Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquabis(4-carboxy-2-propyl-1*H*-imidazole-5-carboxylato-κ^2N^3,O^4)-copper(II) *N*,*N*-dimethylformamide disolvate

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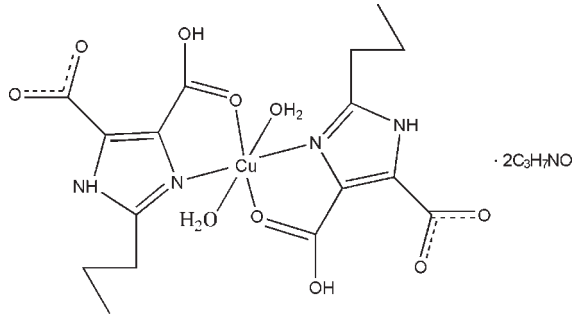
Received 4 June 2010; accepted 27 June 2010

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.039; wR factor = 0.097; data-to-parameter ratio = 12.8.

In the title complex, $[Cu(C_8H_9N_2O_4)_2(H_2O)_2]\cdot 2C_3H_7NO$, the Cu^{II} ion, lying on an inversion center, is six-coordinated in a slightly distorted octahedral geometry. Two N atoms and two O atoms from two H_2pimda (H_3pimda is 2-propyl-1*H*-4,5-dicarboxylic acid) ligands are in the equatorial plane. The axial positions are occupied by two O atoms from two water molecules. A two-dimensional supramolecular network parallel to (001) is constructed by N—H···O and O—H···O hydrogen bonds. An intramolecular O—H···O hydrogen bond is also observed.

Related literature

For the potential uses and diverse structural types of metal complexes with imidazole-4,5-dicarboxylic acid, see: Li *et al.* (2006); Liu *et al.* (2004); Sun *et al.* (2005); Zou *et al.* (2006).



Experimental

Crystal data

$[Cu(C_8H_9N_2O_4)_2(H_2O)_2]\cdot 2C_3H_7NO$
M_r = 640.11
Triclinic, $P\overline{1}$
a = 7.2831 (8) Å
b = 9.250 (1) Å
c = 11.3329 (13) Å
α = 75.264 (1)°
β = 87.305 (2)°
γ = 68.416 (1)°
V = 685.68 (13) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.87 mm^{-1}
T = 298 K
0.32 × 0.21 × 0.19 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.768, T_{max} = 0.852
3603 measured reflections
2385 independent reflections
2011 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.097
S = 1.06
2385 reflections
187 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O6^{i}	0.86	1.83	2.679 (3)	167
O2—H2A···O3	0.82	1.67	2.494 (3)	177
O5—H5A···O4^{ii}	0.85	1.91	2.755 (3)	172
O5—H5B···O4^{iii}	0.85	2.07	2.906 (3)	167

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge Guang Dong Ocean University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2320).

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supplementary materials

Acta Cryst. (2010). E**66**, m896 [**doi:10.1107/S1600536810025249**]

Diaquabis(4-carboxy-2-propyl-1*H*-imidazole-5-carboxylato-κ^2N^3,O^4)copper(II) *N*,*N*-dimethylformamide disolvate

L.-Z. He, S.-J. Li, W.-D. Song and D.-L. Miao

Comment

Design and synthesis of metal-organic complexes *via* deliberate selection of metal ions and organic ligands have been one of the most attractive subjects due to their fascinating structures and potential applications in many field. It is well known that ligands containing N and O atoms which are highly accessible to metal ions are good candidates for the design and synthesis. For example, imidazole-4,5-dicarboxylic acid (H_3idc) containing N and O coordination sites can be deprotonated to form $(H_2idc)^-$, $(Hidc)^{2-}$ and $(idc)^{3-}$ anions at different pH values. H_3idc has been widely used to react with metal salts to obtain a series of metal-organic frameworks with different structures and useful properties (Li *et al.*, 2006; Liu *et al.*, 2004; Sun *et al.*, 2005; Zou *et al.*, 2006). Therefore, we chose 2-propyl-imidazole-4,5-dicarboxylic acid (H_3pimda) as ligand for the synthesis of fascinating structures and we report a new Cu^{II} complex here.

As illustrated in Fig. 1, the asymmetric unit of the title complex comprises one H_2pimda ligand, one Cu^{II} ion lying on an inversion center, one coordinated water molecule and one solvent DMF molecule. The Cu^{II} ion is six-coordinated in a slightly distorted octahedral geometry, formed by two N atoms and two O atoms from two H_2pimda ligands in the equatorial plane. The Cu—O bond length with the value of 2.458 (2) Å is somewhat longer than the Cu—N bond with the value of 1.987 (2) Å. The axial positions are occupied by two O atoms from two water molecules [Cu—O = 2.020 (2) Å]. The H_2pimda ligand adopts a bidentate mode to chelate the metal atom through one imidazole N atom and one O atom from the protonated carboxyl group. The other carboxyl group is deprotonated, indicated by a difference of the bond lengths. The two imidazole rings are coplanar. The DMF molecules are linked to the H_2pimda ligand *via* N—H···O hydrogen bonds. The two-dimensional supramolecular network is stabilized by N—H···O and O—H···O hydrogen bonds (Fig. 2, Table 1).

Experimental

A mixture of $Cu(NO_3)_2$ (0.5 mmol, 0.05 g) and 2-propyl-1*H*-imidazole-4,5-dicarboxylic acid (0.5 mmol, 0.99 g) in 15 ml of DMF solution was sealed in an autoclave equipped with a Teflon liner (20 ml) and then heated at 433 K for 4 d. Blue crystals were obtained by slow evaporation of the solvent at room temperature.

Refinement

C- and N-bound H atoms were placed at calculated positions and were treated as riding on the parent atoms, with C—H = 0.93 (CH), 0.97 (CH_2) and 0.96 (CH_3) Å, N—H = 0.86 Å, and with U_{iso}(H) = 1.2(1.5 for methyl)U_{eq}(C, N). H atoms of the water molecule and hydroxyl group were located in a difference map and were allowed to ride on the parent atom, with O—H = 0.85 and 0.82 Å and U_{iso}(H) = 1.2(1.5 for hydroxyl)U_{eq}(O).

Figures

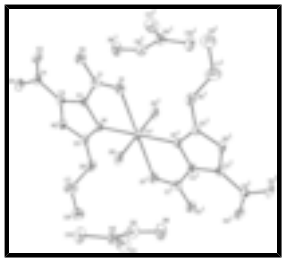

Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are shown at the 30% probability level. H atoms are omitted for clarity. [Symmetry code: (i) 1-x, 1-y, 1-z.]

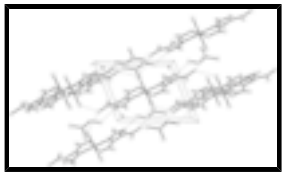

Fig. 2. A view of the two-dimensional network constructed by O—H···O and N—H···O hydrogen bonding interactions. H atoms are omitted for clarity.

Diaquabis(4-carboxy-2-propyl-1*H*-imidazole-5-carboxylato- κ^2N^3,O^4)copper(II) *N*,*N*-dimethylformamide disolvate

Crystal data

$[Cu(C_8H_9N_2O_4)_2(H_2O)_2]\cdot 2C_3H_7NO$	$Z = 1$
$M_r = 640.11$	$F(000) = 335$
Triclinic, $P\overline{1}$	$D_x = 1.550$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.2831$ (8) Å	Cell parameters from 1702 reflections
$b = 9.250$ (1) Å	$\theta = 2.5$–$25.9°$
$c = 11.3329$ (13) Å	$\mu = 0.87$ mm^{-1}
$\alpha = 75.264$ (1)°	$T = 298$ K
$\beta = 87.305$ (2)°	Cubic, blue
$\gamma = 68.416$ (1)°	0.32 × 0.21 × 0.19 mm
$V = 685.68$ (13) Å^3	

Data collection

Bruker SMART 1000 CCD diffractometer	2385 independent reflections
Radiation source: fine-focus sealed tube	2011 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.017$
φ and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -8\rightarrow7$
$T_{min} = 0.768$, $T_{max} = 0.852$	$k = -10\rightarrow10$
3603 measured reflections	$l = -10\rightarrow13$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.039$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.097$	H-atom parameters constrained
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2 + 0.548P]$ where $P = (F_o^2 + 2F_c^2)/3$
2385 reflections	$(\Delta/\sigma)_{max} < 0.001$
187 parameters	$\Delta\rho_{max} = 0.38$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.29$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.5000	0.5000	0.5000	0.02632 (17)
N1	0.6271 (3)	0.2621 (3)	0.5343 (2)	0.0251 (5)
N2	0.7981 (3)	0.0045 (3)	0.5992 (2)	0.0295 (6)
H2	0.8707	−0.0862	0.6461	0.035*
N3	0.1268 (4)	0.4896 (3)	0.8656 (3)	0.0434 (7)
O1	0.4276 (3)	0.4348 (2)	0.31460 (19)	0.0387 (5)
O2	0.4952 (3)	0.2191 (3)	0.24467 (19)	0.0422 (6)
H2A	0.5573	0.1221	0.2687	0.063*
O3	0.6933 (4)	−0.0740 (3)	0.3193 (2)	0.0442 (6)
O4	0.8653 (3)	−0.2477 (2)	0.4863 (2)	0.0398 (5)
O5	0.2402 (3)	0.4858 (2)	0.56026 (19)	0.0353 (5)
H5A	0.2186	0.4061	0.5485	0.042*
H5B	0.1412	0.5701	0.5293	0.042*
O6	0.0414 (4)	0.7502 (3)	0.7641 (2)	0.0568 (7)
C1	0.5080 (4)	0.2896 (3)	0.3284 (3)	0.0305 (7)
C2	0.6222 (4)	0.1888 (3)	0.4434 (3)	0.0255 (6)
C3	0.7286 (4)	0.0262 (3)	0.4834 (3)	0.0265 (6)
C4	0.7665 (4)	−0.1092 (3)	0.4254 (3)	0.0305 (7)
C5	0.7356 (4)	0.1463 (3)	0.6284 (3)	0.0289 (7)
C6	0.7787 (5)	0.1646 (4)	0.7491 (3)	0.0414 (8)
H6A	0.7328	0.2782	0.7460	0.050*
H6B	0.9208	0.1199	0.7659	0.050*
C7	0.6827 (7)	0.0825 (6)	0.8528 (4)	0.0694 (12)
H7A	0.5414	0.1240	0.8336	0.083*
H7B	0.7328	−0.0316	0.8573	0.083*
C8	0.7160 (7)	0.1037 (5)	0.9754 (3)	0.0659 (12)
H8A	0.8439	0.0288	1.0098	0.099*
H8B	0.6159	0.0845	1.0282	0.099*
H8C	0.7097	0.2114	0.9668	0.099*
C9	0.0181 (5)	0.6215 (4)	0.7857 (3)	0.0451 (8)

H9	−0.0840	0.6167	0.7424	0.054*
C10	0.0974 (8)	0.3399 (5)	0.8779 (4)	0.0779 (14)
H10A	−0.0212	0.3605	0.8322	0.117*
H10B	0.0856	0.2932	0.9625	0.117*
H10C	0.2082	0.2669	0.8471	0.117*
C11	0.2925 (6)	0.4885 (5)	0.9321 (4)	0.0625 (11)
H11A	0.4116	0.4480	0.8910	0.094*
H11B	0.3049	0.4207	1.0134	0.094*
H11C	0.2709	0.5959	0.9361	0.094*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0281 (3)	0.0167 (3)	0.0329 (3)	−0.0064 (2)	−0.0004 (2)	−0.0065 (2)
N1	0.0284 (13)	0.0187 (11)	0.0282 (13)	−0.0084 (10)	0.0010 (10)	−0.0066 (10)
N2	0.0300 (14)	0.0166 (11)	0.0365 (14)	−0.0047 (10)	−0.0039 (11)	−0.0025 (10)
N3	0.0490 (18)	0.0311 (14)	0.0453 (17)	−0.0112 (13)	−0.0017 (13)	−0.0060 (12)
O1	0.0464 (14)	0.0227 (11)	0.0391 (13)	−0.0053 (10)	−0.0048 (10)	−0.0045 (9)
O2	0.0540 (15)	0.0332 (12)	0.0363 (13)	−0.0100 (11)	−0.0097 (10)	−0.0105 (10)
O3	0.0579 (16)	0.0319 (12)	0.0443 (14)	−0.0110 (11)	−0.0031 (12)	−0.0194 (10)
O4	0.0397 (13)	0.0185 (11)	0.0580 (15)	−0.0045 (9)	−0.0025 (11)	−0.0125 (10)
O5	0.0289 (11)	0.0218 (10)	0.0565 (14)	−0.0094 (9)	0.0037 (10)	−0.0123 (9)
O6	0.0589 (17)	0.0316 (13)	0.0649 (17)	−0.0080 (12)	−0.0174 (13)	0.0038 (12)
C1	0.0282 (16)	0.0297 (16)	0.0334 (17)	−0.0103 (13)	0.0012 (13)	−0.0082 (13)
C2	0.0263 (15)	0.0228 (14)	0.0309 (16)	−0.0122 (12)	0.0038 (12)	−0.0086 (12)
C3	0.0237 (15)	0.0227 (14)	0.0340 (17)	−0.0091 (12)	0.0046 (12)	−0.0083 (12)
C4	0.0256 (16)	0.0236 (15)	0.0445 (19)	−0.0096 (13)	0.0060 (13)	−0.0128 (14)
C5	0.0304 (16)	0.0222 (14)	0.0340 (17)	−0.0100 (12)	−0.0013 (13)	−0.0060 (12)
C6	0.053 (2)	0.0267 (16)	0.0416 (19)	−0.0119 (15)	−0.0131 (16)	−0.0051 (14)
C7	0.085 (3)	0.094 (3)	0.052 (3)	−0.050 (3)	0.019 (2)	−0.035 (2)
C8	0.079 (3)	0.067 (3)	0.051 (2)	−0.024 (2)	0.006 (2)	−0.018 (2)
C9	0.0362 (19)	0.047 (2)	0.048 (2)	−0.0092 (16)	−0.0039 (16)	−0.0138 (17)
C10	0.105 (4)	0.041 (2)	0.094 (3)	−0.033 (2)	0.015 (3)	−0.019 (2)
C11	0.050 (2)	0.058 (2)	0.062 (3)	−0.0083 (19)	−0.0161 (19)	0.001 (2)

Geometric parameters (Å, °)

Cu1—N1^{i}	1.987 (2)	C1—C2	1.475 (4)
Cu1—N1	1.987 (2)	C2—C3	1.377 (4)
Cu1—O5^{i}	2.020 (2)	C3—C4	1.491 (4)
Cu1—O5	2.020 (2)	C5—C6	1.481 (4)
Cu1—O1	2.458 (2)	C6—C7	1.519 (5)
N1—C5	1.336 (3)	C6—H6A	0.9700
N1—C2	1.378 (3)	C6—H6B	0.9700
N2—C5	1.344 (3)	C7—C8	1.494 (5)
N2—C3	1.368 (4)	C7—H7A	0.9700
N2—H2	0.8600	C7—H7B	0.9700
N3—C9	1.315 (4)	C8—H8A	0.9600

N3—C11	1.448 (4)	C8—H8B	0.9600
N3—C10	1.449 (4)	C8—H8C	0.9600
O1—C1	1.222 (3)	C9—H9	0.9300
O2—C1	1.305 (3)	C10—H10A	0.9600
O2—H2A	0.8200	C10—H10B	0.9600
O3—C4	1.253 (4)	C10—H10C	0.9600
O4—C4	1.247 (3)	C11—H11A	0.9600
O5—H5A	0.8499	C11—H11B	0.9600
O5—H5B	0.8500	C11—H11C	0.9600
O6—C9	1.226 (4)		
$N1^{i}$—Cu1—N1	180.00 (6)	N1—C5—N2	109.4 (2)
$N1^{i}$—Cu1—$O5^{i}$	91.57 (9)	N1—C5—C6	127.0 (3)
N1—Cu1—$O5^{i}$	88.44 (9)	N2—C5—C6	123.6 (3)
$N1^{i}$—Cu1—O5	88.43 (9)	C5—C6—C7	113.2 (3)
N1—Cu1—O5	91.56 (9)	C5—C6—H6A	108.9
$O5^{i}$—Cu1—O5	180.0	C7—C6—H6A	108.9
$N1^{i}$—Cu1—O1	104.94 (8)	C5—C6—H6B	108.9
N1—Cu1—O1	75.06 (8)	C7—C6—H6B	108.9
$O5^{i}$—Cu1—O1	92.58 (8)	H6A—C6—H6B	107.7
O5—Cu1—O1	87.42 (8)	C8—C7—C6	114.9 (3)
C5—N1—C2	106.6 (2)	C8—C7—H7A	108.6
C5—N1—Cu1	134.39 (19)	C6—C7—H7A	108.6
C2—N1—Cu1	118.83 (18)	C8—C7—H7B	108.6
C5—N2—C3	109.7 (2)	C6—C7—H7B	108.6
C5—N2—H2	125.2	H7A—C7—H7B	107.5
C3—N2—H2	125.2	C7—C8—H8A	109.5
C9—N3—C11	119.9 (3)	C7—C8—H8B	109.5
C9—N3—C10	120.6 (3)	H8A—C8—H8B	109.5
C11—N3—C10	119.1 (3)	C7—C8—H8C	109.5
C1—O1—Cu1	108.15 (18)	H8A—C8—H8C	109.5
C1—O2—H2A	109.5	H8B—C8—H8C	109.5
Cu1—O5—H5A	114.3	O6—C9—N3	124.8 (3)
Cu1—O5—H5B	113.0	O6—C9—H9	117.6
H5A—O5—H5B	107.6	N3—C9—H9	117.6
O1—C1—O2	122.2 (3)	N3—C10—H10A	109.5
O1—C1—C2	119.7 (3)	N3—C10—H10B	109.5
O2—C1—C2	118.1 (2)	H10A—C10—H10B	109.5
C3—C2—N1	109.4 (2)	N3—C10—H10C	109.5
C3—C2—C1	132.5 (3)	H10A—C10—H10C	109.5
N1—C2—C1	118.1 (2)	H10B—C10—H10C	109.5
N2—C3—C2	104.9 (2)	N3—C11—H11A	109.5
N2—C3—C4	122.9 (2)	N3—C11—H11B	109.5
C2—C3—C4	132.2 (3)	H11A—C11—H11B	109.5
O4—C4—O3	125.3 (3)	N3—C11—H11C	109.5
O4—C4—C3	117.8 (3)	H11A—C11—H11C	109.5
O3—C4—C3	116.9 (3)	H11B—C11—H11C	109.5
$O5^{i}$—Cu1—N1—C5	85.3 (3)	C5—N2—C3—C4	−177.9 (3)

O5—Cu1—N1—C5	−94.7 (3)	N1—C2—C3—N2	−0.5 (3)
O1—Cu1—N1—C5	178.4 (3)	C1—C2—C3—N2	−178.9 (3)
O5^{i}—Cu1—N1—C2	−89.3 (2)	N1—C2—C3—C4	177.8 (3)
O5—Cu1—N1—C2	90.7 (2)	C1—C2—C3—C4	−0.7 (5)
O1—Cu1—N1—C2	3.76 (19)	N2—C3—C4—O4	0.3 (4)
N1^{i}—Cu1—O1—C1	177.7 (2)	C2—C3—C4—O4	−177.7 (3)
N1—Cu1—O1—C1	−2.3 (2)	N2—C3—C4—O3	179.4 (3)
O5^{i}—Cu1—O1—C1	85.4 (2)	C2—C3—C4—O3	1.4 (5)
O5—Cu1—O1—C1	−94.6 (2)	C2—N1—C5—N2	0.1 (3)
Cu1—O1—C1—O2	179.8 (2)	Cu1—N1—C5—N2	−175.00 (19)
Cu1—O1—C1—C2	0.4 (3)	C2—N1—C5—C6	−178.0 (3)
C5—N1—C2—C3	0.3 (3)	Cu1—N1—C5—C6	6.9 (5)
Cu1—N1—C2—C3	176.24 (18)	C3—N2—C5—N1	−0.4 (3)
C5—N1—C2—C1	179.0 (2)	C3—N2—C5—C6	177.8 (3)
Cu1—N1—C2—C1	−5.1 (3)	N1—C5—C6—C7	112.5 (4)
O1—C1—C2—C3	−179.0 (3)	N2—C5—C6—C7	−65.4 (4)
O2—C1—C2—C3	1.7 (5)	C5—C6—C7—C8	−177.7 (3)
O1—C1—C2—N1	2.7 (4)	C11—N3—C9—O6	−2.4 (6)
O2—C1—C2—N1	−176.7 (2)	C10—N3—C9—O6	−175.2 (4)
C5—N2—C3—C2	0.5 (3)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O6^{ii}	0.86	1.83	2.679 (3)	167
O2—H2A···O3	0.82	1.67	2.494 (3)	177
O5—H5A···O4^{iii}	0.85	1.91	2.755 (3)	172
O5—H5B···O4^{iv}	0.85	2.07	2.906 (3)	167

Symmetry codes: (ii) *x*+1, *y*−1, *z*; (iii) −*x*+1, −*y*, −*z*+1; (iv) *x*−1, *y*+1, *z*.

Fig. 1

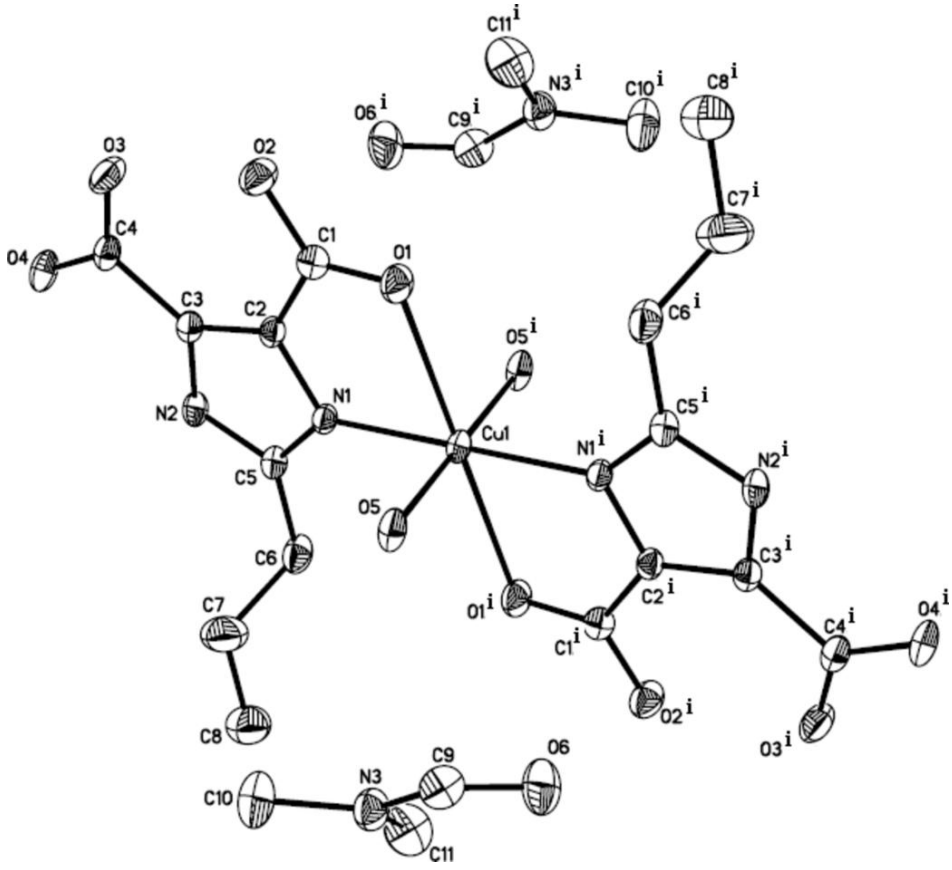
C11i
N3i
C10i
C8i
O6i
C9i
O3
O2
C7i
C4
C1
O1
O4
C3
C2
C6i
O5i
N1
N2
Cu1
C5i
N1i
N2i
C5
O5
C6
C3i
C7
O1i
C2i
C4i
O4i
C1i
O2i
C8
O3i
C9
O6
N3
C10
C11

Fig. 2