⁱ —Cu1—N2—C5 ⁱ	14.83 (14)	C7—C8—C9—C10	0.1 (4)
O1W—Cu1—N2—C5 ⁱ	106.10 (14)	F2—C9—C10—F3	-1.8 (3)
N1—Cu1—N2—C1	-38.68 (15)	C8—C9—C10—F3	178.2 (2)
N1 ⁱ —Cu1—N2—C1	141.32 (15)	F2—C9—C10—C11	179.7 (2)
O1W—Cu1—N2—C1	-127.41 (15)	C8—C9—C10—C11	-0.3 (3)
C5 ⁱ —N2—C1—C2	179.95 (17)	F3—C10—C11—F4	0.7 (3)
Cu1—N2—C1—C2	56.8 (2)	C9—C10—C11—F4	179.1 (2)
N2—C1—C2—C3	-69.8 (2)	F3—C10—C11—C12	-178.7 (2)
C4—N1—C3—C2	-179.63 (17)	C9—C10—C11—C12	-0.3 (3)
Cu1—N1—C3—C2	-56.8 (2)	F4—C11—C12—F5	-0.2 (3)
C1—C2—C3—N1	69.8 (2)	C10—C11—C12—F5	179.2 (2)
C3—N1—C4—C5	172.46 (17)	F4—C11—C12—C7	-178.4 (2)
Cu1—N1—C4—C5	42.67 (18)	C10—C11—C12—C7	1.0 (4)
N1—C4—C5—N2 ⁱ	-58.0 (2)	C8—C7—C12—F5	-179.24 (19)
O2—C6—C7—C8	-132.7 (2)	C6—C7—C12—F5	0.1 (3)
O1—C6—C7—C8	47.8 (3)	C8—C7—C12—C11	-1.1 (3)
O2—C6—C7—C12	48.0 (3)	C6—C7—C12—C11	178.2 (2)
O1—C6—C7—C12	-131.5 (2)		

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 \cdots O2w ⁱⁱ	0.86 (1)	2.17 (2)	2.997 (2)	157 (3)
N2—H2 \cdots O1w	0.86 (1)	2.70 (3)	3.123 (2)	112 (2)
O1w—H11 \cdots O2 ⁱⁱ	0.83 (1)	1.98 (1)	2.785 (2)	162 (3)
O1w—H12 \cdots O2w	0.83 (1)	2.10 (2)	2.898 (2)	160 (3)
O2w—H21 \cdots O1	0.83 (1)	1.90 (1)	2.723 (2)	169 (3)
O2w—H22 \cdots O1 ⁱⁱⁱ	0.83 (1)	2.08 (2)	2.842 (2)	152 (4)

Symmetry codes: (ii) $-x, -y+1, -z+1$; (iii) $-x, -y+2, -z+1$.