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(4,4,12,12-Tetramethyl-5,8,11-triazapenta-2,14-dione 2-oxime 14-oximato-κ^5N)copper(II) perchlorate: a copper(II) compound with a pentadentate triamine–oxime–oximate ligand

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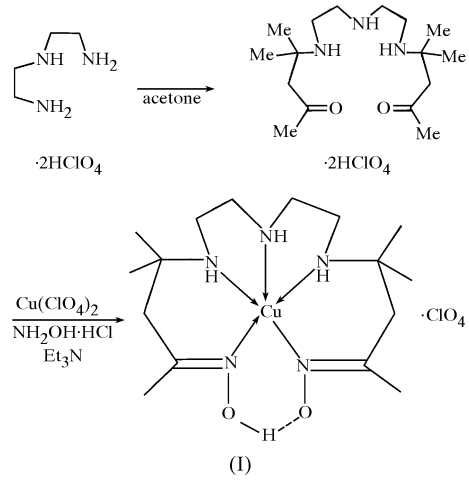
The title compound, $[Cu(C_{16}H_{34}N_5O_2)]ClO_4$, has discrete square-pyramidal (triamine–oxime–oximato)copper(II) cations and perchlorate anions. The cations have very approximate mirror symmetry, with the oxime [Cu—N = 2.066 (2) Å], oximate [Cu—N = 2.087 (2) Å] and amine N atoms [Cu—N = 2.138 (2) and 2.095 (2) Å] in the tetrahedrally twisted basal plane, and the 'central' amine N atom coordinated axially [Cu—N = 2.183 (2) Å]. The oxime and oximate groups are linked by an O—H···O hydrogen bond, forming a pseudo-cyclic pentadentate ligand, with an O···O distance of 2.395 (3) Å.

Comment

The structure of the title copper(II) compound, (I), with a pentadentate triamino–oxime–oximate ligand, is reported. The ligand is the mono-deprotonated dioxime of the triamine–diketone 4,4,12,12-tetramethyl-5,8,11-triazapenta-2,14-dione, which is formed (as the dihydroperchlorate salt) by reaction of 3-azapentane-1,5-diamine dihydroperchlorate with acetone (see scheme) (Morgan *et al.*, 1982).

Compound (I) has discrete cations, with Cu^{II} in a square-pyramidal coordination (Fig. 1), and perchlorate anions. Oxime atom N2, oximate atom N14, and secondary amine atoms N5 and N11, are coordinated in the tetrahedrally twisted basal plane, with the bond to the axially coordinated secondary amine atom N8 being significantly longer. Displacements from the mean-square plane defined by atoms N2, N5, N11 and N14 are: N2 0.154, N5 −0.158, N11 0.158, N14 −0.154, Cu 0.100, N8 2.213, O2 0.793 and O14 0.082 Å (s.u. 0.003 Å), and the *trans* angles are N2—Cu—N11 = 175.75 (8)° and N14—Cu—N5 = 165.87 (8)°. The five-membered chelate rings both have asymmetrical *gauche* conformations [displacements of atoms from the Cu/N5/N8 plane: C6 0.145 and C7 0.697 Å; from the Cu/N8/N11 plane: C9 0.035 and C10 0.683 Å], while the six-membered chelate rings have 'half-chair' conformations, with methyl substituents C41 and C121 axially oriented [displacements from the Cu/N2/N5 plane: C2 0.052, C3 0.445, C4 0.948, C41 −2.323 and C42 1.050 Å; from the Cu/N11/N14 plane: C12 0.984, C121 2.355, C122 1.039, C13 0.590 and C14 0.263 Å].



(I)

Atom O2 of the oxime and O14 of the oximate group are linked by a short hydrogen bond (Table 2), as is common for oxime–oximate compounds, forming a pseudo-macrocyclic ligand. The cations are linked into a one-dimensional chain, with base vector 001, by weak intramolecular hydrogen bonding. The perchlorate ion shows rotational disorder which was not modelled.

The structures of a number of copper(II) compounds with tetradentate diaza–oxime–oximate ligands with short O—H···O hydrogen-bonded 14- to 16-membered pseudo-cyclic structures have been reported. These generally have square-pyramidal coordination, with water (Nunes *et al.*, 1999; Anderson & Packard, 1979; Lee *et al.*, 1990; Pal *et al.*, 1986; Kiani *et al.*, 2002) or an anion (Tahirov *et al.*, 1993, 1995; Jiang *et al.*, 1993; Nunes *et al.*, 1999; Gavel & Schlemper, 1979; Lee *et al.*, 1991; Liss *et al.*, 1975; Schlemper *et al.*, 1981) coordinated axially, or have dinuclear (Tahirov *et al.*, 1993; Fraser *et al.*,

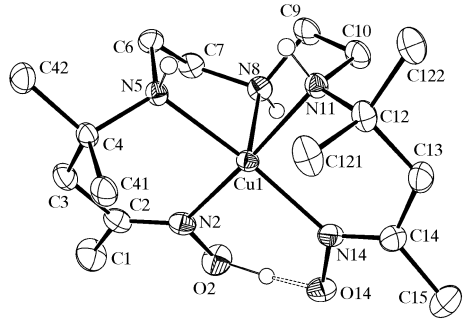


Figure 1
The cation of (I), drawn with displacement ellipsoids at the 50% probability level. H atoms bonded to C atoms have been omitted for clarity, and H atoms bonded to N or O atoms are shown as circles of arbitrary radii.

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1972; Timmons *et al.*, 1981; Kiani *et al.*, 2002; Pal *et al.*, 1986; Fun *et al.*, 1993) or chain polymeric structures (Bertrand *et al.*, 1977) with an oximate O atom bridging to the axial site. The work presented here is the first report of a triaza–oxime–oximate compound in which the pentadentate ligand donor atoms occupy all five coordination sites about the copper(II).

Experimental

The starting material, 4,4,12,12-tetramethyl-5,8,11-triazapenta-2,14-dione dihydroperchlorate, was prepared by reaction of 3-azapentane-1,5-diamine (diethylenetriamine) dihydroperchlorate with acetone (Morgan *et al.*, 1982). The title compound was prepared by reaction of the starting material with $[Cu(H_2O)_6](ClO_4)_2$, hydroxylamine hydrochloride and triethylamine in a 1:1:2:5 molar ratio in methanol. The green product which crystallized on addition of propan-2-ol was recrystallized by dissolving in methanol, adding propan-2-ol until just turbid, and allowing the solvent to evaporate.

Crystal data

$[Cu(C_{16}H_{34}N_5O_2)]ClO_4$
M_r = 491.47
Monoclinic, $P2_1/c$
a = 10.8307 (7) Å
b = 23.9974 (15) Å
c = 8.6318 (6) Å
β = 90.058 (2)°
V = 2243.5 (3) Å^3
Z = 4
D_x = 1.455 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9707 reflections
θ = 2.1–28.4°
μ = 1.13 mm^{-1}
T = 160 (2) K
Plate, green
0.62 × 0.28 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω rotation scans with narrow frame
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.540, T_{max} = 0.895
12 927 measured reflections
4845 independent reflections
4392 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 28.4°
$h = -10 \rightarrow 14$
$k = -26 \rightarrow 30$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.100
S = 1.12
4845 reflections
271 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2 + 3.1169P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	2.067 (2)	N2—C2	1.285 (3)
Cu1—N14	2.088 (2)	N2—O2	1.420 (3)
Cu1—N11	2.096 (2)	C14—N14	1.292 (3)
Cu1—N5	2.138 (2)	N14—O14	1.426 (3)
Cu1—N8	2.182 (2)		
N2—Cu1—N14	93.32 (9)	O2—N2—Cu1	113.9 (2)
N2—Cu1—N11	175.79 (8)	N2—C2—C3	122.7 (2)
N14—Cu1—N11	89.90 (8)	C1—C2—C3	118.1 (2)
N2—Cu1—N5	89.33 (8)	C2—C3—C4	121.8 (2)
N14—Cu1—N5	165.85 (8)	C14—C13—C12	122.3 (2)
N11—Cu1—N5	88.20 (8)	N14—C14—C15	118.9 (3)
N2—Cu1—N8	93.82 (8)	N14—C14—C13	122.8 (2)
N14—Cu1—N8	110.13 (8)	C15—C14—C13	118.2 (2)
N11—Cu1—N8	82.52 (8)	C14—N14—O14	113.6 (2)
N5—Cu1—N8	83.53 (7)	C14—N14—Cu1	129.3 (2)
C2—N2—O2	113.4 (2)	O14—N14—Cu1	117.1 (2)
C2—N2—Cu1	130.4 (2)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O14	1.14 (4)	1.27 (4)	2.395 (3)	171 (4)
O2—H2···N14	1.14 (4)	2.16 (4)	3.044 (3)	132 (3)
N5—H5···O5	0.93	2.34	3.257 (4)	167
N8—H8···O14^{i}	0.93	2.12	3.009 (3)	160
N11—H11···O4	0.93	2.58	3.437 (4)	154

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

For atom H2, the positional coordinates were refined, with U_{iso} = 1.5U_{eq}(O2). All other H atoms were treated as riding atoms, with N—H distances of 0.93 Å and C—H distances of 0.98 or 0.99 Å, and with U_{iso}(H) = 1.2U_{eq}(N) or 1.5U_{eq}(C).

Data collection: *SMART* (Siemens, 1995); cell refinement: local programs; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GD1308). Services for accessing these data are described at the back of the journal.

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supporting information

Acta Cryst. (2004). C**60**, m256–m257 [doi:10.1107/S0108270104008765]

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Data collection: *SMART* (Siemens, 1995); cell refinement: local programs; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Cell parameters from 9707 reflections
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4845 independent reflections
4392 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 28.4°, θ_{min} = 1.7°
h = −10→14
k = −26→30
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.100
S = 1.12
4845 reflections
271 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2 + 3.1169P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.64$ e Å^{-3}
$\Delta\rho_{min} = -0.70$ e Å^{-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.

Refinement. Refinement on F^2 for ALL reflections except for 16 with very negative F^2 or flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factor(obs.) 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.
H(2) located from difference syntheses and the position refined, other H atoms are riding in calculated positions.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.26542 (2)	0.346322 (12)	0.81688 (3)	0.01749 (9)
N2	0.4077 (2)	0.28900 (9)	0.8262 (2)	0.0238 (4)
O2	0.37197 (19)	0.23610 (8)	0.8847 (2)	0.0346 (4)
H2	0.275 (3)	0.2292 (15)	0.838 (4)	0.052*
C1	0.6098 (3)	0.24921 (13)	0.8809 (4)	0.0403 (7)
H1A	0.6958	0.2620	0.8798	0.060*
H1B	0.6011	0.2168	0.8128	0.060*
H1C	0.5866	0.2388	0.9868	0.060*
C2	0.5252 (2)	0.29625 (11)	0.8237 (3)	0.0260 (5)
C3	0.5853 (2)	0.35189 (11)	0.7758 (3)	0.0264 (5)
H3A	0.6483	0.3430	0.6965	0.032*
H3B	0.6304	0.3660	0.8676	0.032*
C4	0.5073 (2)	0.40154 (10)	0.7113 (3)	0.0199 (5)
C41	0.4550 (2)	0.38715 (11)	0.5513 (3)	0.0255 (5)
H4A	0.5231	0.3821	0.4779	0.038*
H4B	0.4016	0.4175	0.5156	0.038*
H4C	0.4069	0.3526	0.5579	0.038*
C42	0.5873 (2)	0.45630 (11)	0.6981 (3)	0.0281 (5)
H4D	0.6510	0.4512	0.6188	0.042*
H4E	0.6266	0.4641	0.7980	0.042*
H4F	0.5339	0.4876	0.6692	0.042*
N5	0.39863 (17)	0.41209 (8)	0.8164 (2)	0.0183 (4)
H5	0.3582	0.4428	0.7749	0.022*
C6	0.4288 (2)	0.42768 (11)	0.9806 (3)	0.0237 (5)
H6A	0.3852	0.4626	1.0074	0.028*
H6B	0.5186	0.4347	0.9895	0.028*
C7	0.3911 (2)	0.38126 (11)	1.0982 (3)	0.0250 (5)
H7A	0.4504	0.3500	1.0914	0.030*
H7B	0.3947	0.3964	1.2048	0.030*

N8	0.26537 (19)	0.36052 (9)	1.0665 (2)	0.0226 (4)
H8	0.2503	0.3276	1.1199	0.027*
C9	0.1673 (2)	0.40327 (12)	1.1010 (3)	0.0285 (6)
H9A	0.2049	0.4408	1.1050	0.034*
H9B	0.1298	0.3954	1.2032	0.034*
C10	0.0682 (2)	0.40182 (12)	0.9764 (3)	0.0269 (5)
H10A	0.0221	0.3663	0.9823	0.032*
H10B	0.0091	0.4327	0.9926	0.032*
N11	0.12680 (17)	0.40724 (9)	0.8219 (2)	0.0196 (4)
H11	0.1661	0.4417	0.8198	0.024*
C12	0.0397 (2)	0.40594 (11)	0.6866 (3)	0.0241 (5)
C121	0.1177 (2)	0.40810 (13)	0.5394 (3)	0.0325 (6)
H12A	0.0634	0.4110	0.4489	0.049*
H12B	0.1674	0.3741	0.5316	0.049*
H12C	0.1724	0.4406	0.5433	0.049*
C122	−0.0472 (2)	0.45843 (12)	0.6906 (3)	0.0320 (6)
H12D	−0.0980	0.4593	0.5966	0.048*
H1DE	0.0031	0.4923	0.6959	0.048*
H1DF	−0.1008	0.4564	0.7818	0.048*
C13	−0.0378 (2)	0.35071 (12)	0.6889 (3)	0.0297 (6)
H13A	−0.0991	0.3546	0.7732	0.036*
H14B	−0.0850	0.3496	0.5907	0.036*
C14	0.0225 (2)	0.29281 (12)	0.7086 (3)	0.0301 (6)
C15	−0.0560 (3)	0.24084 (15)	0.6724 (5)	0.0522 (9)
H15A	−0.0257	0.2233	0.5772	0.078*
H15B	−0.1424	0.2519	0.6585	0.078*
H15C	−0.0497	0.2144	0.7585	0.078*
N14	0.13391 (19)	0.28621 (9)	0.7588 (2)	0.0244 (4)
O14	0.16859 (18)	0.22928 (8)	0.7772 (2)	0.0332 (4)
Cl1	0.24086 (5)	0.57184 (3)	0.78760 (7)	0.02500 (14)
O3	0.1308 (2)	0.59374 (10)	0.7192 (3)	0.0506 (6)
O4	0.2130 (2)	0.53993 (12)	0.9258 (3)	0.0582 (7)
O5	0.2965 (4)	0.53074 (15)	0.6855 (4)	0.0956 (13)
O6	0.3219 (3)	0.61731 (13)	0.8189 (5)	0.0952 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01918 (15)	0.01854 (16)	0.01474 (14)	0.00032 (11)	0.00124 (10)	−0.00069 (10)
N2	0.0294 (10)	0.0197 (10)	0.0224 (10)	0.0034 (8)	0.0008 (8)	0.0003 (8)
O2	0.0387 (11)	0.0239 (10)	0.0413 (11)	0.0000 (8)	−0.0028 (9)	0.0111 (8)
C1	0.0339 (15)	0.0363 (16)	0.0507 (18)	0.0111 (13)	−0.0039 (13)	0.0069 (14)
C2	0.0280 (12)	0.0275 (13)	0.0227 (11)	0.0079 (10)	−0.0008 (9)	−0.0017 (10)
C3	0.0198 (11)	0.0309 (14)	0.0285 (12)	0.0048 (10)	0.0010 (9)	−0.0023 (10)
C4	0.0177 (10)	0.0247 (12)	0.0172 (10)	−0.0002 (9)	0.0030 (8)	−0.0013 (9)
C41	0.0255 (12)	0.0344 (14)	0.0168 (11)	−0.0013 (10)	0.0047 (9)	−0.0005 (10)
C42	0.0254 (12)	0.0334 (14)	0.0254 (12)	−0.0056 (11)	0.0053 (10)	−0.0007 (11)
N5	0.0182 (9)	0.0228 (10)	0.0139 (8)	0.0003 (7)	0.0013 (7)	0.0003 (7)

C6	0.0267 (12)	0.0264 (13)	0.0181 (11)	−0.0037 (10)	0.0013 (9)	−0.0049 (9)
C7	0.0291 (12)	0.0311 (14)	0.0147 (10)	0.0003 (10)	−0.0017 (9)	−0.0013 (9)
N8	0.0270 (10)	0.0259 (11)	0.0150 (9)	−0.0018 (8)	0.0024 (8)	0.0021 (8)
C9	0.0293 (13)	0.0379 (15)	0.0182 (11)	0.0019 (11)	0.0072 (10)	−0.0051 (10)
C10	0.0249 (12)	0.0347 (15)	0.0213 (11)	0.0008 (10)	0.0084 (9)	−0.0021 (10)
N11	0.0184 (9)	0.0232 (10)	0.0172 (9)	0.0001 (8)	0.0015 (7)	−0.0003 (8)
C12	0.0194 (11)	0.0321 (14)	0.0210 (11)	0.0020 (10)	0.0001 (9)	0.0021 (10)
C121	0.0255 (12)	0.0510 (18)	0.0209 (12)	0.0069 (12)	0.0005 (10)	0.0068 (11)
C122	0.0236 (12)	0.0378 (16)	0.0346 (14)	0.0065 (11)	−0.0008 (10)	0.0037 (12)
C13	0.0201 (11)	0.0388 (16)	0.0304 (13)	−0.0011 (11)	−0.0024 (10)	−0.0060 (11)
C14	0.0264 (12)	0.0340 (15)	0.0299 (13)	−0.0049 (11)	0.0025 (10)	−0.0097 (11)
C15	0.0358 (16)	0.0418 (19)	0.079 (3)	−0.0086 (14)	−0.0065 (16)	−0.0214 (18)
N14	0.0263 (10)	0.0222 (11)	0.0249 (10)	−0.0010 (8)	0.0031 (8)	−0.0046 (8)
O14	0.0359 (10)	0.0207 (10)	0.0430 (11)	−0.0020 (8)	0.0031 (9)	−0.0059 (8)
Cl1	0.0210 (3)	0.0289 (3)	0.0250 (3)	0.0016 (2)	−0.0004 (2)	0.0049 (2)
O3	0.0359 (12)	0.0545 (15)	0.0613 (15)	0.0046 (10)	−0.0212 (11)	0.0138 (12)
O4	0.0479 (13)	0.0808 (19)	0.0460 (13)	0.0167 (13)	0.0181 (11)	0.0349 (13)
O5	0.137 (3)	0.098 (3)	0.0518 (17)	0.078 (2)	0.0264 (18)	0.0059 (16)
O6	0.079 (2)	0.068 (2)	0.138 (3)	−0.0430 (17)	−0.067 (2)	0.045 (2)

Geometric parameters (Å, º)

Cu1—N2	2.067 (2)	N8—C9	1.507 (3)
Cu1—N14	2.088 (2)	N8—H8	0.9300
Cu1—N11	2.096 (2)	C9—C10	1.519 (4)
Cu1—N5	2.138 (2)	C9—H9A	0.9900
Cu1—N8	2.1816 (19)	C9—H9B	0.9900
N2—C2	1.285 (3)	C10—N11	1.483 (3)
N2—O2	1.420 (3)	C10—H10A	0.9900
O2—H2	1.14 (4)	C10—H10B	0.9900
C1—C2	1.535 (4)	N11—C12	1.500 (3)
C1—H1A	0.9800	N11—H11	0.9300
C1—H1B	0.9800	C12—C121	1.527 (3)
C1—H1C	0.9800	C12—C13	1.569 (4)
C2—C3	1.542 (4)	C12—C122	1.573 (4)
C3—C4	1.563 (3)	C121—H12A	0.9800
C3—H3A	0.9900	C121—H12B	0.9800
C3—H3B	0.9900	C121—H12C	0.9800
C4—N5	1.508 (3)	C122—H12D	0.9800
C4—C41	1.532 (3)	C122—H1DE	0.9800
C4—C42	1.578 (3)	C122—H1DF	0.9800
C41—H4A	0.9800	C13—C14	1.545 (4)
C41—H4B	0.9800	C13—H13A	0.9900
C41—H4C	0.9800	C13—H14B	0.9900
C42—H4D	0.9800	C14—N14	1.292 (3)
C42—H4E	0.9800	C14—C15	1.541 (4)
C42—H4F	0.9800	C15—H15A	0.9800
N5—C6	1.501 (3)	C15—H15B	0.9800

N5—H5	0.9300	C15—H15C	0.9800
C6—C7	1.561 (3)	N14—O14	1.426 (3)
C6—H6A	0.9900	O14—H2	1.27 (4)
C6—H6B	0.9900	Cl1—O6	1.426 (3)
C7—N8	1.475 (3)	Cl1—O3	1.429 (2)
C7—H7A	0.9900	Cl1—O4	1.449 (2)
C7—H7B	0.9900	Cl1—O5	1.454 (3)
N2—Cu1—N14	93.32 (9)	C7—N8—Cu1	103.58 (13)
N2—Cu1—N11	175.79 (8)	C9—N8—Cu1	107.60 (14)
N14—Cu1—N11	89.90 (8)	C7—N8—H8	110.9
N2—Cu1—N5	89.33 (8)	C9—N8—H8	110.9
N14—Cu1—N5	165.85 (8)	Cu1—N8—H8	110.9
N11—Cu1—N5	88.20 (8)	N8—C9—C10	110.0 (2)
N2—Cu1—N8	93.82 (8)	N8—C9—H9A	109.7
N14—Cu1—N8	110.13 (8)	C10—C9—H9A	109.7
N11—Cu1—N8	82.52 (8)	N8—C9—H9B	109.7
N5—Cu1—N8	83.53 (7)	C10—C9—H9B	109.7
C2—N2—O2	113.4 (2)	H9A—C9—H9B	108.2
C2—N2—Cu1	130.37 (18)	N11—C10—C9	109.4 (2)
O2—N2—Cu1	113.90 (15)	N11—C10—H10A	109.8
N2—O2—H2	104.9 (19)	C9—C10—H10A	109.8
C2—C1—H1A	109.5	N11—C10—H10B	109.8
C2—C1—H1B	109.5	C9—C10—H10B	109.8
H1A—C1—H1B	109.5	H10A—C10—H10B	108.2
C2—C1—H1C	109.5	C10—N11—C12	115.38 (18)
H1A—C1—H1C	109.5	C10—N11—Cu1	105.33 (15)
H1B—C1—H1C	109.5	C12—N11—Cu1	114.78 (15)
N2—C2—C1	119.1 (2)	C10—N11—H11	106.9
N2—C2—C3	122.7 (2)	C12—N11—H11	106.9
C1—C2—C3	118.1 (2)	Cu1—N11—H11	106.9
C2—C3—C4	121.8 (2)	N11—C12—C121	107.40 (19)
C2—C3—H3A	106.9	N11—C12—C13	110.1 (2)
C4—C3—H3A	106.9	C121—C12—C13	109.6 (2)
C2—C3—H3B	106.9	N11—C12—C122	110.0 (2)
C4—C3—H3B	106.9	C121—C12—C122	108.8 (2)
H3A—C3—H3B	106.7	C13—C12—C122	110.8 (2)
N5—C4—C41	107.01 (18)	C12—C121—H12A	109.5
N5—C4—C3	109.59 (19)	C12—C121—H12B	109.5
C41—C4—C3	110.4 (2)	H12A—C121—H12B	109.5
N5—C4—C42	109.42 (19)	C12—C121—H12C	109.5
C41—C4—C42	108.95 (19)	H12A—C121—H12C	109.5
C3—C4—C42	111.35 (19)	H12B—C121—H12C	109.5
C4—C41—H4A	109.5	C12—C122—H12D	109.5
C4—C41—H4B	109.5	C12—C122—H1DE	109.5
H4A—C41—H4B	109.5	H12D—C122—H1DE	109.5
C4—C41—H4C	109.5	C12—C122—H1DF	109.5
H4A—C41—H4C	109.5	H12D—C122—H1DF	109.5

H4B—C41—H4C	109.5	H1DE—C122—H1DF	109.5
C4—C42—H4D	109.5	C14—C13—C12	122.3 (2)
C4—C42—H4E	109.5	C14—C13—H13A	106.7
H4D—C42—H4E	109.5	C12—C13—H13A	106.7
C4—C42—H4F	109.5	C14—C13—H14B	106.7
H4D—C42—H4F	109.5	C12—C13—H14B	106.7
H4E—C42—H4F	109.5	H13A—C13—H14B	106.6
C6—N5—C4	116.16 (18)	N14—C14—C15	118.9 (3)
C6—N5—Cu1	109.17 (14)	N14—C14—C13	122.8 (2)
C4—N5—Cu1	113.83 (14)	C15—C14—C13	118.2 (2)
C6—N5—H5	105.6	C14—C15—H15A	109.5
C4—N5—H5	105.6	C14—C15—H15B	109.5
Cu1—N5—H5	105.6	H15A—C15—H15B	109.5
N5—C6—C7	112.28 (19)	C14—C15—H15C	109.5
N5—C6—H6A	109.1	H15A—C15—H15C	109.5
C7—C6—H6A	109.1	H15B—C15—H15C	109.5
N5—C6—H6B	109.1	C14—N14—O14	113.6 (2)
C7—C6—H6B	109.1	C14—N14—Cu1	129.26 (19)
H6A—C6—H6B	107.9	O14—N14—Cu1	117.11 (15)
N8—C7—C6	111.22 (19)	N14—O14—H2	106.7 (17)
N8—C7—H7A	109.4	O6—Cl1—O3	108.03 (17)
C6—C7—H7A	109.4	O6—Cl1—O4	112.1 (2)
N8—C7—H7B	109.4	O3—Cl1—O4	111.10 (15)
C6—C7—H7B	109.4	O6—Cl1—O5	112.3 (3)
H7A—C7—H7B	108.0	O3—Cl1—O5	110.19 (19)
C7—N8—C9	112.6 (2)	O4—Cl1—O5	103.13 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O14	1.14 (4)	1.27 (4)	2.395 (3)	171 (4)
O2—H2···N14	1.14 (4)	2.16 (4)	3.044 (3)	132 (3)
N5—H5···O5	0.93	2.34	3.257 (4)	167
N8—H8···O14^{i}	0.93	2.12	3.009 (3)	160
N11—H11···O4	0.93	2.58	3.437 (4)	154

Symmetry code: (i) $x, -y+1/2, z+1/2$.