Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetrachlorido-1κCl,2$\kappa^2 Cl$,3κCl-bis[μ-4-undecyl-1,4,7-triazacyclonon-1-yl)acetato]-1$\kappa^4 N,N',N'',O$:2$\kappa O'$;2$\kappa O'$:3$\kappa^4 N,N',N'',O$-tricopper(II) dihydrate

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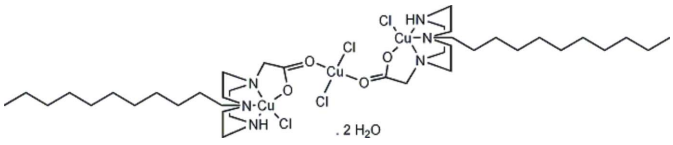
Received 6 July 2007; accepted 14 July 2007

Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.008 Å; R factor = 0.084; wR factor = 0.142; data-to-parameter ratio = 20.8.

In the trinuclear title compound, $[Cu_3Cl_4(C_{17}H_{38}N_3O_2)_2]\cdot 2H_2O$ or $[Cu(AcC_{11}tacn)Cl\cdot H_2O]_2\cdot CuCl_2$ [tacn is 1,4,7-triazacyclononone], two Cu atoms are coordinated by a bifunctionalized 1-acetato-4-undecyl-1,4,7-triazacyclononone ($AcC_{11}tacn$) macrocycle and are five-coordinate, while the third Cu atom, located on a centre of inversion, bridges these two units between two keto O atoms, with two Cl atoms completing a four-coordinate square-planar geometry. The long C_{11} tails on the macrocycle create well ordered multilayer packing.

Related literature

There are several reports of carboxylate-functionalized 1,4,7-triazacyclononane (Mondal *et al.*, 2003; Neves *et al.*, 1988; Graham *et al.*, 1997; Studer *et al.*, 1989; Schulz *et al.*, 1996). In contrast, the arrangement of long hydrophobic carbon tails has been under-represented (Fallis *et al.*, 1998; Battle & Martin, 2006). The title complex combines both groups and results in a trinuclear copper complex. For synthesis, see: Zhang *et al.* (1995).



Experimental

Crystal data

$[Cu_3Cl_4(C_{17}H_{38}N_3O_2)_2]\cdot 2H_2O$
M_r = 1049.50
Monoclinic, $P2_1/c$
a = 22.1182 (11) Å
b = 7.8330 (4) Å
c = 14.6177 (7) Å
β = 104.570 (2)°
V = 2451.1 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.56 mm^{-1}
T = 123 (2) K
0.20 × 0.10 × 0.05 mm

Data collection

Bruker X8 APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.746, T_{max} = 0.926
25491 measured reflections
5625 independent reflections
4994 reflections with $I > 2\sigma(I)$
R_{int} = 0.071

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.084
$wR(F^2)$ = 0.142
S = 1.32
5625 reflections
271 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −1.02 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H31···Cl1	0.90 (2)	2.37 (3)	3.267 (7)	172 (12)
N3—H3···Cl2^{i}	0.89 (2)	2.31 (3)	3.161 (5)	160 (7)

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

We acknowledge support from Monash University and the Australian Research Council.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2179).

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supplementary materials

Acta Cryst. (2007). E**63**, m2193 [**doi:10.1107/S1600536807034538**]

Tetrachlorido-1κCl,2$\kappa^2 Cl$,3κCl-bis[μ-4-undecyl-1,4,7-triazacyclonon-1-yl)acetato]-1$\kappa^4 N,N',N'',O$:2$\kappa O'$;2$\kappa O'$:3$\kappa^4 N,N',N'',O$-tricopper(II) dihydrate

L. Nagel, C. M. Forsyth and L. L. Martin

Comment

The title complex, (I), crystallizes in the monoclinic space group ($P2_1/c$), with the asymmetric unit comprising one half of the molecule $[Cu(AcC_{11}tacn)Cl{\cdot}H_2O]_2{\cdot}CuCl_2$, Fig. 1; the Cu2 atom is located on a crystallographic inversion centre. The three N atoms from the macrocycle coordinate facially to Cu1, which is also bound to a terminal Cl with the fifth coordination site completed by the O atom derived from the *N*-acetyl group. Two of these units are further connected *via* the keto-O atoms to a four coordinate copper dichloride entity. The Cu1—Cl1 bond distance (2.2645 (14) Å) is slightly longer than the Cu2—Cl2 distance of 2.2512 (14) Å, but this may also reflect the interaction of Cl1 with the water molecule *via* a O3—H31···Cl1 (2.37 (3) Å) hydrogen bond. The Cu—N distances are inequivalent with the C_{11} substituted N atom having the longest bond (Cu1—N2 2.289 (4) Å) whilst the secondary amine has the shortest (Cu1—N3 1.985 (4) Å).

The cell contents, when viewed along the *b* axis, Fig. 2, show the straight chain C_{11} units form interdigitated layers which separate the hydrophilic $\{Cu(Actacn)Cl\}{\cdot}CuCl_2$ moieties, the latter associated *via* intermolecular N3—H3···$Cl2^i$ hydrogen bonds (Table 1).

Experimental

The title complex was synthesized using a modification of the published procedure (Zhang *et al.*, 1995). 1-Acetato-4-undecyl-1,4,7-triazacyclononane trihydrochloride (0.1 g, 0.22 mmol) was dissolved in MeOH (5 ml) and mixed with 1 equivalent of $CuCl_2{\cdot}6H_2O$ (0.038 g, 0.22 mmol) dissolved in MeOH (1 ml). Addition of 1.1 equivalent NaOAc (0.0076 g, 0.2 4 mmol) dissolved in MeOH resulted in a dark-green solution. Slow evaporation of the solution resulted in the deposition of blue-green crystals suitable for X-ray diffraction analysis. The solid was collected by filtration and air-dried (0.04 g, 18%). IR (KBr): 3199, 2920, 1578 (νC—O), 1491, 1466, 1445, 1403, 1313 (νC—O) cm^{-1}. UV/vis (MeCN): $\lambda_{max}(\varepsilon)$ 265 (934), 461 (114) nm (L.mol^{-1}.cm).

Refinement

The amine-H3 atom and the water-H31 and H32 atoms and were located and refined with the latter having O—H distances restrained to approximately 0.90 Å. Otherwise, all H atoms were included in the riding model approximation with C—H = 0.95–0.99 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$. The maximum and minimum electron density peaks were located 1.23 and 1.81 Å from the H3A and H6A atoms, respectively.

Figures

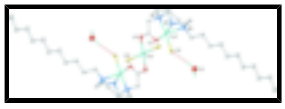

Fig. 1. A view of (I) showing atomic labelling and displacement ellipsoids at the 50% probability level.

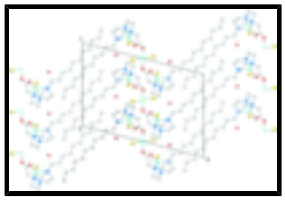

Fig. 2. Cell contents as viewed down the *b* axis. H atoms have been omitted for clarity.

Tetrachlorido-1κ*Cl*,2κ^2*Cl*,3κ*Cl*- bis[μ-4-undecyl-1,4,7-triazacyclonon-1-yl)acetato]-1κ^4*N*,*N*',*N*'',*O*:2κ*O*';2κ*O*':3κ^4*N*,*N*',*N*'',*O*-tricopper(II) dihydrate

Crystal data

$[Cu_3Cl_4(C_{17}H_{38}N_3O_2)_2]\cdot 2H_2O$	F_{000} = 1106
M_r = 1049.50	D_x = 1.422 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 25491 reflections
a = 22.1182 (11) Å	θ = 2.8–27.5º
b = 7.8330 (4) Å	μ = 1.56 mm^{-1}
c = 14.6177 (7) Å	T = 123 (2) K
β = 104.570 (2)º	Plate, blue-green
V = 2451.1 (2) Å^3	0.20 × 0.10 × 0.05 mm
Z = 2	

Data collection

Bruker X8 APEX CCD diffractometer	5625 independent reflections
Radiation source: fine-focus sealed tube	4994 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.071
T = 123(2) K	θ_{max} = 27.5º
φ scans	θ_{min} = 2.8º
Absorption correction: multi-scan (SADABS; Bruker, 2005)	h = −28→28
T_{min} = 0.746, T_{max} = 0.926	k = −10→10
25491 measured reflections	l = −18→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.084$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.142$	$w = 1/[\sigma^2(F_o^2) + 12.2399P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.32$	$(\Delta/\sigma)_{max} = 0.001$
5625 reflections	$\Delta\rho_{max} = 0.62$ e Å^{-3}
271 parameters	$\Delta\rho_{min} = -1.02$ e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.61289 (3)	0.74292 (8)	−0.20823 (4)	0.01211 (15)
Cu2	0.5000	0.5000	0.0000	0.0165 (2)
Cl1	0.61753 (6)	1.00100 (16)	−0.13697 (9)	0.0193 (3)
Cl2	0.41046 (7)	0.64527 (17)	−0.05565 (10)	0.0252 (3)
O1	0.56465 (17)	0.6326 (5)	−0.1290 (2)	0.0154 (8)
O2	0.49883 (18)	0.4205 (5)	−0.1271 (3)	0.0189 (8)
O3	0.7218 (3)	1.1587 (10)	0.0423 (4)	0.0563 (16)
N1	0.5975 (2)	0.5189 (5)	−0.2818 (3)	0.0145 (9)
N2	0.7136 (2)	0.6474 (6)	−0.1574 (3)	0.0147 (9)
N3	0.6437 (2)	0.8278 (6)	−0.3163 (3)	0.0167 (9)
C1	0.6565 (2)	0.4132 (6)	−0.2570 (4)	0.0150 (10)
H1A	0.6788	0.4268	−0.3073	0.018*
H1B	0.6451	0.2913	−0.2549	0.018*
C2	0.6998 (3)	0.4626 (6)	−0.1629 (4)	0.0176 (11)
H2A	0.6804	0.4307	−0.1113	0.021*
H2B	0.7394	0.3982	−0.1537	0.021*
C3	0.7453 (3)	0.7104 (7)	−0.2280 (4)	0.0191 (11)
H3A	0.7463	0.6189	−0.2744	0.023*
H3B	0.7889	0.7416	−0.1964	0.023*
C4	0.7115 (3)	0.8647 (7)	−0.2790 (4)	0.0212 (12)
H4A	0.7169	0.9627	−0.2349	0.025*
H4B	0.7298	0.8961	−0.3319	0.025*

C5	0.6297 (3)	0.7046 (7)	−0.3966 (4)	0.0182 (11)
H5A	0.6685	0.6444	−0.4000	0.022*
H5B	0.6137	0.7668	−0.4568	0.022*
C6	0.5813 (3)	0.5755 (7)	−0.3828 (3)	0.0166 (11)
H6A	0.5392	0.6282	−0.3992	0.020*
H6B	0.5807	0.4759	−0.4247	0.020*
C7	0.5455 (2)	0.4318 (7)	−0.2560 (4)	0.0167 (11)
H7A	0.5541	0.3077	−0.2505	0.020*
H7B	0.5068	0.4494	−0.3066	0.020*
C8	0.5361 (2)	0.4972 (7)	−0.1645 (4)	0.0164 (11)
C9	0.7438 (2)	0.7052 (7)	−0.0614 (4)	0.0195 (12)
H9A	0.7154	0.6792	−0.0205	0.023*
H9B	0.7481	0.8309	−0.0628	0.023*
C10	0.8079 (3)	0.6299 (8)	−0.0148 (4)	0.0269 (14)
H10A	0.8035	0.5073	−0.0014	0.032*
H10B	0.8354	0.6397	−0.0585	0.032*
C11	0.8375 (2)	0.7237 (8)	0.0771 (4)	0.0214 (12)
H11A	0.8443	0.8442	0.0618	0.026*
H11B	0.8075	0.7230	0.1172	0.026*
C12	0.8988 (3)	0.6509 (8)	0.1337 (4)	0.0258 (13)
H12A	0.9311	0.6706	0.0987	0.031*
H12B	0.8942	0.5260	0.1398	0.031*
C13	0.9208 (3)	0.7283 (8)	0.2317 (4)	0.0274 (14)
H13A	0.9258	0.8529	0.2251	0.033*
H13B	0.8879	0.7107	0.2658	0.033*
C14	0.9817 (3)	0.6562 (8)	0.2914 (4)	0.0265 (13)
H14A	1.0155	0.6814	0.2600	0.032*
H14B	0.9779	0.5306	0.2947	0.032*
C15	0.9999 (3)	0.7275 (9)	0.3913 (4)	0.0276 (14)
H15A	1.0033	0.8532	0.3877	0.033*
H15B	0.9661	0.7018	0.4225	0.033*
C16	1.0606 (3)	0.6581 (9)	0.4518 (4)	0.0278 (14)
H16A	1.0946	0.6851	0.4211	0.033*
H16B	1.0575	0.5323	0.4549	0.033*
C17	1.0781 (3)	0.7283 (8)	0.5517 (4)	0.0289 (14)
H17A	1.0442	0.7010	0.5825	0.035*
H17B	1.0810	0.8542	0.5486	0.035*
C18	1.1396 (3)	0.6591 (9)	0.6132 (4)	0.0301 (15)
H18A	1.1369	0.5333	0.6172	0.036*
H18B	1.1738	0.6866	0.5831	0.036*
C19	1.1551 (3)	0.7339 (11)	0.7131 (5)	0.0417 (18)
H19A	1.1947	0.6861	0.7499	0.063*
H19B	1.1217	0.7051	0.7436	0.063*
H19C	1.1588	0.8582	0.7096	0.063*
H3	0.622 (3)	0.919 (6)	−0.343 (5)	0.05 (2)*
H31	0.695 (5)	1.105 (16)	−0.006 (6)	0.16 (6)*
H32	0.714 (8)	1.266 (8)	0.059 (11)	0.22 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0141 (3)	0.0100 (3)	0.0124 (3)	−0.0002 (2)	0.0038 (2)	−0.0010 (2)
Cu2	0.0238 (5)	0.0127 (4)	0.0126 (4)	−0.0055 (4)	0.0041 (4)	0.0013 (3)
Cl1	0.0247 (7)	0.0129 (6)	0.0199 (6)	−0.0012 (5)	0.0051 (5)	−0.0045 (5)
Cl2	0.0362 (8)	0.0131 (6)	0.0223 (7)	0.0035 (6)	0.0000 (6)	−0.0011 (5)
O1	0.021 (2)	0.0137 (18)	0.0123 (18)	−0.0014 (15)	0.0064 (15)	−0.0017 (14)
O2	0.021 (2)	0.023 (2)	0.0146 (19)	−0.0062 (16)	0.0069 (16)	−0.0001 (15)
O3	0.051 (4)	0.075 (5)	0.042 (3)	−0.008 (3)	0.008 (3)	−0.007 (3)
N1	0.016 (2)	0.012 (2)	0.014 (2)	0.0021 (17)	0.0015 (17)	−0.0001 (17)
N2	0.013 (2)	0.017 (2)	0.015 (2)	−0.0003 (17)	0.0032 (17)	0.0002 (18)
N3	0.020 (2)	0.017 (2)	0.013 (2)	0.0017 (19)	0.0038 (18)	−0.0005 (18)
C1	0.021 (3)	0.006 (2)	0.017 (3)	0.001 (2)	0.003 (2)	0.0011 (19)
C2	0.020 (3)	0.011 (2)	0.020 (3)	0.005 (2)	0.003 (2)	0.005 (2)
C3	0.017 (3)	0.022 (3)	0.021 (3)	−0.001 (2)	0.009 (2)	0.001 (2)
C4	0.021 (3)	0.018 (3)	0.027 (3)	−0.005 (2)	0.010 (2)	0.001 (2)
C5	0.027 (3)	0.014 (3)	0.016 (3)	0.001 (2)	0.010 (2)	0.001 (2)
C6	0.023 (3)	0.016 (3)	0.009 (2)	0.002 (2)	0.000 (2)	−0.001 (2)
C7	0.018 (3)	0.015 (3)	0.019 (3)	−0.002 (2)	0.007 (2)	−0.008 (2)
C8	0.018 (3)	0.018 (3)	0.014 (3)	0.001 (2)	0.005 (2)	−0.001 (2)
C9	0.015 (3)	0.025 (3)	0.016 (3)	0.000 (2)	0.000 (2)	0.001 (2)
C10	0.021 (3)	0.034 (3)	0.023 (3)	0.007 (3)	−0.001 (2)	−0.008 (3)
C11	0.018 (3)	0.028 (3)	0.017 (3)	0.000 (2)	0.001 (2)	−0.002 (2)
C12	0.019 (3)	0.030 (3)	0.026 (3)	0.000 (3)	0.001 (2)	0.002 (3)
C13	0.022 (3)	0.034 (3)	0.022 (3)	−0.004 (3)	−0.002 (2)	0.006 (3)
C14	0.021 (3)	0.030 (3)	0.025 (3)	−0.002 (3)	0.001 (2)	0.004 (3)
C15	0.018 (3)	0.035 (4)	0.026 (3)	−0.002 (3)	−0.001 (2)	0.001 (3)
C16	0.019 (3)	0.035 (4)	0.026 (3)	−0.001 (3)	0.000 (2)	0.002 (3)
C17	0.025 (3)	0.034 (4)	0.024 (3)	−0.005 (3)	0.000 (2)	0.009 (3)
C18	0.021 (3)	0.034 (4)	0.030 (3)	−0.001 (3)	−0.002 (3)	0.007 (3)
C19	0.026 (3)	0.063 (5)	0.032 (4)	−0.004 (4)	0.000 (3)	−0.002 (4)

Geometric parameters (Å, °)

Cu1—O1	1.962 (4)	C7—C8	1.495 (7)
Cu1—N3	1.986 (5)	C7—H7A	0.9900
Cu1—N1	2.041 (4)	C7—H7B	0.9900
Cu1—Cl1	2.2645 (14)	C9—C10	1.529 (7)
Cu1—N2	2.289 (4)	C9—H9A	0.9900
Cu2—O2	1.954 (4)	C9—H9B	0.9900
Cu2—O2^{i}	1.954 (4)	C10—C11	1.526 (7)
Cu2—Cl2	2.2512 (14)	C10—H10A	0.9900
Cu2—Cl2^{i}	2.2512 (15)	C10—H10B	0.9900
O1—C8	1.276 (6)	C11—C12	1.512 (7)
O2—C8	1.251 (6)	C11—H11A	0.9900
O3—H31	0.90 (2)	C11—H11B	0.9900

O3—H32	0.90 (2)	C12—C13	1.519 (8)
N1—C7	1.466 (7)	C12—H12A	0.9900
N1—C6	1.496 (6)	C12—H12B	0.9900
N1—C1	1.510 (6)	C13—C14	1.518 (8)
N2—C9	1.466 (6)	C13—H13A	0.9900
N2—C3	1.470 (7)	C13—H13B	0.9900
N2—C2	1.477 (6)	C14—C15	1.520 (8)
N3—C4	1.490 (7)	C14—H14A	0.9900
N3—C5	1.491 (7)	C14—H14B	0.9900
N3—H3	0.89 (2)	C15—C16	1.511 (8)
C1—C2	1.516 (7)	C15—H15A	0.9900
C1—H1A	0.9900	C15—H15B	0.9900
C1—H1B	0.9900	C16—C17	1.516 (8)
C2—H2A	0.9900	C16—H16A	0.9900
C2—H2B	0.9900	C16—H16B	0.9900
C3—C4	1.515 (8)	C17—C18	1.529 (8)
C3—H3A	0.9900	C17—H17A	0.9900
C3—H3B	0.9900	C17—H17B	0.9900
C4—H4A	0.9900	C18—C19	1.529 (9)
C4—H4B	0.9900	C18—H18A	0.9900
C5—C6	1.523 (7)	C18—H18B	0.9900
C5—H5A	0.9900	C19—H19A	0.9800
C5—H5B	0.9900	C19—H19B	0.9800
C6—H6A	0.9900	C19—H19C	0.9800
C6—H6B	0.9900		
O1—Cu1—N3	164.51 (17)	N1—C7—H7A	109.3
O1—Cu1—N1	83.65 (16)	C8—C7—H7A	109.3
N3—Cu1—N1	85.07 (18)	N1—C7—H7B	109.3
O1—Cu1—Cl1	95.16 (11)	C8—C7—H7B	109.3
N3—Cu1—Cl1	94.70 (14)	H7A—C7—H7B	108.0
N1—Cu1—Cl1	172.72 (13)	O2—C8—O1	122.3 (5)
O1—Cu1—N2	107.10 (15)	O2—C8—C7	118.8 (5)
N3—Cu1—N2	82.35 (17)	O1—C8—C7	118.9 (5)
N1—Cu1—N2	84.80 (16)	N2—C9—C10	117.1 (5)
Cl1—Cu1—N2	102.39 (12)	N2—C9—H9A	108.0
O2—Cu2—O2^{i}	180	C10—C9—H9A	108.0
O2—Cu2—Cl2	91.00 (12)	N2—C9—H9B	108.0
O2^{i}—Cu2—Cl2	89.00 (12)	C10—C9—H9B	108.0
O2—Cu2—Cl2^{i}	89.00 (12)	H9A—C9—H9B	107.3
O2^{i}—Cu2—Cl2^{i}	91.00 (12)	C11—C10—C9	110.5 (5)
Cl2—Cu2—Cl2^{i}	180	C11—C10—H10A	109.5
C8—O1—Cu1	114.3 (3)	C9—C10—H10A	109.5
C8—O2—Cu2	114.2 (3)	C11—C10—H10B	109.5
H31—O3—H32	120 (10)	C9—C10—H10B	109.5
C7—N1—C6	112.5 (4)	H10A—C10—H10B	108.1
C7—N1—C1	111.7 (4)	C12—C11—C10	115.3 (5)
C6—N1—C1	112.2 (4)	C12—C11—H11A	108.5
C7—N1—Cu1	107.6 (3)	C10—C11—H11A	108.5

C6—N1—Cu1	103.4 (3)	C12—C11—H11B	108.5
C1—N1—Cu1	109.0 (3)	C10—C11—H11B	108.5
C9—N2—C3	112.7 (4)	H11A—C11—H11B	107.5
C9—N2—C2	113.1 (4)	C11—C12—C13	113.4 (5)
C3—N2—C2	114.7 (4)	C11—C12—H12A	108.9
C9—N2—Cu1	112.4 (3)	C13—C12—H12A	108.9
C3—N2—Cu1	105.0 (3)	C11—C12—H12B	108.9
C2—N2—Cu1	97.6 (3)	C13—C12—H12B	108.9
C4—N3—C5	113.8 (4)	H12A—C12—H12B	107.7
C4—N3—Cu1	106.8 (3)	C14—C13—C12	114.9 (5)
C5—N3—Cu1	111.4 (3)	C14—C13—H13A	108.5
C4—N3—H3	113 (5)	C12—C13—H13A	108.5
C5—N3—H3	101 (5)	C14—C13—H13B	108.5
Cu1—N3—H3	111 (5)	C12—C13—H13B	108.5
N1—C1—C2	112.9 (4)	H13A—C13—H13B	107.5
N1—C1—H1A	109.0	C13—C14—C15	113.4 (5)
C2—C1—H1A	109.0	C13—C14—H14A	108.9
N1—C1—H1B	109.0	C15—C14—H14A	108.9
C2—C1—H1B	109.0	C13—C14—H14B	108.9
H1A—C1—H1B	107.8	C15—C14—H14B	108.9
N2—C2—C1	112.0 (4)	H14A—C14—H14B	107.7
N2—C2—H2A	109.2	C16—C15—C14	114.3 (5)
C1—C2—H2A	109.2	C16—C15—H15A	108.7
N2—C2—H2B	109.2	C14—C15—H15A	108.7
C1—C2—H2B	109.2	C16—C15—H15B	108.7
H2A—C2—H2B	107.9	C14—C15—H15B	108.7
N2—C3—C4	110.5 (4)	H15A—C15—H15B	107.6
N2—C3—H3A	109.6	C15—C16—C17	114.0 (5)
C4—C3—H3A	109.6	C15—C16—H16A	108.8
N2—C3—H3B	109.6	C17—C16—H16A	108.8
C4—C3—H3B	109.6	C15—C16—H16B	108.8
H3A—C3—H3B	108.1	C17—C16—H16B	108.8
N3—C4—C3	110.6 (4)	H16A—C16—H16B	107.6
N3—C4—H4A	109.5	C16—C17—C18	114.2 (6)
C3—C4—H4A	109.5	C16—C17—H17A	108.7
N3—C4—H4B	109.5	C18—C17—H17A	108.7
C3—C4—H4B	109.5	C16—C17—H17B	108.7
H4A—C4—H4B	108.1	C18—C17—H17B	108.7
N3—C5—C6	109.8 (4)	H17A—C17—H17B	107.6
N3—C5—H5A	109.7	C19—C18—C17	112.2 (6)
C6—C5—H5A	109.7	C19—C18—H18A	109.2
N3—C5—H5B	109.7	C17—C18—H18A	109.2
C6—C5—H5B	109.7	C19—C18—H18B	109.2
H5A—C5—H5B	108.2	C17—C18—H18B	109.2
N1—C6—C5	109.0 (4)	H18A—C18—H18B	107.9
N1—C6—H6A	109.9	C18—C19—H19A	109.5
C5—C6—H6A	109.9	C18—C19—H19B	109.5
N1—C6—H6B	109.9	H19A—C19—H19B	109.5
C5—C6—H6B	109.9	C18—C19—H19C	109.5

H6A—C6—H6B	108.3	H19A—C19—H19C	109.5
N1—C7—C8	111.4 (4)	H19B—C19—H19C	109.5

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H31···Cl1	0.90 (2)	2.37 (3)	3.267 (7)	172 (12)
N3—H3···Cl2^{ii}	0.89 (2)	2.31 (3)	3.161 (5)	160 (7)

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

Fig. 1

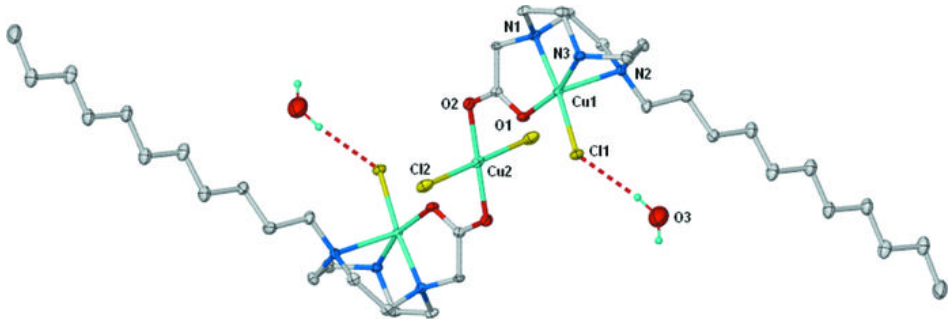

Fig. 2