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Crystal structures of *trans*-diaqua(3-*R*-1,3,5,8,12-pentaazacyclotetradecane)copper(II) isophthalate hydrates (*R* = benzyl or pyridin-3-ylmethyl)

Irina L. Andriichuk,[a] Liudmyla V. Tsymbal,[a] Vladimir B. Arion[b] and Yaroslaw D. Lampeka[a]*

[a]L. V. Pisarzhevskii Institute of Physical Chemistry of the National Academy of Sciences of Ukraine, Prospekt Nauki 31, 03028 Kiev, Ukraine, and [b]Institute of Inorganic Chemistry of the University of Vienna, Wahringer Str., 42, 1090 Vienna, Austria. *Correspondence e-mail: lampeka@adamant.net

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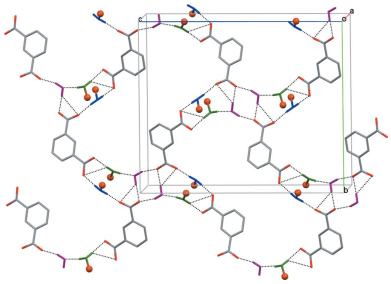
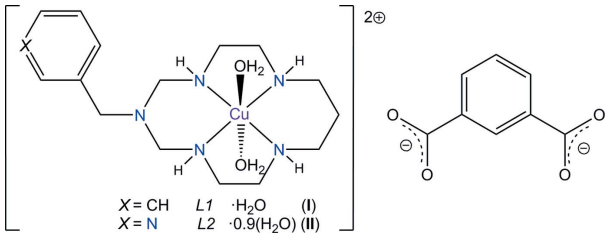
The asymmetric units of the title compounds, *trans*-diaqua(3-benzyl-1,3,5,8,12-pentaazacyclotetradecane-$\kappa^4N^1,N^5,N^8,N^{12}$)copper(II) isophthalate monohydrate, $[Cu(C_{16}H_{29}N_5)(H_2O)_2](C_8H_4O_4)\cdot H_2O$, (I), and *trans*-diaqua[3-(pyridin-3-ylmethyl)-1,3,5,8,12-pentaazacyclotetradecane-$\kappa^4N^1,N^5,N^8,N^{12}$]copper(II) isophthalate 0.9-hydrate, $[Cu(C_{15}H_{28}N_6)(H_2O)_2](C_8H_4O_4)\cdot 0.9H_2O$, (II) consist of one diaqua macrocyclic cation, one dicarboxylate anion and uncoordinated water molecule(s). In each compound, the metal ion is coordinated by the four secondary N atoms of the macrocyclic ligand and the mutually *trans* O atoms of the water molecules in a tetragonally distorted octahedral geometry. The average equatorial Cu—N bond lengths are significantly shorter than the average axial Cu—O bond lengths [2.020 (9) *versus* 2.495 (12) Å and 2.015 (4) *versus* 2.507 (7) Å for (I) and (II), respectively]. The coordinated macrocyclic ligand in the cations of both compounds adopts the most energetically favorable *trans*-III conformation. In the crystals, the complex cations and counter-anions are connected *via* hydrogen-bonding interactions between the N—H groups of the macrocycles and the O—H groups of coordinated water molecules as the proton donors and the O atoms of the carboxylate as the proton acceptors. Additionally, as a result of O—H···O hydrogen bonding with the coordinated and water molecules of crystallization, the isophthalate dianions form layers lying parallel to the $(\bar{1}01)$ and (100) planes in (I) and (II), respectively.

1. Chemical context

Transition-metal complexes of the versatile macrocyclic 14-membered tetraamine ligand cyclam (cyclam = 1,4,8,11-tetraazacyclotetradecane) are popular metal-containing building units for the construction of metal–organic frameworks (MOFs) possessing many promising applications (Lampeka & Tsymbal, 2004; Suh & Moon, 2007; Suh *et al.*, 2012; Stackhouse & Ma, 2018; Lee & Moon, 2018). Such an interest is explained by the exceptionally high thermodynamic stability and kinetic inertness of these species (Melson, 1979; Yatsimirskii & Lampeka, 1985), implying a preservation of their structural features (equatorial arrangement of the macrocycle in the coordination sphere of the metal ion, availability of two *trans* vacant sites in the axial positions suitable for coordination of bridging ligands), thus making the architecture of MOFs more predictable. The complexes of N^3,N^{10}-disubstituted diazacyclam (diazacyclam = 1,3,5,8,10,12-hexaazacyclotetradecane), readily obtainable *via* template-



directed Mannich condensation of bis(ethylenediamine) complexes with formaldehyde and primary amines (Costisor & Linert, 2000), also represent widespread systems in this kind of investigations. At the same time, the complexes of N^3-substituted azacyclam (azacyclam = 1,3,5,8,12-pentaazacyclotetradecane) – a middle member of this series of ligands – have attracted considerably less attention, presumably because of the necessity of using a more sophisticated non-cyclic precursor, *i.e.* 3,7-diazanonane-1,9-diamine, in the Mannich condensation (Rosokha *et al.*, 1993).



Though the isophthalate (1,3-benzenedicarboxylate) dianion is often used as bridging ligand in the construction of MOFs, a very limited number of its compounds with aza-macrocyclic cations have been described to date and all they are complexes of the Ni^{II} ion.

Herein, we describe the syntheses and crystal structures of the title Cu^{II} complexes with azacyclam ligands and an isophthalate dianion, namely, *trans*-diaqua(3-benzyl-1,3,5,8,12-pentaazacyclotetradecane-$\kappa^4N^1,N^5,N^8,N^{12}$)copper(II) isophthalate hydrate, [Cu(*L1*)(H_2O)$_2$](ip)·H_2O, (I), and *trans*-diaqua[3-(pyridin-3-ylmethyl)-1,3,5,8,12-pentaazacyclotetradecane-$\kappa^4N^1,N^5,N^8,N^{12}$]copper(II) isophthalate 0.9-hydrate, [Cu(*L2*)(H_2O)$_2$](ip)·0.9(H_2O), (II).

2. Structural commentary

Each Cu^{II} ion in the complex cations in the title compounds (I) and (II) is coordinated in the equatorial plane by four secondary amine N atoms of the azamacrocyclic ligand in a square-planar fashion, and by two O atoms from the water molecules in the axial positions, resulting in a tetragonally distorted octahedral geometry (Table 1, Fig. 1 and Fig. 2).

The average equatorial Cu—N bond lengths are significantly shorter than the average axial Cu—O bond lengths [2.020 (9) *versus* 2.495 (12) Å for (I) and 2.015 (4) *versus* 2.507 (7) Å for (II)], which can be attributed to a large Jahn–Teller distortion. The Cu^{II} ions are displaced from the nearly planar (r.m.s. deviations less than 0.01 Å) mean planes of the N_4 donor atoms towards the O1*W* water molecule by 0.024 and 0.033 Å in (I) and (II), respectively. Both coordinated macrocyclic ligands adopt the most energetically favourable *trans*-III (*R,R,S,S*) conformation (Bosnich *et al.*, 1965) with the five-membered chelate rings in *gauche* [bite angles 86.28 (1) for (I) and 86.30 (7)° for (II)] and six-membered chelate rings in *chair* [bite angles 93.7 (2) for (I) and 93.7 (9)° for (II)] conformations. The methylene group of the substituent at the non-coordinated nitrogen atoms N3 in the six-membered chelate rings is axially oriented and the sum of the C—N—C angles around these atoms [345.6 and 348.1° for (I) and (II), respectively] indicates their partial sp^2 character (Tsymbal *et al.*, 2019).

Table 1
Selected bond lengths (Å).

	(I)	(II)
Cu1—N1	2.0146 (17)	2.011 (3)
Cu1—N2	2.0290 (17)	2.019 (3)
Cu1—N4	2.0119 (17)	2.019 (3)
Cu1—N5	2.0206 (17)	2.009 (3)
Cu1—O1*W*	2.5071 (16)	2.514 (2)
Cu1—O2*W*	2.4832 (15)	2.499 (2)

The isophthalate dianions in the title compounds counterbalance the charge of the complex cations. One carboxylic group of the isophthalate (O1/O2/C) is nearly coplanar with the mean plane of the aromatic fragment [dihedral angles being 2.4 (3) and 3.6 (4)° in (I) and (II), respectively], while the second (O3/O4/C) is tilted by 11.6 (3) and 21.1 (4)° in (I) and (II), respectively. The C—O bond lengths in the carboxylic groups are nearly equal, thus indicating essential electron delocalization.

Among the water molecules of crystallization, O3*W* in (I) is fully occupied, while that in (II) has a site occupancy of 50%.

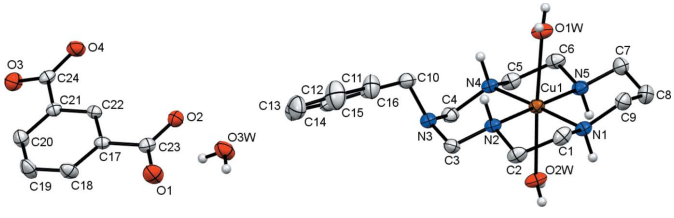


Figure 1
View of the asymmetric unit of (I), showing the atom-labelling scheme, with displacement ellipsoids drawn at the 30% probability level. H atoms attached to carbon atoms have been omitted for clarity.

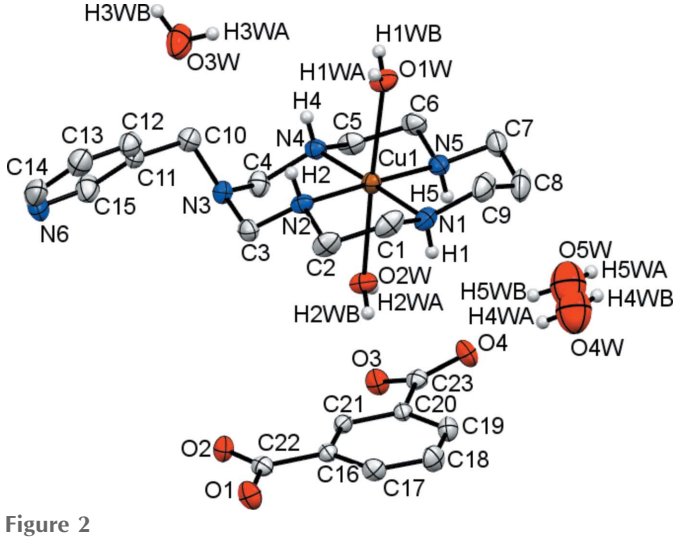


Figure 2
View of the asymmetric unit of (II), showing the atom-labelling scheme, with displacement ellipsoids drawn at the 30% probability level. H atoms attached to carbon atoms have been omitted for clarity.

Table 2
Hydrogen-bond geometry (Å, °) for (I).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O4^{i}	0.98	2.04	2.950 (2)	154
N2—H2···O3^{ii}	0.98	2.15	3.118 (2)	170
N4—H4···O2^{iii}	0.98	2.00	2.949 (2)	161
N5—H5···O3W^{iv}	0.98	2.35	3.230 (3)	149
O1W—H1WB···O4^{ii}	0.87	2.01	2.884 (2)	176
O1W—H1WB···O3^{ii}	0.87	2.60	3.213 (2)	128
O1W—H1WA···O3W^{iii}	0.85	1.97	2.813 (2)	173
O2W—H2WA···O2^{iv}	0.84	1.96	2.795 (2)	174
O2W—H2WB···O3^{i}	0.85	1.95	2.798 (2)	178
O3W—H3WA···O1^{v}	0.88	1.92	2.779 (2)	163
O3W—H3WB···O1	0.87	1.85	2.720 (2)	176
O3W—H3WB···O2	0.87	2.66	3.248 (2)	126

Symmetry codes: (i) $x-1, y+1, z$; (ii) $x, y+1, z$; (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (v) $-x+1, -y+1, -z+1$.

Table 3
Hydrogen-bond geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O4	0.79 (4)	2.37 (4)	3.115 (4)	157 (4)
N2—H2···O3^{i}	0.81 (3)	2.25 (4)	3.044 (4)	167 (3)
N4—H4···O1^{ii}	0.78 (3)	2.31 (3)	3.037 (4)	157 (3)
N5—H5···O2^{iii}	0.83 (4)	2.10 (4)	2.910 (4)	163 (3)
O1W—H1WA···O4^{i}	0.85	2.00	2.849 (3)	174
O1W—H1WB···O2^{ii}	0.76	2.07	2.831 (3)	176
O2W—H2WA···O1^{iii}	0.71	2.15	2.859 (3)	178
O2W—H2WB···O3	0.82	1.90	2.722 (3)	180
O3W—H3WA···O1^{ii}	0.85	1.88	2.731 (6)	179
O3W—H3WB···O1^{iv}	0.85	2.18	2.760 (6)	126
C1—H1A···O4^{i}	1.05 (4)	2.64 (4)	3.662 (5)	164 (3)
C4—H4B···O3W^{v}	0.98 (4)	2.60 (4)	3.274 (7)	125 (3)
C5—H5B···O3W^{v}	0.94 (4)	2.62 (4)	3.415 (7)	142 (3)
C10—H10A···O3W	0.92 (4)	2.49 (4)	3.367 (8)	161 (3)
C13—H13···O2^{i}	1.03 (4)	2.53 (4)	3.446 (6)	147 (3)
C1—H1B···N6^{vi}	0.84 (4)	2.66 (4)	3.474 (5)	165 (4)

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

Additionally, two positions for disordered water molecules (O4W and O5W), each with 20% population, were found in (II). Because of their low partial population, these were not considered further in the analysis of the hydrogen-bonding network.

3. Supramolecular features

Three secondary amino groups of the coordinated macrocycle in (I) act as proton donors by the formation of N—H···O hydrogen bonds with the carboxylic groups of three different adjacent anions, while the fourth group forms hydrogen bond with the water molecule of crystallization O3W (Fig. 3, Table 2). In turn, the coordinated water molecules donate protons to the carboxylic group of the anion {bifurcated hydrogen bonding O1W—H1WB···[O3,O4(x, $y+1$, z)] and O2W—H2WA···O2($-x+\frac{1}{2}$, $y+\frac{1}{2}$, $-z+\frac{3}{2}$) and O2W—H2WB···O3($x-1$, $y+1$, z)}, as well as to the O3W molecule [O1W—H1WA···O3W($-x+\frac{3}{2}$, $y+\frac{1}{2}$, $-z+\frac{3}{2}$)]. Additionally, the uncoordinated water molecule O3W acts as a proton donor by the formation of bifurcated O3W—H3WB···(O1,O2) and O3W—H3WA···O1($-x+1$, $-y+1$, $-z+1$) hydrogen bonds.

The hydrogen-bonded network in (II), though slightly different, has much in common with that in (I). In particular, all secondary amino groups of the macrocycle form N—H···O hydrogen bonds acting as proton donors with the carboxylic groups of four different adjacent anions (Fig. 4, Table 3). Each coordinated water molecule, as well as the water molecule of crystallization O3W, donates protons to two carboxylic groups of different isophthalate anions. Additionally, in the crystal of (II) there are a number of C—H···O and C—H···N contacts

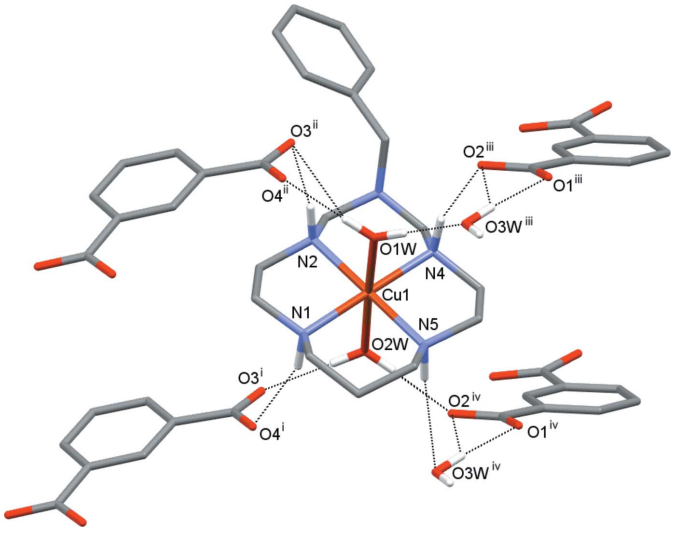


Figure 3
Nearest surrounding of the macrocyclic cation in (I) formed by hydrogen bonding (dashed lines). [Symmetry codes: (i) $x-1, y+1, z$; (ii) $x, y+1, z$; (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.]

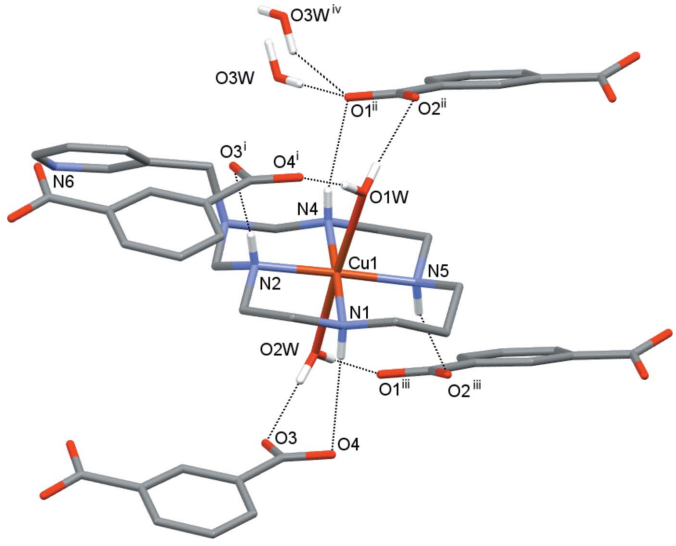


Figure 4
Nearest surrounding of the macrocyclic cation in (II) formed by hydrogen bonding (dashed lines). [Symmetry codes: (i) $x+1, y, z$; (ii) $x+1, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $-x+2, -y, -z+1$.] The contact C1—H1B···N6 ($-x+1$, $y+\frac{1}{2}$, $-z+\frac{1}{2}$) is not shown.

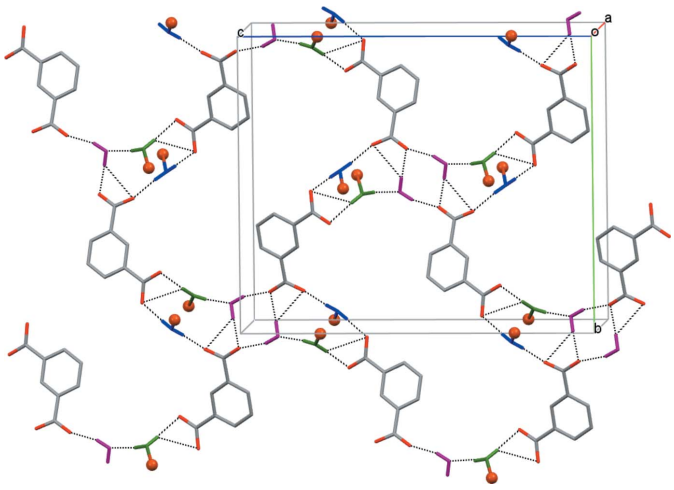


Figure 5
Sheets of isophthalate dianions parallel to the ($\bar{1}$01) plane in (I). Macrocyclic ligands and H atoms at carbon atoms of the carboxylate anions are omitted, only water molecules coordinated to Cu^{II} (balls) participating in the formation of a carboxylate layer are shown (O1*W* – green, O2*W* – dark blue, O3*W* – violet). Hydrogen bonds are shown as dashed lines.

between the methylene and methine groups of the macrocyclic ligand and oxygen atoms of carboxylic groups, the water molecule O3*W* and atom N6 of the substituent in the neighbouring macrocycle (Table 3).

As can be seen from Figs. 3 and 4, because of the hydrogen bonding, two pairs of isophthalate anions are situated above and below the imaginary plane of the macrocyclic ligand. Each pair is further bound with symmetry-related partners *via* hydrogen bonding with the water molecule of crystallization, O3*W*, thus forming layers of anions lying parallel to the ($\bar{1}$01)

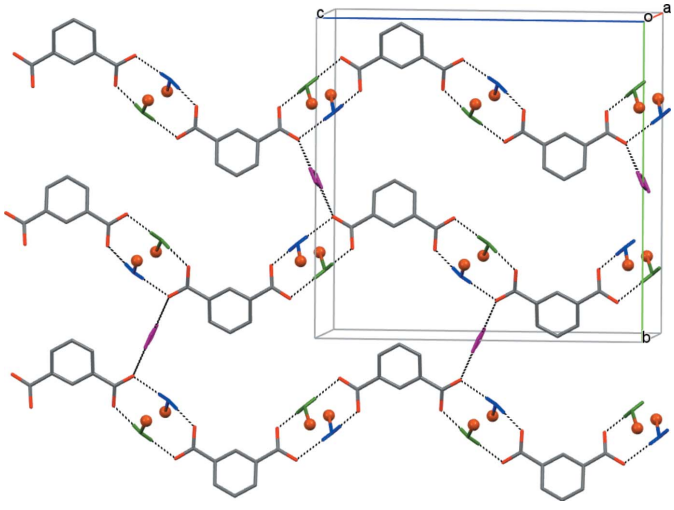


Figure 6
Sheets of isophthalate dianions parallel to the (100) plane in (II). Macrocyclic ligands and H atoms at carbon atoms of the carboxylate anions are omitted, only water molecules coordinated to Cu^{II} (balls) participating in the formation of a carboxylate layer are shown (O1*W* – green, O2*W* – dark blue, O3*W* – violet). Hydrogen bonds are shown as dashed lines.

and (100) planes in (I) and (II), respectively (Figs. 5 and 6), which thus are pillared with macrocyclic cations.

4. Database survey

A search of the Cambridge Structural Database (CSD, version 5.39, last update August 2018; Groom *et al.*, 2016) indicated that only three Cu^{II}–perchlorate complexes of azacyclam macrocycles bearing *N*-alkyl groups decorated with aromatic rings have been reported (Tsymbal *et al.*, 2010). In addition, four related dicopper(II) complexes with a *p*-xylylene-bridged bis(azacyclam) ligand and terephthalate anion have been described, none of which includes the diaqua Cu^{II} azacyclam cation (Park & Suh, 2012). At the same time, four complexes containing macrocyclic cations and an isophthalate dianion have been reported, all of them being formed by an Ni^{II} ion coordinated to a C-methyl-substituted cyclam. Thus, the title compounds (I) and (II) are the first examples of diaqua Cu^{II} azacyclam cations described so far.

5. Synthesis and crystallization

All chemicals and solvents used in this work were purchased from Sigma–Aldrich and used without further purification. The starting complexes, [Cu(*L1*)](ClO$_4$)$_2$ and [Cu(*L2*)](ClO$_4$)$_2$, were prepared by a method reported in the literature (Tsymbal *et al.*, 2010) using benzylamine or 3-picolylamine, respectively, as locking reagents.

Compound (I) was prepared as follows: To a hot solution of [Cu(*L1*)](ClO$_4$)$_2$ (138 mg, 0.25 mmol) in 8 ml of DMF were added 3 ml of an aqueous solution of Na$_2$ip (84 mg, 40 mmol). A violet precipitate formed in 24 h; this was filtered off, washed with diethyl ether and dried in air. Yield: 27 mg (19%). Analysis calculated for $C_{24}H_{39}N_5CuO_7$: C 50.29, H 6.86, N 12.22%. Found: C 50.42, H 6.96, N 12.02%.

Compound (II) was prepared analogously starting from [Cu(*L2*)](ClO$_4$)$_2$. Yield: 30 mg (21%). Analysis calculated for $C_{23}H_{37.8}N_6CuO_{6.9}$: C 48.12, H 6.67, N 14.64%. Found: C 48.31, H 6.84, N 14.32%. Violet plates of (I) and violet needles of (II) suitable for X-ray diffraction analysis were selected from the samples resulting from the syntheses.

Safety note: perchlorate salts of metal complexes are potentially explosive and should be handled with care.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. All H atoms in (I) were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 (ring H atoms) or 0.97 Å (open-chain H atoms), an N—H distance of 0.98 Å, and aqua O—H distances of 0.84–0.87 Å with U_{iso}(H) values of 1.2 or 1.5U_{eq} of the parent atoms. Water H atoms in (II) were positioned geometrically (O—H = 0.71–0.85 Å) and refined as riding with U_{iso}(H) = 1.5U_{eq}(O). All other H atoms were freely refined.

Table 4
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$[Cu(C_{16}H_{29}N_5)(H_2O)_2](C_8H_4O_4)\cdot H_2O$	$[Cu(C_{15}H_{28}N_6)(H_2O)_2](C_8H_4O_4)\cdot 0.9H_2O$
M_r	573.14	572.33
Crystal system, space group	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/c$
Temperature (K)	296	296
a, b, c (Å)	7.2625 (3), 17.8132 (7), 21.1511 (9)	7.1955 (3), 19.0463 (8), 19.4426 (8)
β (°)	92.159 (3)	94.276 (2)
V (Å^3)	2734.34 (19)	2657.15 (19)
Z	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.85	0.88
Crystal size (mm)	0.30 × 0.25 × 0.04	0.16 × 0.04 × 0.04
Data cocollection		
Diffractometer	Bruker X8 APEXII CCD	Bruker X8 APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)	Multi-scan (*SADABS*; Bruker, 2007)
T_{min}, T_{max}	0.785, 0.967	0.873, 0.966
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	137978, 5555, 4193	76082, 4532, 2834
R_{int}	0.070	0.106
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.624	0.589
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.084, 1.02	0.040, 0.097, 1.00
No. of reflections	5555	4532
No. of parameters	334	439
No. of restraints	9	0
H-atom treatment	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.24	0.29, −0.34

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2008) and *publCIF* (Westrip, 2010).

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Crystal structures of *trans*-diaqua(3-*R*-1,3,5,8,12-pentaazacyclotetradecane)-copper(II) isophthalate hydrates (*R* = benzyl or pyridin-3-ylmethyl)

Irina L. Andriichuk, Liudmyla V. Tsymbal, Vladimir B. Arion and Yaroslaw D. Lampeka

Computing details

For both structures, data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS2014* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

trans-Diaqua(3-benzyl-1,3,5,8,12-pentaazacyclotetradecane-$\kappa^4N^1,N^5,N^8,N^{12}$)copper(II) isophthalate monohydrate (I)

Crystal data

$[Cu(C_{16}H_{29}N_5)(H_2O)_2](C_8H_4O_4)\cdot H_2O$
$M_r = 573.14$
Monoclinic, $P2_1/n$
$a = 7.2625$ (3) Å
$b = 17.8132$ (7) Å
$c = 21.1511$ (9) Å
$\beta = 92.159$ (3)°
$V = 2734.34$ (19) Å^3
$Z = 4$
$F(000) = 1212$
$D_x = 1.392$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6434 reflections
$\theta = 2.9$–$24.8°$
$\mu = 0.85$ mm^{-1}
$T = 296$ K
Plate, violet
0.30 × 0.25 × 0.04 mm

Data collection

Bruker X8 APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2007)
$T_{min} = 0.785$, $T_{max} = 0.967$
137978 measured reflections
5555 independent reflections
4193 reflections with $I > 2\sigma(I)$
$R_{int} = 0.070$
$\theta_{max} = 26.3°$, $\theta_{min} = 2.5°$
$h = -9\rightarrow9$
$k = -22\rightarrow22$
$l = -26\rightarrow26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.084$
$S = 1.02$
5555 reflections
334 parameters
9 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 1.2028P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.37585 (3)	1.01815 (2)	0.78932 (2)	0.03694 (9)
O1	0.5450 (3)	0.40229 (9)	0.54740 (8)	0.0648 (5)
O2	0.6548 (2)	0.39430 (8)	0.64621 (7)	0.0487 (4)
O3	0.8446 (2)	0.05140 (8)	0.67653 (8)	0.0532 (4)
O4	0.9001 (2)	0.15648 (9)	0.73008 (7)	0.0498 (4)
O3W	0.5996 (3)	0.55120 (10)	0.56962 (8)	0.0648 (5)
H3WA	0.5628	0.5751	0.5349	0.097*
H3WB	0.5787	0.5037	0.5639	0.097*
N1	0.2874 (2)	1.12200 (10)	0.76576 (8)	0.0401 (4)
H1	0.1526	1.1199	0.7621	0.048*
N2	0.4363 (2)	1.00637 (9)	0.69696 (8)	0.0375 (4)
H2	0.5687	1.0154	0.6936	0.045*
N3	0.4758 (2)	0.86889 (10)	0.70197 (9)	0.0429 (4)
N4	0.4561 (2)	0.91310 (9)	0.81190 (8)	0.0374 (4)
H4	0.5906	0.9132	0.8175	0.045*
N5	0.3123 (2)	1.02892 (11)	0.88106 (8)	0.0432 (4)
H5	0.1787	1.0222	0.8828	0.052*
C1	0.3531 (3)	1.13819 (13)	0.70214 (11)	0.0502 (6)
H1A	0.4803	1.1548	0.7051	0.060*
H1B	0.2794	1.1778	0.6825	0.060*
C2	0.3377 (3)	1.06781 (13)	0.66276 (10)	0.0478 (6)
H2A	0.2091	1.0545	0.6555	0.057*
H2B	0.3916	1.0760	0.6221	0.057*
C3	0.3946 (3)	0.93131 (12)	0.66827 (10)	0.0441 (5)
H3A	0.2620	0.9245	0.6658	0.053*
H3B	0.4374	0.9309	0.6254	0.053*
C4	0.4046 (3)	0.85523 (12)	0.76317 (11)	0.0446 (5)
H4A	0.4487	0.8067	0.7781	0.054*
H4B	0.2713	0.8525	0.7590	0.054*
C5	0.3781 (3)	0.89603 (13)	0.87395 (10)	0.0473 (6)
H5A	0.4432	0.8541	0.8936	0.057*
H5B	0.2491	0.8826	0.8684	0.057*
C6	0.3982 (3)	0.96466 (14)	0.91516 (10)	0.0478 (6)
H6A	0.3382	0.9565	0.9548	0.057*
H6B	0.5276	0.9749	0.9245	0.057*
C7	0.3557 (4)	1.10175 (14)	0.91163 (11)	0.0547 (6)
H7A	0.4882	1.1091	0.9133	0.066*
H7B	0.3146	1.1009	0.9547	0.066*
C8	0.2646 (4)	1.16677 (15)	0.87651 (12)	0.0619 (7)

H8A	0.1334	1.1569	0.8722	0.074*
H8B	0.2807	1.2117	0.9020	0.074*
C9	0.3361 (3)	1.18222 (13)	0.81163 (12)	0.0533 (6)
H9A	0.2854	1.2294	0.7961	0.064*
H9B	0.4691	1.1873	0.8149	0.064*
C10	0.6775 (3)	0.86203 (15)	0.69872 (11)	0.0517 (6)
H10A	0.7207	0.8244	0.7290	0.062*
H10B	0.7337	0.9095	0.7109	0.062*
C11	0.7397 (3)	0.84076 (13)	0.63423 (12)	0.0471 (6)
C12	0.7251 (3)	0.76725 (14)	0.61308 (14)	0.0579 (7)
H12	0.6735	0.7310	0.6387	0.069*
C13	0.7863 (4)	0.74730 (17)	0.55453 (16)	0.0745 (9)
H13	0.7773	0.6977	0.5412	0.089*
C14	0.8599 (5)	0.7999 (2)	0.51605 (17)	0.0875 (10)
H14	0.9000	0.7864	0.4764	0.105*
C15	0.8740 (5)	0.8718 (2)	0.53593 (17)	0.0938 (11)
H15	0.9238	0.9077	0.5097	0.113*
C16	0.8155 (4)	0.89255 (16)	0.59478 (14)	0.0696 (8)
H16	0.8276	0.9422	0.6079	0.084*
C17	0.6606 (3)	0.28470 (11)	0.58309 (9)	0.0336 (4)
C18	0.6232 (3)	0.25013 (13)	0.52558 (10)	0.0467 (6)
H18	0.5736	0.2779	0.4918	0.056*
C19	0.6587 (4)	0.17463 (14)	0.51781 (11)	0.0573 (7)
H19	0.6332	0.1519	0.4789	0.069*
C20	0.7320 (3)	0.13288 (12)	0.56760 (10)	0.0473 (5)
H20	0.7542	0.0819	0.5623	0.057*
C21	0.7726 (3)	0.16653 (11)	0.62556 (9)	0.0333 (4)
C22	0.7357 (3)	0.24223 (11)	0.63274 (9)	0.0321 (4)
H22	0.7617	0.2651	0.6716	0.039*
C23	0.6174 (3)	0.36688 (12)	0.59299 (10)	0.0391 (5)
C24	0.8464 (3)	0.12152 (12)	0.68160 (10)	0.0372 (5)
O2W	0.05598 (19)	0.97303 (9)	0.76801 (8)	0.0524 (4)
H2WA	−0.0020	0.9507	0.7957	0.079*
H2WB	−0.0090	0.9958	0.7401	0.079*
O1W	0.6919 (2)	1.06796 (10)	0.81644 (7)	0.0537 (4)
H1WA	0.7519	1.0591	0.8508	0.081*
H1WB	0.7511	1.0939	0.7887	0.081*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.03746 (15)	0.03986 (14)	0.03343 (14)	0.00188 (11)	0.00046 (10)	0.00340 (11)
O1	0.0916 (14)	0.0464 (9)	0.0544 (10)	0.0095 (9)	−0.0229 (10)	0.0123 (8)
O2	0.0523 (10)	0.0434 (8)	0.0498 (9)	0.0096 (7)	−0.0069 (8)	−0.0060 (7)
O3	0.0622 (11)	0.0351 (8)	0.0616 (10)	0.0028 (7)	−0.0075 (8)	0.0095 (8)
O4	0.0569 (10)	0.0465 (9)	0.0449 (9)	0.0043 (7)	−0.0150 (8)	0.0056 (7)
O3W	0.0889 (14)	0.0498 (10)	0.0538 (10)	0.0027 (9)	−0.0241 (10)	0.0014 (8)
N1	0.0305 (9)	0.0447 (10)	0.0450 (10)	0.0021 (8)	0.0004 (8)	0.0029 (8)

N2	0.0298 (9)	0.0452 (10)	0.0374 (9)	0.0005 (7)	0.0000 (7)	0.0046 (8)
N3	0.0361 (10)	0.0463 (10)	0.0461 (10)	0.0027 (8)	−0.0019 (8)	−0.0040 (8)
N4	0.0302 (9)	0.0430 (10)	0.0388 (9)	0.0005 (7)	−0.0001 (7)	0.0053 (8)
N5	0.0323 (10)	0.0586 (12)	0.0386 (10)	0.0044 (8)	0.0018 (8)	0.0006 (9)
C1	0.0470 (14)	0.0473 (13)	0.0569 (15)	0.0057 (11)	0.0096 (11)	0.0173 (11)
C2	0.0450 (13)	0.0606 (15)	0.0380 (12)	0.0058 (11)	0.0027 (10)	0.0151 (11)
C3	0.0384 (12)	0.0541 (13)	0.0394 (12)	−0.0003 (10)	−0.0054 (10)	−0.0062 (10)
C4	0.0380 (12)	0.0415 (12)	0.0542 (14)	−0.0048 (10)	0.0008 (10)	0.0006 (10)
C5	0.0426 (13)	0.0539 (14)	0.0455 (13)	0.0003 (11)	0.0051 (10)	0.0159 (11)
C6	0.0404 (13)	0.0688 (16)	0.0343 (11)	0.0036 (11)	0.0019 (10)	0.0103 (11)
C7	0.0524 (15)	0.0682 (16)	0.0436 (13)	0.0079 (12)	0.0010 (11)	−0.0132 (12)
C8	0.0598 (17)	0.0633 (16)	0.0624 (16)	0.0155 (13)	0.0003 (13)	−0.0174 (13)
C9	0.0513 (15)	0.0437 (13)	0.0643 (16)	0.0066 (11)	−0.0051 (12)	−0.0030 (12)
C10	0.0400 (13)	0.0639 (15)	0.0507 (14)	0.0025 (11)	−0.0046 (11)	−0.0016 (12)
C11	0.0353 (12)	0.0454 (13)	0.0602 (15)	0.0056 (10)	−0.0024 (11)	−0.0046 (11)
C12	0.0420 (14)	0.0463 (13)	0.0846 (19)	0.0036 (11)	−0.0067 (13)	−0.0028 (13)
C13	0.0559 (18)	0.0638 (18)	0.103 (2)	0.0145 (14)	−0.0066 (17)	−0.0377 (18)
C14	0.077 (2)	0.103 (3)	0.083 (2)	0.005 (2)	0.0206 (18)	−0.037 (2)
C15	0.108 (3)	0.088 (2)	0.088 (2)	−0.008 (2)	0.044 (2)	−0.007 (2)
C16	0.079 (2)	0.0523 (15)	0.079 (2)	−0.0034 (14)	0.0246 (16)	−0.0112 (14)
C17	0.0288 (10)	0.0382 (11)	0.0336 (10)	−0.0040 (8)	−0.0005 (8)	0.0051 (8)
C18	0.0556 (15)	0.0505 (13)	0.0333 (11)	−0.0019 (11)	−0.0086 (10)	0.0068 (10)
C19	0.0835 (19)	0.0545 (14)	0.0330 (12)	−0.0011 (13)	−0.0084 (12)	−0.0083 (11)
C20	0.0591 (15)	0.0392 (12)	0.0437 (13)	0.0008 (11)	0.0013 (11)	−0.0041 (10)
C21	0.0292 (11)	0.0360 (10)	0.0349 (10)	−0.0020 (8)	0.0025 (8)	0.0041 (8)
C22	0.0288 (10)	0.0375 (10)	0.0299 (10)	−0.0036 (8)	−0.0005 (8)	0.0007 (8)
C23	0.0341 (12)	0.0401 (11)	0.0430 (12)	−0.0015 (9)	−0.0011 (9)	0.0060 (10)
C24	0.0277 (11)	0.0413 (12)	0.0428 (12)	0.0004 (9)	0.0026 (9)	0.0069 (10)
O2W	0.0305 (8)	0.0620 (10)	0.0642 (10)	−0.0010 (7)	−0.0034 (7)	0.0196 (8)
O1W	0.0393 (9)	0.0735 (11)	0.0481 (9)	−0.0017 (8)	−0.0029 (7)	0.0129 (8)

Geometric parameters (Å, º)

Cu1—N4	2.0119 (17)	C7—C8	1.515 (3)
Cu1—N1	2.0146 (17)	C7—H7A	0.9700
Cu1—N5	2.0206 (17)	C7—H7B	0.9700
Cu1—N2	2.0290 (17)	C8—C9	1.511 (4)
O1—C23	1.251 (2)	C8—H8A	0.9700
O2—C23	1.247 (2)	C8—H8B	0.9700
O3—C24	1.254 (3)	C9—H9A	0.9700
O4—C24	1.249 (3)	C9—H9B	0.9700
O3W—H3WA	0.8814	C10—C11	1.502 (3)
O3W—H3WB	0.8671	C10—H10A	0.9700
N1—C1	1.473 (3)	C10—H10B	0.9700
N1—C9	1.480 (3)	C11—C16	1.373 (4)
N1—H1	0.9800	C11—C12	1.386 (3)
N2—C2	1.481 (3)	C12—C13	1.378 (4)
N2—C3	1.495 (3)	C12—H12	0.9300

N2—H2	0.9800	C13—C14	1.364 (5)
N3—C4	1.433 (3)	C13—H13	0.9300
N3—C3	1.435 (3)	C14—C15	1.350 (5)
N3—C10	1.474 (3)	C14—H14	0.9300
N4—C5	1.480 (3)	C15—C16	1.381 (4)
N4—C4	1.495 (3)	C15—H15	0.9300
N4—H4	0.9800	C16—H16	0.9300
N5—C6	1.478 (3)	C17—C18	1.381 (3)
N5—C7	1.478 (3)	C17—C22	1.389 (3)
N5—H5	0.9800	C17—C23	1.513 (3)
C1—C2	1.507 (3)	C18—C19	1.380 (3)
C1—H1A	0.9700	C18—H18	0.9300
C1—H1B	0.9700	C19—C20	1.380 (3)
C2—H2A	0.9700	C19—H19	0.9300
C2—H2B	0.9700	C20—C21	1.386 (3)
C3—H3A	0.9700	C20—H20	0.9300
C3—H3B	0.9700	C21—C22	1.384 (3)
C4—H4A	0.9700	C21—C24	1.513 (3)
C4—H4B	0.9700	C22—H22	0.9300
C5—C6	1.505 (3)	O2W—H2WA	0.8360
C5—H5A	0.9700	O2W—H2WB	0.8450
C5—H5B	0.9700	O1W—H1WA	0.8473
C6—H6A	0.9700	O1W—H1WB	0.8730
C6—H6B	0.9700		

N4—Cu1—N1	178.13 (7)	H6A—C6—H6B	108.4
N4—Cu1—N5	86.27 (7)	N5—C7—C8	112.00 (19)
N1—Cu1—N5	93.91 (7)	N5—C7—H7A	109.2
N4—Cu1—N2	93.51 (7)	C8—C7—H7A	109.2
N1—Cu1—N2	86.29 (7)	N5—C7—H7B	109.2
N5—Cu1—N2	179.15 (8)	C8—C7—H7B	109.2
H3WA—O3W—H3WB	108.0	H7A—C7—H7B	107.9
C1—N1—C9	112.30 (18)	C9—C8—C7	115.2 (2)
C1—N1—Cu1	107.13 (13)	C9—C8—H8A	108.5
C9—N1—Cu1	115.94 (13)	C7—C8—H8A	108.5
C1—N1—H1	107.0	C9—C8—H8B	108.5
C9—N1—H1	107.0	C7—C8—H8B	108.5
Cu1—N1—H1	107.0	H8A—C8—H8B	107.5
C2—N2—C3	112.08 (17)	N1—C9—C8	112.4 (2)
C2—N2—Cu1	106.01 (13)	N1—C9—H9A	109.1
C3—N2—Cu1	115.82 (13)	C8—C9—H9A	109.1
C2—N2—H2	107.5	N1—C9—H9B	109.1
C3—N2—H2	107.5	C8—C9—H9B	109.1
Cu1—N2—H2	107.5	H9A—C9—H9B	107.8
C4—N3—C3	115.14 (18)	N3—C10—C11	113.38 (18)
C4—N3—C10	114.89 (18)	N3—C10—H10A	108.9
C3—N3—C10	115.56 (19)	C11—C10—H10A	108.9
C5—N4—C4	112.06 (17)	N3—C10—H10B	108.9

C5—N4—Cu1	106.53 (13)	C11—C10—H10B	108.9
C4—N4—Cu1	114.52 (13)	H10A—C10—H10B	107.7
C5—N4—H4	107.8	C16—C11—C12	117.8 (2)
C4—N4—H4	107.8	C16—C11—C10	121.6 (2)
Cu1—N4—H4	107.8	C12—C11—C10	120.6 (2)
C6—N5—C7	112.77 (18)	C13—C12—C11	120.7 (3)
C6—N5—Cu1	106.72 (13)	C13—C12—H12	119.7
C7—N5—Cu1	116.79 (15)	C11—C12—H12	119.7
C6—N5—H5	106.7	C14—C13—C12	120.4 (3)
C7—N5—H5	106.7	C14—C13—H13	119.8
Cu1—N5—H5	106.7	C12—C13—H13	119.8
N1—C1—C2	108.80 (18)	C15—C14—C13	119.5 (3)
N1—C1—H1A	109.9	C15—C14—H14	120.2
C2—C1—H1A	109.9	C13—C14—H14	120.2
N1—C1—H1B	109.9	C14—C15—C16	120.8 (3)
C2—C1—H1B	109.9	C14—C15—H15	119.6
H1A—C1—H1B	108.3	C16—C15—H15	119.6
N2—C2—C1	108.68 (18)	C11—C16—C15	120.8 (3)
N2—C2—H2A	110.0	C11—C16—H16	119.6
C1—C2—H2A	110.0	C15—C16—H16	119.6
N2—C2—H2B	110.0	C18—C17—C22	118.79 (19)
C1—C2—H2B	110.0	C18—C17—C23	121.21 (18)
H2A—C2—H2B	108.3	C22—C17—C23	119.98 (18)
N3—C3—N2	114.72 (17)	C19—C18—C17	120.5 (2)
N3—C3—H3A	108.6	C19—C18—H18	119.7
N2—C3—H3A	108.6	C17—C18—H18	119.7
N3—C3—H3B	108.6	C20—C19—C18	120.2 (2)
N2—C3—H3B	108.6	C20—C19—H19	119.9
H3A—C3—H3B	107.6	C18—C19—H19	119.9
N3—C4—N4	114.61 (17)	C19—C20—C21	120.3 (2)
N3—C4—H4A	108.6	C19—C20—H20	119.8
N4—C4—H4A	108.6	C21—C20—H20	119.8
N3—C4—H4B	108.6	C22—C21—C20	118.86 (19)
N4—C4—H4B	108.6	C22—C21—C24	119.66 (18)
H4A—C4—H4B	107.6	C20—C21—C24	121.41 (18)
N4—C5—C6	108.34 (18)	C21—C22—C17	121.31 (18)
N4—C5—H5A	110.0	C21—C22—H22	119.3
C6—C5—H5A	110.0	C17—C22—H22	119.3
N4—C5—H5B	110.0	O2—C23—O1	124.7 (2)
C6—C5—H5B	110.0	O2—C23—C17	117.66 (18)
H5A—C5—H5B	108.4	O1—C23—C17	117.66 (19)
N5—C6—C5	108.45 (17)	O4—C24—O3	124.7 (2)
N5—C6—H6A	110.0	O4—C24—C21	118.00 (18)
C5—C6—H6A	110.0	O3—C24—C21	117.30 (19)
N5—C6—H6B	110.0	H2WA—O2W—H2WB	115.8
C5—C6—H6B	110.0	H1WA—O1W—H1WB	115.1
C9—N1—C1—C2	167.12 (18)	N3—C10—C11—C12	−77.4 (3)

Cu1—N1—C1—C2	38.7 (2)	C16—C11—C12—C13	0.4 (4)
C3—N2—C2—C1	167.77 (18)	C10—C11—C12—C13	−178.4 (2)
Cu1—N2—C2—C1	40.5 (2)	C11—C12—C13—C14	−0.9 (4)
N1—C1—C2—N2	−54.0 (2)	C12—C13—C14—C15	0.6 (5)
C4—N3—C3—N2	67.2 (2)	C13—C14—C15—C16	0.2 (6)
C10—N3—C3—N2	−70.5 (2)	C12—C11—C16—C15	0.3 (4)
C2—N2—C3—N3	−175.81 (18)	C10—C11—C16—C15	179.2 (3)
Cu1—N2—C3—N3	−54.0 (2)	C14—C15—C16—C11	−0.7 (6)
C3—N3—C4—N4	−70.0 (2)	C22—C17—C18—C19	0.4 (3)
C10—N3—C4—N4	68.0 (2)	C23—C17—C18—C19	−178.2 (2)
C5—N4—C4—N3	179.82 (18)	C17—C18—C19—C20	0.1 (4)
Cu1—N4—C4—N3	58.3 (2)	C18—C19—C20—C21	−0.8 (4)
C4—N4—C5—C6	−166.99 (17)	C19—C20—C21—C22	1.0 (3)
Cu1—N4—C5—C6	−41.01 (19)	C19—C20—C21—C24	177.7 (2)
C7—N5—C6—C5	−168.77 (19)	C20—C21—C22—C17	−0.5 (3)
Cu1—N5—C6—C5	−39.2 (2)	C24—C21—C22—C17	−177.30 (18)
N4—C5—C6—N5	54.5 (2)	C18—C17—C22—C21	−0.2 (3)
C6—N5—C7—C8	−179.3 (2)	C23—C17—C22—C21	178.41 (18)
Cu1—N5—C7—C8	56.6 (2)	C18—C17—C23—O2	179.9 (2)
N5—C7—C8—C9	−67.4 (3)	C22—C17—C23—O2	1.3 (3)
C1—N1—C9—C8	178.50 (19)	C18—C17—C23—O1	0.6 (3)
Cu1—N1—C9—C8	−57.9 (2)	C22—C17—C23—O1	−178.0 (2)
C7—C8—C9—N1	68.5 (3)	C22—C21—C24—O4	−11.4 (3)
C4—N3—C10—C11	153.0 (2)	C20—C21—C24—O4	171.9 (2)
C3—N3—C10—C11	−69.1 (3)	C22—C21—C24—O3	166.69 (19)
N3—C10—C11—C16	103.8 (3)	C20—C21—C24—O3	−10.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O4^{i}	0.98	2.04	2.950 (2)	154
N2—H2···O3^{ii}	0.98	2.15	3.118 (2)	170
N4—H4···O2^{iii}	0.98	2.00	2.949 (2)	161
N5—H5···O3*W*^{iv}	0.98	2.35	3.230 (3)	149
O1*W*—H1*WB*···O4^{ii}	0.87	2.01	2.884 (2)	176
O1*W*—H1*WB*···O3^{ii}	0.87	2.60	3.213 (2)	128
O1*W*—H1*WA*···O3*W*^{iii}	0.85	1.97	2.813 (2)	173
O2*W*—H2*WA*···O2^{iv}	0.84	1.96	2.795 (2)	174
O2*W*—H2*WB*···O3^{i}	0.85	1.95	2.798 (2)	178
O3*W*—H3*WA*···O1^{v}	0.88	1.92	2.779 (2)	163
O3*W*—H3*WB*···O1	0.87	1.85	2.720 (2)	176
O3*W*—H3*WB*···O2	0.87	2.66	3.248 (2)	126

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

trans-Diaqua[3-(pyridin-3-ylmethyl)-1,3,5,8,12-pentaazacyclotetradecane-$\kappa^4N^1,N^5,N^8,N^{12}$]copper(II) isophthalate 0.9-hydrate (II)

Crystal data

$[Cu(C_{15}H_{28}N_6)(H_2O)_2](C_8H_4O_4)\cdot 0.9H_2O$
$M_r = 572.33$
Monoclinic, $P2_1/c$
$a = 7.1955$ (3) Å
$b = 19.0463$ (8) Å
$c = 19.4426$ (8) Å
$\beta = 94.276$ (2)°
$V = 2657.15$ (19) Å^3
$Z = 4$
$F(000) = 1208$
$D_x = 1.431$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6756 reflections
$\theta = 3.5$–$24.1°$
$\mu = 0.88$ mm^{-1}
$T = 296$ K
Needle, violet
0.16 × 0.04 × 0.04 mm

Data collection

Bruker X8 APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2007)
$T_{min} = 0.873$, $T_{max} = 0.966$
76082 measured reflections
4532 independent reflections
2834 reflections with $I > 2\sigma(I)$
$R_{int} = 0.106$
$\theta_{max} = 24.7°$, $\theta_{min} = 2.4°$
$h = -8\rightarrow 8$
$k = -22\rightarrow 22$
$l = -22\rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.097$
$S = 1.00$
4532 reflections
439 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0305P)^2 + 2.3396P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.43303 (5)	0.24763 (2)	0.48049 (2)	0.03543 (14)	
O1W	0.7535 (3)	0.29360 (13)	0.51575 (12)	0.0526 (7)	
H1WA	0.8135	0.3174	0.4879	0.079*	
H1WB	0.8207	0.2732	0.5405	0.079*	
O2W	0.1108 (3)	0.20190 (13)	0.45250 (12)	0.0489 (7)	
H2WA	0.0608	0.1826	0.4762	0.073*	
H2WB	0.0448	0.2250	0.4244	0.073*	
O2	−0.0118 (3)	0.28246 (13)	0.11247 (12)	0.0458 (6)	

O1	−0.0810 (4)	0.37745 (13)	0.05000 (12)	0.0514 (7)	
O3	−0.1053 (3)	0.27854 (13)	0.35932 (12)	0.0477 (6)	
O4	−0.0716 (4)	0.37804 (13)	0.41829 (12)	0.0520 (7)	
O3W	0.8843 (8)	−0.0087 (3)	0.4939 (3)	0.090 (2)	0.5
H3WA	0.8940	0.0323	0.5112	0.135*	0.5
H3WB	0.9961	−0.0217	0.4903	0.135*	0.5
N5	0.3655 (4)	0.25100 (17)	0.57886 (14)	0.0422 (7)	
H5	0.252 (5)	0.2428 (18)	0.5797 (17)	0.051*	
N4	0.5142 (4)	0.14778 (15)	0.50045 (15)	0.0380 (7)	
H4	0.622 (5)	0.1491 (18)	0.5042 (18)	0.046*	
N3	0.5197 (4)	0.11268 (15)	0.37866 (14)	0.0422 (7)	
N2	0.4917 (4)	0.24119 (15)	0.38076 (14)	0.0375 (7)	
H2	0.604 (5)	0.2455 (18)	0.3789 (17)	0.045*	
N1	0.3470 (4)	0.34611 (16)	0.45862 (17)	0.0459 (8)	
H1	0.237 (5)	0.342 (2)	0.4524 (19)	0.055*	
N6	0.7057 (5)	0.0207 (2)	0.1924 (2)	0.0773 (12)	
C6	0.4550 (6)	0.1900 (2)	0.6144 (2)	0.0517 (11)	
H6A	0.400 (5)	0.1804 (19)	0.658 (2)	0.062*	
H6B	0.579 (6)	0.2040 (19)	0.6278 (19)	0.062*	
C5	0.4414 (6)	0.1282 (2)	0.56692 (19)	0.0472 (10)	
H5A	0.511 (5)	0.0884 (19)	0.5869 (18)	0.057*	
H5B	0.317 (5)	0.1139 (18)	0.5564 (17)	0.057*	
C4	0.4585 (6)	0.0962 (2)	0.4450 (2)	0.0475 (10)	
H4A	0.504 (5)	0.052 (2)	0.4583 (18)	0.057*	
H4B	0.322 (5)	0.0956 (18)	0.4417 (17)	0.057*	
C3	0.4360 (5)	0.1735 (2)	0.34625 (19)	0.0454 (10)	
H3A	0.305 (5)	0.1701 (18)	0.3498 (17)	0.055*	
H3B	0.475 (5)	0.1762 (17)	0.2977 (18)	0.055*	
C2	0.4032 (6)	0.3025 (2)	0.3452 (2)	0.0558 (12)	
H2A	0.275 (6)	0.291 (2)	0.3319 (19)	0.067*	
H2B	0.461 (5)	0.3108 (19)	0.303 (2)	0.067*	
C1	0.4203 (6)	0.3651 (2)	0.3917 (2)	0.0594 (12)	
H1A	0.561 (6)	0.379 (2)	0.4029 (19)	0.071*	
H1B	0.370 (6)	0.402 (2)	0.375 (2)	0.071*	
C9	0.3921 (7)	0.3989 (2)	0.5132 (3)	0.0637 (13)	
H9A	0.349 (6)	0.441 (2)	0.496 (2)	0.076*	
H9B	0.529 (6)	0.405 (2)	0.522 (2)	0.076*	
C8	0.3075 (7)	0.3790 (3)	0.5796 (3)	0.0730 (15)	
H8A	0.321 (6)	0.414 (2)	0.609 (2)	0.088*	
H8B	0.167 (6)	0.372 (2)	0.575 (2)	0.088*	
C7	0.3989 (7)	0.3169 (3)	0.6173 (2)	0.0603 (12)	
H7A	0.527 (6)	0.323 (2)	0.625 (2)	0.072*	
H7B	0.352 (6)	0.313 (2)	0.664 (2)	0.072*	
C10	0.7173 (6)	0.1022 (2)	0.3693 (2)	0.0500 (10)	
H10A	0.756 (5)	0.064 (2)	0.3953 (19)	0.060*	
H10B	0.798 (5)	0.1392 (19)	0.3909 (18)	0.060*	
C11	0.7527 (5)	0.09148 (19)	0.29454 (19)	0.0433 (9)	
C15	0.6836 (6)	0.0338 (2)	0.2589 (3)	0.0634 (13)	

H15	0.622 (6)	0.003 (2)	0.280 (2)	0.076*	
C14	0.8046 (7)	0.0681 (3)	0.1601 (2)	0.0711 (14)	
H14	0.834 (6)	0.060 (2)	0.117 (2)	0.085*	
C13	0.8791 (6)	0.1269 (3)	0.1905 (2)	0.0639 (12)	
H13	0.957 (6)	0.161 (2)	0.163 (2)	0.077*	
C12	0.8528 (6)	0.1385 (2)	0.2583 (2)	0.0514 (10)	
H12	0.903 (5)	0.177 (2)	0.2834 (19)	0.062*	
C16	−0.0922 (4)	0.38525 (17)	0.17181 (16)	0.0315 (8)	
C17	−0.1431 (5)	0.45554 (19)	0.17099 (19)	0.0419 (9)	
H17	−0.154 (5)	0.4782 (18)	0.1319 (18)	0.050*	
C18	−0.1798 (5)	0.4895 (2)	0.2311 (2)	0.0484 (10)	
H18	−0.212 (5)	0.535 (2)	0.2291 (18)	0.058*	
C19	−0.1628 (5)	0.45471 (19)	0.2933 (2)	0.0423 (9)	
H19	−0.178 (5)	0.4782 (18)	0.3327 (18)	0.051*	
C20	−0.1130 (4)	0.38455 (17)	0.29563 (16)	0.0322 (8)	
C21	−0.0791 (4)	0.35064 (18)	0.23471 (18)	0.0333 (8)	
H21	−0.049 (4)	0.3043 (17)	0.2347 (16)	0.040*	
C22	−0.0577 (4)	0.3458 (2)	0.10677 (17)	0.0377 (8)	
C23	−0.0942 (4)	0.34456 (19)	0.36318 (18)	0.0366 (8)	
O4W	0.018 (3)	0.5169 (8)	0.4782 (9)	0.138 (5)	0.2
H4WA	−0.0066	0.4764	0.4615	0.207*	0.2
H4WB	0.0112	0.5119	0.5213	0.207*	0.2
O5W	0.086 (3)	0.5056 (8)	0.4928 (9)	0.138 (5)	0.2
H5WA	0.0741	0.4989	0.5361	0.207*	0.2
H5WB	0.0812	0.4718	0.4661	0.207*	0.2

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0391 (2)	0.0350 (2)	0.0325 (2)	0.0007 (2)	0.00440 (15)	0.0006 (2)
O1W	0.0417 (15)	0.0661 (18)	0.0504 (16)	0.0018 (12)	0.0065 (12)	0.0141 (14)
O2W	0.0363 (14)	0.0672 (18)	0.0431 (15)	−0.0005 (12)	0.0028 (11)	0.0152 (13)
O2	0.0547 (16)	0.0430 (16)	0.0411 (15)	0.0053 (12)	0.0118 (12)	−0.0040 (12)
O1	0.0723 (18)	0.0507 (16)	0.0320 (15)	−0.0058 (13)	0.0091 (12)	0.0048 (13)
O3	0.0655 (17)	0.0388 (16)	0.0385 (15)	0.0013 (12)	0.0034 (12)	0.0051 (12)
O4	0.0690 (18)	0.0542 (17)	0.0323 (15)	−0.0054 (13)	0.0008 (12)	−0.0085 (13)
O3W	0.085 (4)	0.059 (4)	0.129 (6)	−0.009 (3)	0.025 (4)	−0.033 (4)
N5	0.0338 (15)	0.0535 (19)	0.0395 (17)	−0.0023 (17)	0.0042 (13)	−0.0067 (17)
N4	0.0367 (16)	0.0421 (18)	0.0349 (17)	0.0003 (14)	0.0015 (13)	0.0025 (14)
N3	0.0411 (18)	0.047 (2)	0.0386 (18)	0.0035 (14)	0.0065 (13)	−0.0064 (15)
N2	0.0330 (15)	0.0432 (19)	0.0360 (16)	0.0024 (15)	0.0016 (13)	0.0069 (15)
N1	0.0358 (17)	0.0402 (19)	0.063 (2)	0.0030 (15)	0.0099 (16)	0.0016 (16)
N6	0.066 (3)	0.086 (3)	0.079 (3)	−0.001 (2)	0.004 (2)	−0.048 (2)
C6	0.047 (2)	0.076 (3)	0.031 (2)	0.005 (2)	0.0010 (19)	0.006 (2)
C5	0.045 (2)	0.056 (3)	0.041 (2)	0.002 (2)	0.0042 (18)	0.018 (2)
C4	0.052 (2)	0.038 (2)	0.053 (3)	−0.0043 (19)	0.011 (2)	−0.004 (2)
C3	0.041 (2)	0.063 (3)	0.033 (2)	0.0004 (19)	0.0044 (17)	−0.009 (2)
C2	0.057 (3)	0.064 (3)	0.046 (3)	0.014 (2)	0.007 (2)	0.023 (2)

C1	0.055 (3)	0.046 (3)	0.079 (3)	0.011 (2)	0.016 (2)	0.024 (3)
C9	0.061 (3)	0.036 (2)	0.095 (4)	0.001 (2)	0.012 (3)	−0.014 (3)
C8	0.076 (3)	0.060 (3)	0.086 (4)	−0.001 (3)	0.027 (3)	−0.035 (3)
C7	0.059 (3)	0.071 (3)	0.053 (3)	−0.005 (2)	0.011 (2)	−0.025 (3)
C10	0.047 (2)	0.050 (3)	0.053 (3)	0.0033 (19)	0.0030 (19)	−0.006 (2)
C11	0.036 (2)	0.042 (2)	0.051 (2)	0.0065 (17)	0.0032 (17)	−0.0141 (19)
C15	0.053 (3)	0.061 (3)	0.078 (3)	−0.010 (2)	0.017 (2)	−0.022 (3)
C14	0.064 (3)	0.095 (4)	0.055 (3)	0.026 (3)	0.009 (3)	−0.015 (3)
C13	0.068 (3)	0.065 (3)	0.060 (3)	0.015 (2)	0.011 (2)	0.003 (3)
C12	0.049 (2)	0.041 (3)	0.064 (3)	0.0016 (19)	0.005 (2)	−0.006 (2)
C16	0.0283 (17)	0.034 (2)	0.032 (2)	−0.0023 (14)	0.0050 (14)	−0.0003 (16)
C17	0.048 (2)	0.041 (2)	0.037 (2)	0.0002 (17)	0.0023 (17)	0.0075 (19)
C18	0.063 (3)	0.029 (2)	0.053 (3)	0.0046 (19)	0.0011 (19)	0.002 (2)
C19	0.048 (2)	0.038 (2)	0.042 (2)	−0.0016 (17)	0.0083 (17)	−0.0067 (19)
C20	0.0277 (18)	0.035 (2)	0.034 (2)	−0.0026 (14)	0.0044 (14)	−0.0048 (16)
C21	0.0295 (18)	0.0323 (19)	0.038 (2)	0.0029 (15)	0.0023 (14)	−0.0015 (19)
C22	0.0327 (19)	0.047 (3)	0.034 (2)	−0.0061 (16)	0.0050 (15)	0.0005 (19)
C23	0.0298 (19)	0.044 (2)	0.037 (2)	−0.0023 (16)	0.0060 (15)	0.0016 (19)
O4W	0.16 (2)	0.121 (12)	0.135 (14)	−0.018 (11)	0.049 (10)	−0.014 (10)
O5W	0.16 (2)	0.121 (12)	0.135 (14)	−0.018 (11)	0.049 (10)	−0.014 (10)

Geometric parameters (Å, º)

Cu1—N5	2.009 (3)	C3—H3B	1.01 (3)
Cu1—N1	2.011 (3)	C2—C1	1.496 (6)
Cu1—N4	2.019 (3)	C2—H2A	0.96 (4)
Cu1—N2	2.019 (3)	C2—H2B	0.95 (4)
Cu1—O2W	2.499 (2)	C1—H1A	1.05 (4)
Cu1—O1W	2.514 (2)	C1—H1B	0.84 (4)
O1W—H1WA	0.8490	C9—C8	1.518 (7)
O1W—H1WB	0.7628	C9—H9A	0.91 (4)
O2W—H2WA	0.7075	C9—H9B	0.99 (4)
O2W—H2WB	0.8243	C8—C7	1.515 (7)
O2—C22	1.253 (4)	C8—H8A	0.88 (5)
O1—C22	1.258 (4)	C8—H8B	1.01 (5)
O3—C23	1.262 (4)	C7—H7A	0.93 (4)
O4—C23	1.247 (4)	C7—H7B	1.00 (4)
O3W—H3WA	0.8501	C10—C11	1.508 (5)
O3W—H3WB	0.8500	C10—H10A	0.92 (4)
N5—C7	1.472 (5)	C10—H10B	0.99 (4)
N5—C6	1.475 (5)	C11—C15	1.373 (5)
N5—H5	0.83 (4)	C11—C12	1.376 (5)
N4—C5	1.478 (4)	C15—H15	0.85 (4)
N4—C4	1.491 (5)	C14—C13	1.358 (7)
N4—H4	0.78 (3)	C14—H14	0.90 (4)
N3—C4	1.428 (5)	C13—C12	1.365 (6)
N3—C3	1.430 (5)	C13—H13	1.03 (4)
N3—C10	1.460 (5)	C12—H12	0.94 (4)

N2—C2	1.477 (5)	C16—C21	1.386 (4)
N2—C3	1.494 (5)	C16—C17	1.388 (5)
N2—H2	0.81 (3)	C16—C22	1.507 (4)
N1—C9	1.480 (5)	C17—C18	1.378 (5)
N1—C1	1.484 (5)	C17—H17	0.87 (3)
N1—H1	0.79 (4)	C18—C19	1.377 (5)
N6—C14	1.335 (6)	C18—H18	0.90 (4)
N6—C15	1.337 (6)	C19—C20	1.383 (5)
C6—C5	1.494 (6)	C19—H19	0.90 (3)
C6—H6A	0.98 (4)	C20—C21	1.387 (4)
C6—H6B	0.95 (4)	C20—C23	1.516 (4)
C5—H5A	0.97 (4)	C21—H21	0.91 (3)
C5—H5B	0.94 (4)	O4W—H4WA	0.8499
C4—H4A	0.94 (4)	O4W—H4WB	0.8499
C4—H4B	0.98 (4)	O5W—H5WA	0.8621
C3—H3A	0.95 (4)	O5W—H5WB	0.8273

N5—Cu1—N1	94.53 (13)	C1—C2—H2A	112 (2)
N5—Cu1—N4	86.23 (12)	N2—C2—H2B	109 (2)
N1—Cu1—N4	178.43 (13)	C1—C2—H2B	111 (2)
N5—Cu1—N2	177.48 (12)	H2A—C2—H2B	106 (3)
N1—Cu1—N2	86.37 (12)	N1—C1—C2	108.5 (3)
N4—Cu1—N2	92.82 (12)	N1—C1—H1A	106 (2)
N5—Cu1—O2W	86.10 (10)	C2—C1—H1A	111 (2)
N1—Cu1—O2W	90.74 (10)	N1—C1—H1B	111 (3)
N4—Cu1—O2W	87.94 (10)	C2—C1—H1B	115 (3)
N2—Cu1—O2W	91.54 (10)	H1A—C1—H1B	105 (4)
N5—Cu1—O1W	90.65 (10)	N1—C9—C8	111.0 (4)
N1—Cu1—O1W	89.69 (10)	N1—C9—H9A	106 (3)
N4—Cu1—O1W	91.68 (10)	C8—C9—H9A	113 (3)
N2—Cu1—O1W	91.71 (10)	N1—C9—H9B	111 (2)
O2W—Cu1—O1W	176.75 (8)	C8—C9—H9B	110 (2)
Cu1—O1W—H1WA	120.8	H9A—C9—H9B	106 (4)
Cu1—O1W—H1WB	121.4	C7—C8—C9	114.8 (4)
H1WA—O1W—H1WB	110.2	C7—C8—H8A	105 (3)
Cu1—O2W—H2WA	123.2	C9—C8—H8A	109 (3)
Cu1—O2W—H2WB	115.9	C7—C8—H8B	109 (3)
H2WA—O2W—H2WB	114.4	C9—C8—H8B	114 (2)
H3WA—O3W—H3WB	104.5	H8A—C8—H8B	103 (4)
C7—N5—C6	112.7 (3)	N5—C7—C8	111.8 (4)
C7—N5—Cu1	117.9 (3)	N5—C7—H7A	108 (2)
C6—N5—Cu1	107.0 (2)	C8—C7—H7A	111 (3)
C7—N5—H5	106 (2)	N5—C7—H7B	110 (2)
C6—N5—H5	104 (3)	C8—C7—H7B	110 (2)
Cu1—N5—H5	109 (2)	H7A—C7—H7B	106 (3)
C5—N4—C4	111.9 (3)	N3—C10—C11	112.0 (3)
C5—N4—Cu1	106.8 (2)	N3—C10—H10A	107 (2)
C4—N4—Cu1	115.0 (2)	C11—C10—H10A	111 (2)

C5—N4—H4	110 (3)	N3—C10—H10B	113 (2)
C4—N4—H4	108 (3)	C11—C10—H10B	112 (2)
Cu1—N4—H4	105 (3)	H10A—C10—H10B	101 (3)
C4—N3—C3	115.3 (3)	C15—C11—C12	116.5 (4)
C4—N3—C10	116.8 (3)	C15—C11—C10	120.9 (4)
C3—N3—C10	116.0 (3)	C12—C11—C10	122.5 (4)
C2—N2—C3	112.3 (3)	N6—C15—C11	124.9 (4)
C2—N2—Cu1	106.7 (2)	N6—C15—H15	116 (3)
C3—N2—Cu1	114.5 (2)	C11—C15—H15	119 (3)
C2—N2—H2	107 (2)	N6—C14—C13	124.0 (4)
C3—N2—H2	108 (2)	N6—C14—H14	120 (3)
Cu1—N2—H2	108 (2)	C13—C14—H14	116 (3)
C9—N1—C1	112.9 (3)	C14—C13—C12	118.5 (5)
C9—N1—Cu1	115.8 (3)	C14—C13—H13	120 (2)
C1—N1—Cu1	106.8 (2)	C12—C13—H13	122 (2)
C9—N1—H1	109 (3)	C13—C12—C11	120.3 (4)
C1—N1—H1	108 (3)	C13—C12—H12	124 (2)
Cu1—N1—H1	104 (3)	C11—C12—H12	116 (2)
C14—N6—C15	115.9 (4)	C21—C16—C17	118.0 (3)
N5—C6—C5	109.0 (3)	C21—C16—C22	119.9 (3)
N5—C6—H6A	111 (2)	C17—C16—C22	122.1 (3)
C5—C6—H6A	112 (2)	C18—C17—C16	120.7 (3)
N5—C6—H6B	106 (2)	C18—C17—H17	120 (2)
C5—C6—H6B	114 (2)	C16—C17—H17	120 (2)
H6A—C6—H6B	104 (3)	C19—C18—C17	120.6 (4)
N4—C5—C6	109.3 (3)	C19—C18—H18	121 (2)
N4—C5—H5A	110 (2)	C17—C18—H18	119 (2)
C6—C5—H5A	111 (2)	C18—C19—C20	120.0 (3)
N4—C5—H5B	106 (2)	C18—C19—H19	120 (2)
C6—C5—H5B	112 (2)	C20—C19—H19	120 (2)
H5A—C5—H5B	108 (3)	C19—C20—C21	118.9 (3)
N3—C4—N4	115.1 (3)	C19—C20—C23	121.3 (3)
N3—C4—H4A	109 (2)	C21—C20—C23	119.7 (3)
N4—C4—H4A	109 (2)	C16—C21—C20	121.8 (3)
N3—C4—H4B	109 (2)	C16—C21—H21	118 (2)
N4—C4—H4B	106 (2)	C20—C21—H21	121 (2)
H4A—C4—H4B	110 (3)	O2—C22—O1	123.8 (3)
N3—C3—N2	114.3 (3)	O2—C22—C16	117.7 (3)
N3—C3—H3A	107 (2)	O1—C22—C16	118.5 (3)
N2—C3—H3A	105 (2)	O4—C23—O3	124.4 (3)
N3—C3—H3B	108 (2)	O4—C23—C20	119.0 (3)
N2—C3—H3B	107 (2)	O3—C23—C20	116.6 (3)
H3A—C3—H3B	115 (3)	H4WA—O4W—H4WB	104.5
N2—C2—C1	109.5 (3)	H5WA—O5W—H5WB	119.6
N2—C2—H2A	109 (2)		

C7—N5—C6—C5	−170.6 (3)	N3—C10—C11—C12	114.6 (4)
Cu1—N5—C6—C5	−39.4 (4)	C14—N6—C15—C11	0.7 (7)

C4—N4—C5—C6	−164.5 (3)	C12—C11—C15—N6	−0.5 (6)
Cu1—N4—C5—C6	−37.7 (3)	C10—C11—C15—N6	178.9 (4)
N5—C6—C5—N4	52.4 (4)	C15—N6—C14—C13	−0.7 (7)
C3—N3—C4—N4	−67.4 (4)	N6—C14—C13—C12	0.4 (7)
C10—N3—C4—N4	74.0 (4)	C14—C13—C12—C11	−0.1 (6)
C5—N4—C4—N3	178.4 (3)	C15—C11—C12—C13	0.1 (6)
Cu1—N4—C4—N3	56.3 (4)	C10—C11—C12—C13	−179.2 (4)
C4—N3—C3—N2	68.6 (4)	C21—C16—C17—C18	−0.1 (5)
C10—N3—C3—N2	−73.2 (4)	C22—C16—C17—C18	177.8 (3)
C2—N2—C3—N3	179.5 (3)	C16—C17—C18—C19	1.3 (6)
Cu1—N2—C3—N3	−58.5 (3)	C17—C18—C19—C20	−1.6 (6)
C3—N2—C2—C1	164.3 (3)	C18—C19—C20—C21	0.6 (5)
Cu1—N2—C2—C1	38.0 (4)	C18—C19—C20—C23	−179.6 (3)
C9—N1—C1—C2	168.2 (3)	C17—C16—C21—C20	−0.8 (5)
Cu1—N1—C1—C2	39.9 (4)	C22—C16—C21—C20	−178.8 (3)
N2—C2—C1—N1	−52.9 (4)	C19—C20—C21—C16	0.6 (5)
C1—N1—C9—C8	177.6 (4)	C23—C20—C21—C16	−179.2 (3)
Cu1—N1—C9—C8	−59.0 (4)	C21—C16—C22—O2	−2.2 (4)
N1—C9—C8—C7	71.4 (5)	C17—C16—C22—O2	179.9 (3)
C6—N5—C7—C8	179.4 (3)	C21—C16—C22—O1	176.0 (3)
Cu1—N5—C7—C8	54.0 (4)	C17—C16—C22—O1	−1.9 (5)
C9—C8—C7—N5	−68.1 (5)	C19—C20—C23—O4	−20.1 (5)
C4—N3—C10—C11	156.2 (3)	C21—C20—C23—O4	159.6 (3)
C3—N3—C10—C11	−62.6 (4)	C19—C20—C23—O3	158.9 (3)
N3—C10—C11—C15	−64.7 (5)	C21—C20—C23—O3	−21.4 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O4	0.79 (4)	2.37 (4)	3.115 (4)	157 (4)
N2—H2···O3^{i}	0.81 (3)	2.25 (4)	3.044 (4)	167 (3)
N4—H4···O1^{ii}	0.78 (3)	2.31 (3)	3.037 (4)	157 (3)
N5—H5···O2^{iii}	0.83 (4)	2.10 (4)	2.910 (4)	163 (3)
O1*W*—H1*WA*···O4^{i}	0.85	2.00	2.849 (3)	174
O1*W*—H1*WB*···O2^{ii}	0.76	2.07	2.831 (3)	176
O2*W*—H2*WA*···O1^{iii}	0.71	2.15	2.859 (3)	178
O2*W*—H2*WB*···O3	0.82	1.90	2.722 (3)	180
O3*W*—H3*WA*···O1^{ii}	0.85	1.88	2.731 (6)	179
O3*W*—H3*WB*···O1^{iv}	0.85	2.18	2.760 (6)	126
C1—H1*A*···O4^{i}	1.05 (4)	2.64 (4)	3.662 (5)	164 (3)
C4—H4*B*···O3*W*^{v}	0.98 (4)	2.60 (4)	3.274 (7)	125 (3)
C5—H5*B*···O3*W*^{v}	0.94 (4)	2.62 (4)	3.415 (7)	142 (3)
C10—H10*A*···O3*W*	0.92 (4)	2.49 (4)	3.367 (8)	161 (3)
C13—H13···O2^{i}	1.03 (4)	2.53 (4)	3.446 (6)	147 (3)
C1—H1*B*···N6^{vi}	0.84 (4)	2.66 (4)	3.474 (5)	165 (4)

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