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catena-Poly[[[hemiaquacopper(II)]-μ-(3,9-dimethyl-4,8-diazaundeca-3,8-diene-2,10-dione dioximato)-$\kappa^4N,N',N'',N'':\kappa O$] perchlorate]

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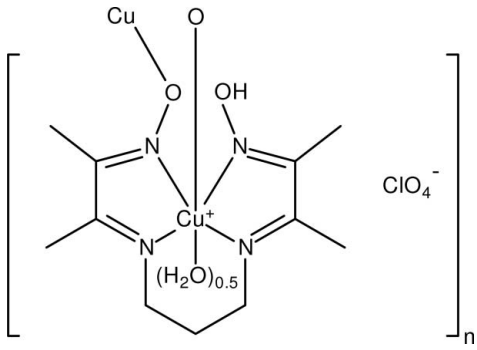
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.034; wR factor = 0.081; data-to-parameter ratio = 21.3.

The structure of the title compound, $\{[Cu(C_{11}H_{19}N_4O_2)(H_2O)_{0.5}]ClO_4\}_n$, consists of perchlorate anions and infinite chain cations. Each Cu atom has a distorted square-pyramidal or octahedral environment, with two oxime and two imine N atoms from the tetradentate ligand in a square-planar arrangement and one or two weak bonds to O atoms in *trans* positions through the coordination of the half-occupancy water molecule and an oxime O atom of the adjacent unit. The dihedral angle between the planes of coordination of the tetradentate ligand in adjacent units of the polymeric cation is 61.92 (4)°. The perchlorate anions are hydrogen bonded to the aqua ligand.

Related literature

For related literature, see: Bertrand *et al.* (1977); Wang *et al.* (1991); Wang, Chung *et al.* (1990); Wang, Wang *et al.* (1990); Tahirov *et al.* (1995); Lu *et al.* (1993); Asadi *et al.* (2005); Movahedi & Golchoubian (2006); Wisemann & Krebs (2000).



Experimental

Crystal data

$[Cu(C_{11}H_{19}N_4O_2)(H_2O)_{0.5}]ClO_4$
M_r = 411.30
Monoclinic, $P2_1/n$
a = 13.0833 (5) Å
b = 6.6401 (3) Å
c = 18.6698 (7) Å
β = 90.445 (1)°
V = 1621.88 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.55 mm^{-1}
T = 100 (2) K
0.36 × 0.35 × 0.12 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.577, T_{max} = 0.832
15994 measured reflections
4717 independent reflections
3609 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.081
S = 1.00
4717 reflections
221 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.97 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2129).

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supplementary materials

Acta Cryst. (2007). E**63**, m2324 [**doi:10.1107/S160053680703886X**]

catena-Poly[[[hemiaquacopper(II)]-μ-(3,9-dimethyl-4,8-diazaundeca-3,8-diene-2,10-dione dioximato)-$\kappa^4N,N',N'',N'':\kappa O$] perchlorate]

H. Golchoubian and O. Nazari

Comment

An investigation to assess the possible use of dioxime–diimine compounds as tetradentate ligands in the production of metal complexes with the copper(II) ion which demonstrates solvatochromism (Asadi *et al.*, 2005; Movahedi & Golchoubian, 2006) motivated us to synthesize the title compound (I). This compound was previously prepared and its structure was investigated by Bertrand *et al.* (1977), but their reported structure has the formula $[Cu(C_{11}H_{19}N_4O_2)]^+ClO_4^-\cdot 0.5CH_3OH$ with a triclinic space group and a density of 1.60 Mg m^{-3}. However, our results show the presence of a water molecule in place of methanol, with a monoclinic space group and a density of 1.684 Mg m^{-3} as well as a different color of the crystals. On the other hand, Wisemann & Krebs (2000) reported a structure for the title compound. The structure appears to be the same as ours except for the full occupancy modeling of the water molecule and the lower precision. Other complexes of this tetradentate ligand with different transition metals and their derivatives have been synthesized (Wang, Chung *et al.*, 1990; Wang, Wang *et al.*, 1990; Wang *et al.*, 1991) and their structures have been examined (Tahirov *et al.*, 1995; Lu *et al.*, 1993). The structure of the title compound contains infinite-chain cations. The dihedral angle between the CuN4 coordination planes of adjacent monomer units is 61.92 (4)°. In each unit the tetradentate ligand is coordinated to copper as shown in Fig. 1 through the two oxime and two imine nitrogen atoms. This coordination forms a six-membered and two five-membered chelate rings. Each five-membered chelate ring includes an imine nitrogen and an oxime nitrogen atoms. However, the six-membered chelate ring includes two imine nitrogen atoms. The four nitrogen atoms of the ligand are coplanar. The displacement of Cu out of this plane is 0.079 Å. The six-membered ring CuN2C5C6C7N3 is puckered with C6 positioned 0.701 Å out of the ring mean plane. This produces an overall chair-like conformation of the ligand. Cationic units are linked together by a weak bond between the copper atom of one unit and an oxygen atom of the oxime of the next unit. The coordination of each copper atom also includes a water molecule which bonds weakly to the other site of the CuN_4 plane to complete a distorted octahedron. The water site is only half-occupied, so that only half of the Cu atoms have their coordination completed by the water molecule, the other half being square pyramidal. Full occupancy would give unacceptably short contacts between water molecules of adjacent chains, so the disorder is correlated between chains, but is random within chains.

The cationic chains are offset, resulting in a zigzag pattern of copper atoms as shown in Fig. 2. The structure is consolidated by hydrogen bonds which form a three-dimensional framework.

Experimental

The complex was prepared by a procedure given by Bertrand *et al.* (1977).

Refinement

C-bound hydrogen atoms were treated in a riding model with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) [1.5U_{eq}(C) for methyl groups]. The O-bound H atoms were located in a difference map and refined as riding in their as-found relative positions, with U_{iso}(H) = 1.5U_{eq}(O). Attempts to refine the model with full occupancy for water led to U_{eq}(O1s) = 0.105 Å^2 and R1 = 0.045. Refinement of the water occupancy gave essentially half-occupancy, and this was fixed in the final refinement.

Figures

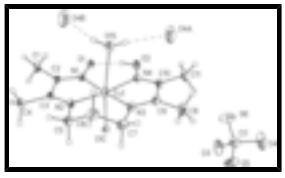

Fig. 1. The asymmetric unit of the title compound with 50% probability displacement ellipsoids. Hydrogen bonds are shown as dashed lines. Symmetry transformations used to generate equivalent atoms: A −*x* + 3/2, *y* + 1/2, −*z* + 1/2; B *x* − 1/2, −*y* + 1/2, *z* + 1/2; C −*x*, −*y* − 1, −*z*.

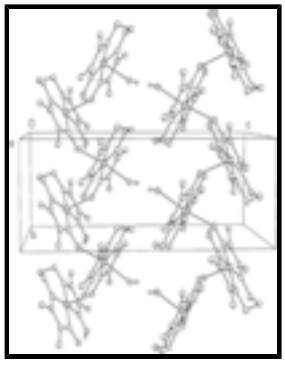

Fig. 2. The crystal packing of the cationic chains (view approximately along the *a* axis). Anions and hydrogen atoms of ligands have been omitted for clarity, and all water sites are shown occupied, illustrating the unacceptably short contacts thus generated.

catena-Poly[[[hemiaquacopper(II)]-μ-3,9-dimethyl-4,8-diazaundeca-3,8-diene- 2,10-dione dioximato-κ^4*N*,*N*',*N*'',*N*''':κ*O*)] perchlorate]

Crystal data

$[Cu(C_{11}H_{19}N_4O_2)(H_2O)_{0.5}]ClO_4$	F_{000} = 848
M_r = 411.30	D_x = 1.684 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 4849 reflections
a = 13.0833 (5) Å	θ = 3.1–34.0º
b = 6.6401 (3) Å	μ = 1.55 mm^{-1}
c = 18.6698 (7) Å	*T* = 100 (2) K
β = 90.445 (1)º	Prism, brown
V = 1621.88 (11) Å^3	0.36 × 0.35 × 0.12 mm
Z = 4	

Data collection

Bruker SMART APEXII CCD area-detector	4717 independent reflections

diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 100(2) K

ω scans

Absorption correction: multi-scan (APEX2; Bruker, 2005)

T_{min} = 0.577, T_{max} = 0.832

15994 measured reflections

3609 reflections with $I > 2\sigma(I)$

R_{int} = 0.035

θ_{max} = 30.0º

θ_{min} = 1.9º

$h = -18 \rightarrow 18$

$k = -9 \rightarrow 8$

$l = -26 \rightarrow 26$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.034

$wR(F^2)$ = 0.081

S = 1.00

4717 reflections

221 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: mixed

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.03P)^2 + 1.5P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.53 e Å^{-3}

$\Delta\rho_{min}$ = −0.97 e Å^{-3}

Extinction correction: none

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}	Occ. (<1)
Cu1	0.337030 (18)	0.28836 (4)	0.333467 (15)	0.02361 (8)	
Cl1	0.73712 (4)	0.02121 (8)	0.07806 (3)	0.02456 (11)	
O1	0.23722 (10)	0.6526 (2)	0.28151 (7)	0.0174 (3)	
O2	0.42009 (10)	0.6102 (2)	0.24366 (7)	0.0209 (3)	
H2A	0.3595	0.6461	0.2511	0.031*	
O3	0.69075 (12)	−0.0705 (3)	0.13955 (9)	0.0362 (4)	
O4	0.84578 (13)	−0.0135 (4)	0.08157 (10)	0.0483 (5)	
O5	0.69497 (15)	−0.0660 (3)	0.01428 (9)	0.0374 (4)	
O6	0.71672 (17)	0.2335 (3)	0.07880 (10)	0.0469 (5)	
N1	0.22697 (12)	0.4842 (2)	0.32114 (8)	0.0155 (3)	

N2	0.23733 (12)	0.1622 (2)	0.39627 (9)	0.0176 (3)	
N3	0.45279 (12)	0.1049 (3)	0.34784 (9)	0.0181 (3)	
N4	0.43956 (12)	0.4366 (3)	0.27955 (8)	0.0156 (3)	
C1	0.05749 (14)	0.5895 (3)	0.36414 (11)	0.0205 (4)	
H1A	0.0744	0.7179	0.3412	0.031*	
H1B	0.0415	0.6128	0.4147	0.031*	
H1C	−0.0019	0.5296	0.3399	0.031*	
C2	0.14635 (13)	0.4499 (3)	0.35890 (10)	0.0151 (4)	
C3	0.15169 (14)	0.2563 (3)	0.39869 (10)	0.0158 (4)	
C4	0.05944 (15)	0.1835 (3)	0.43799 (11)	0.0233 (4)	
H4B	0.0541	0.0369	0.4332	0.035*	
H4C	−0.0019	0.2468	0.4177	0.035*	
H4D	0.0658	0.2191	0.4888	0.035*	
C5	0.25740 (16)	−0.0270 (3)	0.43378 (11)	0.0221 (4)	
H5B	0.2376	−0.1414	0.4026	0.026*	
H5C	0.2154	−0.0332	0.4776	0.026*	
C6	0.36965 (17)	−0.0454 (3)	0.45408 (11)	0.0243 (4)	
H6B	0.3775	−0.1594	0.4878	0.029*	
H6C	0.3904	0.0786	0.4798	0.029*	
C7	0.44309 (16)	−0.0778 (3)	0.39138 (11)	0.0235 (4)	
H7A	0.5112	−0.1166	0.4103	0.028*	
H7B	0.4175	−0.1894	0.3610	0.028*	
C8	0.63399 (16)	0.0489 (4)	0.31626 (12)	0.0300 (5)	
H8A	0.6279	−0.0723	0.3458	0.045*	
H8B	0.6885	0.1349	0.3355	0.045*	
H8C	0.6503	0.0104	0.2670	0.045*	
C9	0.53527 (14)	0.1615 (3)	0.31692 (10)	0.0193 (4)	
C10	0.52860 (14)	0.3557 (3)	0.27613 (10)	0.0187 (4)	
C11	0.61537 (14)	0.4418 (4)	0.23499 (11)	0.0271 (5)	
H11A	0.5951	0.5721	0.2147	0.041*	
H11B	0.6337	0.3495	0.1962	0.041*	
H11C	0.6743	0.4604	0.2670	0.041*	
O1S	0.4279 (2)	0.4681 (5)	0.44200 (16)	0.0267 (7)	0.50
H1S	0.4925	0.4607	0.4464	0.032*	0.50
H2S	0.3888	0.4851	0.4777	0.032*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01772 (12)	0.01642 (13)	0.03693 (16)	0.00581 (10)	0.01567 (10)	0.00905 (11)
Cl1	0.0289 (2)	0.0278 (3)	0.0169 (2)	−0.0001 (2)	−0.00467 (18)	−0.00056 (19)
O1	0.0180 (6)	0.0159 (7)	0.0184 (7)	0.0006 (5)	0.0031 (5)	0.0046 (5)
O2	0.0188 (7)	0.0231 (8)	0.0208 (7)	−0.0013 (6)	0.0045 (5)	0.0053 (6)
O3	0.0218 (8)	0.0559 (12)	0.0308 (9)	0.0033 (8)	0.0004 (6)	0.0138 (8)
O4	0.0239 (8)	0.0888 (17)	0.0321 (9)	−0.0020 (9)	0.0055 (7)	0.0093 (10)
O5	0.0602 (11)	0.0255 (9)	0.0262 (8)	0.0064 (8)	−0.0182 (8)	−0.0078 (7)
O6	0.0786 (14)	0.0260 (10)	0.0360 (10)	−0.0010 (9)	−0.0077 (10)	−0.0084 (8)
N1	0.0167 (7)	0.0142 (8)	0.0155 (7)	−0.0009 (6)	0.0037 (6)	0.0010 (6)

N2	0.0202 (8)	0.0147 (8)	0.0179 (8)	−0.0010 (6)	0.0059 (6)	0.0011 (6)
N3	0.0176 (7)	0.0202 (9)	0.0166 (8)	0.0031 (6)	−0.0016 (6)	−0.0010 (7)
N4	0.0152 (7)	0.0193 (8)	0.0122 (7)	−0.0023 (6)	0.0003 (6)	−0.0014 (6)
C1	0.0125 (8)	0.0301 (11)	0.0191 (9)	0.0030 (7)	0.0014 (7)	0.0027 (8)
C2	0.0137 (8)	0.0186 (9)	0.0130 (8)	−0.0015 (7)	0.0010 (6)	−0.0023 (7)
C3	0.0160 (8)	0.0184 (10)	0.0129 (8)	−0.0037 (7)	0.0033 (6)	−0.0019 (7)
C4	0.0193 (9)	0.0265 (12)	0.0241 (10)	−0.0057 (8)	0.0073 (8)	0.0013 (9)
C5	0.0272 (10)	0.0155 (10)	0.0236 (10)	−0.0012 (8)	0.0053 (8)	0.0024 (8)
C6	0.0327 (11)	0.0207 (10)	0.0196 (9)	0.0027 (9)	−0.0011 (8)	0.0029 (8)
C7	0.0261 (10)	0.0211 (11)	0.0233 (10)	0.0063 (8)	−0.0015 (8)	0.0009 (8)
C8	0.0164 (9)	0.0431 (14)	0.0304 (11)	0.0087 (9)	−0.0017 (8)	−0.0027 (10)
C9	0.0147 (8)	0.0285 (11)	0.0148 (9)	0.0032 (7)	−0.0031 (7)	−0.0056 (8)
C10	0.0117 (8)	0.0300 (11)	0.0143 (8)	−0.0031 (7)	−0.0009 (6)	−0.0063 (8)
C11	0.0116 (8)	0.0478 (15)	0.0220 (10)	−0.0042 (9)	0.0031 (7)	0.0002 (10)
O1S	0.0223 (14)	0.0324 (18)	0.0254 (15)	−0.0045 (13)	0.0071 (12)	−0.0054 (13)

Geometric parameters (Å, °)

Cu1—N2	1.9499 (16)	C4—H4B	0.980
Cu1—N4	1.9502 (16)	C4—H4C	0.980
Cu1—N1	1.9525 (16)	C4—H4D	0.980
Cu1—N3	1.9607 (16)	C5—C6	1.519 (3)
Cl1—O5	1.4309 (16)	C5—H5B	0.990
Cl1—O6	1.4346 (19)	C5—H5C	0.990
Cl1—O3	1.4380 (17)	C6—C7	1.535 (3)
Cl1—O4	1.4411 (18)	C6—H6B	0.990
O1—N1	1.348 (2)	C6—H6C	0.990
O2—N4	1.357 (2)	C7—H7A	0.990
O2—H2A	0.840	C7—H7B	0.990
N1—C2	1.293 (2)	C8—C9	1.492 (3)
N2—C3	1.284 (2)	C8—H8A	0.980
N2—C5	1.461 (3)	C8—H8B	0.980
N3—C9	1.284 (2)	C8—H8C	0.980
N3—C7	1.466 (3)	C9—C10	1.499 (3)
N4—C10	1.285 (2)	C10—C11	1.490 (3)
C1—C2	1.491 (3)	C11—H11A	0.980
C1—H1A	0.980	C11—H11B	0.980
C1—H1B	0.980	C11—H11C	0.980
C1—H1C	0.980	O1S—H1S	0.850
C2—C3	1.486 (3)	O1S—H2S	0.850
C3—C4	1.498 (2)		
N2—Cu1—N4	173.41 (7)	C3—C4—H4D	109.5
N2—Cu1—N1	82.00 (7)	H4B—C4—H4D	109.5
N4—Cu1—N1	96.46 (7)	H4C—C4—H4D	109.5
N2—Cu1—N3	99.81 (7)	N2—C5—C6	111.00 (17)
N4—Cu1—N3	81.41 (7)	N2—C5—H5B	109.4
N1—Cu1—N3	176.58 (7)	C6—C5—H5B	109.4
O5—Cl1—O6	109.57 (11)	N2—C5—H5C	109.4
O5—Cl1—O3	109.31 (11)	C6—C5—H5C	109.4

O6—Cl1—O3	109.19 (12)	H5B—C5—H5C	108.0
O5—Cl1—O4	110.29 (12)	C5—C6—C7	115.52 (17)
O6—Cl1—O4	109.90 (14)	C5—C6—H6B	108.4
O3—Cl1—O4	108.55 (10)	C7—C6—H6B	108.4
N4—O2—H2A	109.5	C5—C6—H6C	108.4
C2—N1—O1	122.01 (16)	C7—C6—H6C	108.4
C2—N1—Cu1	114.99 (13)	H6B—C6—H6C	107.5
O1—N1—Cu1	122.74 (11)	N3—C7—C6	111.36 (17)
C3—N2—C5	123.73 (16)	N3—C7—H7A	109.4
C3—N2—Cu1	113.58 (13)	C6—C7—H7A	109.4
C5—N2—Cu1	122.62 (12)	N3—C7—H7B	109.4
C9—N3—C7	124.64 (17)	C6—C7—H7B	109.4
C9—N3—Cu1	114.03 (14)	H7A—C7—H7B	108.0
C7—N3—Cu1	121.33 (13)	C9—C8—H8A	109.5
C10—N4—O2	119.86 (16)	C9—C8—H8B	109.5
C10—N4—Cu1	116.23 (14)	H8A—C8—H8B	109.5
O2—N4—Cu1	123.83 (11)	C9—C8—H8C	109.5
C2—C1—H1A	109.5	H8A—C8—H8C	109.5
C2—C1—H1B	109.5	H8B—C8—H8C	109.5
H1A—C1—H1B	109.5	N3—C9—C8	126.0 (2)
C2—C1—H1C	109.5	N3—C9—C10	115.75 (17)
H1A—C1—H1C	109.5	C8—C9—C10	118.26 (18)
H1B—C1—H1C	109.5	N4—C10—C11	124.0 (2)
N1—C2—C3	112.90 (16)	N4—C10—C9	112.56 (16)
N1—C2—C1	124.48 (18)	C11—C10—C9	123.38 (18)
C3—C2—C1	122.60 (16)	C10—C11—H11A	109.5
N2—C3—C2	116.17 (16)	C10—C11—H11B	109.5
N2—C3—C4	124.53 (18)	H11A—C11—H11B	109.5
C2—C3—C4	119.29 (17)	C10—C11—H11C	109.5
C3—C4—H4B	109.5	H11A—C11—H11C	109.5
C3—C4—H4C	109.5	H11B—C11—H11C	109.5
H4B—C4—H4C	109.5	H1S—O1S—H2S	122.3

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···O1	0.84	1.70	2.516 (2)	162
O1S—H1S···O4^{i}	0.85	2.19	3.000 (2)	159
O1S—H2S···O4^{ii}	0.85	2.03	2.842 (2)	159

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

Fig. 1

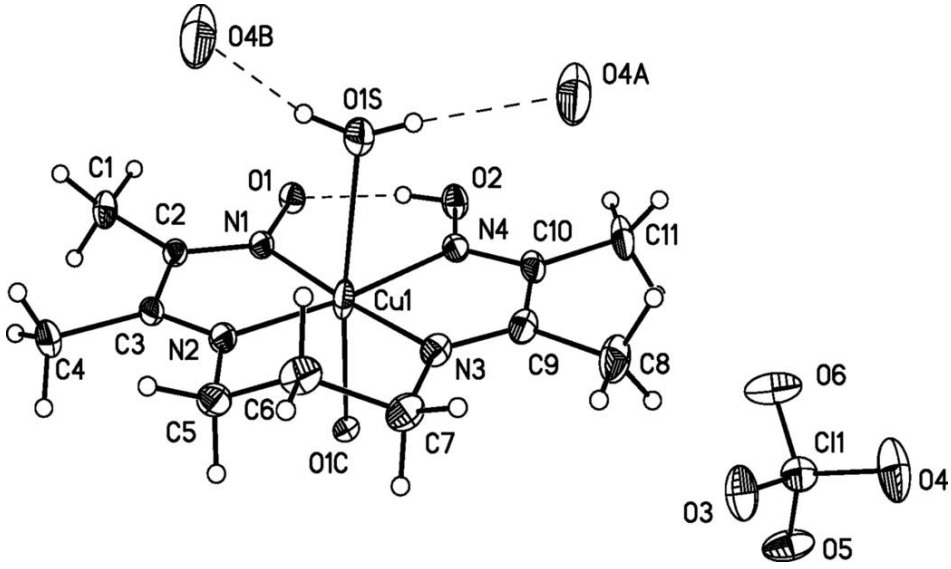
O4B
O1S
O4A
C1
O1
O2
C2
N1
N4
C10
C11
Cu1
C3
N2
N3
C9
C8
C4
C6
C5
O1C
C7
O6
Cl1
O4
O3
O5

Fig. 2