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catena-Poly[[bis(nitrato-κO)copper(II)]-bis[μ-1,4-bis(pyridin-3-ylmethoxy)-benzene-$\kappa^2 N:N'$]]

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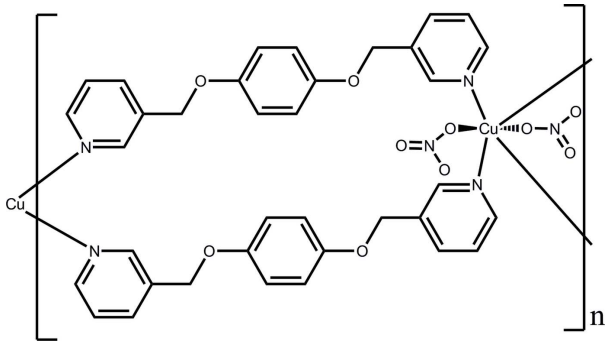
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.037; wR factor = 0.097; data-to-parameter ratio = 15.3.

In the title compound, $[Cu(NO_3)_2(C_{18}H_{16}N_2O_2)_2]_n$, the Cu^{II} ion lies on an inversion center and is six-coordinated in a Jahn–Teller-distored octahedral geometry defined by four N atoms of the pyridine derivative forming a square plane, above and below which are the O atoms of the nitrate anion. The ligand links the metal atoms linto a linear chain running along the *a* axis. One of the nitrate O atoms is equally disordered over two sets of sites.

Related literature

For the synthesis and background to network structures built up from flexible pyridyl-based aromatic ligands and transition metals, see Liu *et al.* (2010*a*,*b*).



Experimental

Crystal data

$[Cu(NO_3)_2(C_{18}H_{16}N_2O_2)_2]$
M_r = 772.22
Monoclinic, $P2_1/c$
a = 8.4859 (17) Å
b = 17.030 (3) Å
c = 12.986 (4) Å
β = 116.22 (2)°
V = 1683.6 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.72 mm^{-1}
T = 291 K
0.20 × 0.18 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.867, T_{max} = 0.889
16256 measured reflections
3831 independent reflections
3067 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.097
S = 1.07
3831 reflections
251 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5152).

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supplementary materials

Acta Cryst. (2011). E**67**, m692 [**doi:10.1107/S1600536811016096**]

catena-Poly[[bis(nitrato-κO)copper(II)]-bis[μ-1,4-bis(pyridin-3-ylmethoxy)benzene-$\kappa^2 N$:N']]

P. Zou, Y. Liu, G.-F. Hou and J.-S. Gao

Comment

The bridging pyridyl ligands can be used to construct interesting 0D to three-dimensional supramolecular architectures. Our group has reported some isolated molecule, chain, plane and three-dimensional network structures built up by flexible pyridyl-based aromatic ligands and transition metals. (Liu *et al.*, 2010*a*; Liu *et al.*, 2010*b*). As our continuing work for pyridyl ligands, we report here the synthesis and crystal structure of the title compound.

An asymmetric unit of the title compound consists of a 1,4-bis(pyridin-3-ylmethoxy)benzene molecule, a nitrate anion and a Cu^{II} cation (Figure 1). The Cu^{II} cations lie on the inversion centers and are six-coordinated in the Jahn-Teller distored octahedral geometry environments defined by four N atoms forming the square planes and two O atoms locating the polar axis.

In the crystal, ribbon structures along [2 0 1] direction are built up by heterocyclic ligands bridging Cu^{II} cations (Figure 2, Table 1).

Experimental

The 1,4-bis(pyridin-3-ylmethoxy)benzene ligand was synthesized as the reference method (Liu *et al.*, 2010*a*): A mixture of 1,4-dihydroxybenzene (1.1 g, 10 mmol), 3-chloromethylpyridine hydrochloride (3.28 g, 20 mmol) and NaOH (1.6 g, 40 mmol) in acetonitrile (50 ml) was refluxed under nitrogen with stirring for 24 h. After cooling to room temperature, the solution was filtered and the residue was washed with acetonitrile for several times. The mixed filtrate was droped into 300 ml water solution to get the powder crude product. A total of 2.51 g (yield 86%) pure product was obtained by recrystallizing from the mixed solution of 10 ml water and 10 ml me thanol. The title compound was synthesized by reaction of 1,4-bis(pyridin-3-ylmethoxy)benzene ligand (0.29 g, 1.0 mmol) and $Cu(NO_3)_2{\cdot}3H_2O$ (0.22 g, 1.0 mmol) in 5 ml water and 5 ml me thanol mixed solution. After filtration, blue block crystals suitable for X-ray diffraction were obtained by slow evaporation at room temperature for several days in 46% yield.

Refinement

O4 atom of nitrate was disordered over two positions with site occupancy factors of *ca* 0.51 and 0.49, and then, the two positions were restraint refined with commond 'Iosr 0.01 O4 O4' '. H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic); C—H = 0.97 Å (methylene), and with U_{iso}(H) = 1.2U_{eq}(C).

Figures

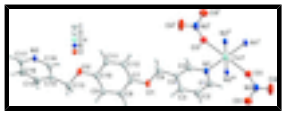

Fig. 1. The molecular structure of the title compound, showing displacement ellipsoids at the 50% probability level for non-H atoms, disordered O4' atom has been omitted for clarity.

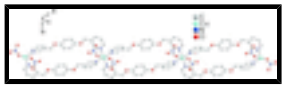

Fig. 2. A partial packing view, showing the ribbon structure along [2 0 1] direction. Disordered O4' atoms and no involving H atoms have been omitted for clarity.

catena-Poly[[bis(nitrato-κ*O*)copper(II)]-bis[μ-1,4- bis(pyridin-3-ylmethoxy)benzene-κ^2*N*:*N*']]

Crystal data

$[Cu(NO_3)_2(C_{18}H_{16}N_2O_2)_2]$	$F(000) = 798$
$M_r = 772.22$	$D_x = 1.523$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 13022 reflections
$a = 8.4859$ (17) Å	$\theta = 3.4$–$27.4°$
$b = 17.030$ (3) Å	$\mu = 0.72$ mm^{-1}
$c = 12.986$ (4) Å	$T = 291$ K
$\beta = 116.22$ (2)°	Block, blue
$V = 1683.6$ (7) Å^3	0.20 × 0.18 × 0.17 mm
$Z = 2$	

Data collection

Rigaku R-AXIS RAPID diffractometer	3831 independent reflections
Radiation source: fine-focus sealed tube	3067 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.039$
ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 3.4°$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$h = -11 \rightarrow 10$
$T_{min} = 0.867$, $T_{max} = 0.889$	$k = -22 \rightarrow 22$
16256 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.037$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.097$	H-atom parameters constrained
$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 0.4137P]$ where $P = (F_o^2 + 2F_c^2)/3$
3831 reflections	$(\Delta/\sigma)_{max} < 0.001$

251 parameters	$\Delta\rho_{max}$ = 0.45 e Å^{-3}
12 restraints	$\Delta\rho_{min}$ = −0.26 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 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)
C1	−0.3511 (2)	0.87028 (12)	0.16557 (18)	0.0353 (4)	
H1	−0.4698	0.8612	0.1432	0.042*	
C2	−0.2290 (3)	0.82377 (13)	0.25037 (19)	0.0383 (5)	
H2	−0.2657	0.7837	0.2833	0.046*	
C3	−0.0520 (3)	0.83705 (12)	0.28601 (18)	0.0351 (4)	
H3	0.0317	0.8065	0.3435	0.042*	
C4	−0.0017 (2)	0.89662 (11)	0.23463 (17)	0.0303 (4)	
C5	−0.1310 (2)	0.93984 (12)	0.14835 (18)	0.0325 (4)	
H5	−0.0970	0.9788	0.1120	0.039*	
C6	0.1879 (2)	0.91934 (13)	0.27306 (19)	0.0385 (5)	
H6A	0.2070	0.9342	0.2073	0.046*	
H6B	0.2181	0.9637	0.3252	0.046*	
C7	0.4713 (2)	0.86583 (12)	0.39043 (19)	0.0372 (5)	
C8	0.5671 (2)	0.80017 (12)	0.44675 (18)	0.0350 (4)	
H8	0.5101	0.7526	0.4415	0.042*	
C9	0.7480 (2)	0.80513 (12)	0.51103 (18)	0.0349 (4)	
H9	0.8124	0.7609	0.5482	0.042*	
C10	0.8320 (2)	0.87615 (12)	0.51957 (18)	0.0360 (5)	
C11	0.7367 (3)	0.94163 (13)	0.4634 (2)	0.0419 (5)	
H11	0.7937	0.9892	0.4690	0.050*	
C12	0.5558 (3)	0.93666 (13)	0.3987 (2)	0.0425 (5)	
H12	0.4917	0.9808	0.3611	0.051*	
C13	1.1170 (2)	0.82248 (12)	0.63460 (19)	0.0381 (5)	
H13A	1.1171	0.7852	0.5781	0.046*	
H13B	1.0739	0.7963	0.6835	0.046*	
C14	1.2990 (2)	0.85426 (11)	0.70499 (17)	0.0305 (4)	
C15	1.4412 (3)	0.83865 (12)	0.68279 (19)	0.0375 (5)	
H15	1.4282	0.8078	0.6205	0.045*	
C16	1.6027 (3)	0.86992 (12)	0.75514 (19)	0.0377 (5)	
H16	1.6998	0.8600	0.7418	0.045*	

C17	1.6204 (2)	0.91564 (11)	0.84668 (18)	0.0319 (4)	
H17	1.7306	0.9354	0.8955	0.038*	
C18	1.3260 (2)	0.90220 (11)	0.79731 (16)	0.0300 (4)	
H18	1.2301	0.9139	0.8113	0.036*	
Cu1	−0.5000	1.0000	0.0000	0.03106 (12)	
N1	−0.30485 (19)	0.92812 (9)	0.11430 (14)	0.0304 (3)	
N2	1.48165 (18)	0.93268 (9)	0.86752 (13)	0.0279 (3)	
N3	−0.8293 (2)	0.86505 (11)	−0.01848 (17)	0.0411 (4)	
O1	0.29285 (18)	0.85382 (9)	0.32890 (17)	0.0579 (5)	
O2	1.01067 (18)	0.88797 (9)	0.57993 (16)	0.0536 (5)	
O3	−0.74035 (19)	0.92569 (8)	0.02595 (14)	0.0421 (4)	
O4	−0.9828 (11)	0.8623 (6)	−0.035 (2)	0.085 (4)	0.49 (4)
O5	−0.7554 (2)	0.80297 (10)	−0.01836 (19)	0.0654 (5)	
O4'	−0.9848 (9)	0.8748 (6)	−0.0923 (18)	0.080 (4)	0.51 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0205 (9)	0.0423 (11)	0.0386 (11)	−0.0021 (8)	0.0088 (8)	−0.0068 (9)
C2	0.0323 (10)	0.0405 (11)	0.0392 (12)	−0.0036 (9)	0.0132 (9)	0.0031 (9)
C3	0.0270 (9)	0.0401 (11)	0.0304 (10)	0.0059 (8)	0.0056 (8)	0.0042 (8)
C4	0.0195 (8)	0.0351 (10)	0.0305 (10)	0.0041 (7)	0.0058 (7)	−0.0003 (8)
C5	0.0216 (9)	0.0352 (10)	0.0343 (10)	0.0040 (7)	0.0065 (8)	0.0048 (8)
C6	0.0194 (9)	0.0427 (11)	0.0436 (12)	0.0033 (8)	0.0049 (9)	0.0093 (9)
C7	0.0152 (8)	0.0442 (11)	0.0429 (12)	0.0024 (8)	0.0044 (8)	0.0069 (9)
C8	0.0236 (9)	0.0351 (10)	0.0415 (12)	−0.0008 (8)	0.0100 (9)	0.0045 (9)
C9	0.0233 (9)	0.0365 (10)	0.0360 (11)	0.0040 (8)	0.0050 (8)	0.0043 (8)
C10	0.0179 (8)	0.0424 (11)	0.0355 (11)	−0.0001 (8)	0.0008 (8)	0.0011 (9)
C11	0.0252 (10)	0.0369 (11)	0.0524 (14)	−0.0033 (8)	0.0069 (9)	0.0042 (10)
C12	0.0247 (10)	0.0383 (11)	0.0518 (13)	0.0057 (8)	0.0054 (9)	0.0119 (10)
C13	0.0216 (9)	0.0371 (10)	0.0417 (12)	0.0011 (8)	0.0012 (8)	−0.0056 (9)
C14	0.0206 (8)	0.0306 (9)	0.0308 (10)	0.0011 (7)	0.0028 (8)	−0.0006 (8)
C15	0.0323 (10)	0.0383 (11)	0.0383 (11)	0.0028 (8)	0.0123 (9)	−0.0087 (9)
C16	0.0251 (9)	0.0400 (11)	0.0489 (13)	0.0013 (8)	0.0172 (9)	−0.0063 (9)
C17	0.0184 (8)	0.0316 (9)	0.0385 (11)	0.0010 (7)	0.0059 (8)	−0.0019 (8)
C18	0.0164 (8)	0.0376 (10)	0.0299 (10)	0.0025 (7)	0.0046 (7)	−0.0007 (8)
Cu1	0.01777 (16)	0.03750 (19)	0.02666 (18)	0.00767 (13)	−0.00042 (12)	−0.00511 (14)
N1	0.0193 (7)	0.0353 (8)	0.0292 (8)	0.0048 (6)	0.0041 (6)	−0.0024 (7)
N2	0.0186 (7)	0.0312 (8)	0.0289 (8)	0.0032 (6)	0.0059 (6)	−0.0011 (6)
N3	0.0276 (9)	0.0427 (10)	0.0492 (11)	−0.0003 (7)	0.0136 (8)	0.0019 (8)
O1	0.0167 (7)	0.0448 (9)	0.0878 (14)	0.0030 (6)	0.0009 (8)	0.0187 (9)
O2	0.0205 (7)	0.0427 (9)	0.0697 (12)	−0.0023 (6)	−0.0055 (7)	0.0095 (8)
O3	0.0392 (8)	0.0356 (7)	0.0475 (9)	−0.0028 (6)	0.0154 (7)	−0.0007 (7)
O4	0.028 (2)	0.096 (4)	0.124 (9)	0.000 (2)	0.027 (4)	0.004 (5)
O5	0.0593 (11)	0.0374 (9)	0.0899 (15)	0.0023 (8)	0.0243 (11)	−0.0022 (9)
O4'	0.022 (2)	0.086 (4)	0.102 (8)	−0.005 (2)	0.001 (3)	−0.006 (4)

Geometric parameters (Å, °)

C1—N1	1.341 (3)	C13—O2	1.413 (2)
C1—C2	1.380 (3)	C13—C14	1.505 (3)
C1—H1	0.9300	C13—H13A	0.9700
C2—C3	1.381 (3)	C13—H13B	0.9700
C2—H2	0.9300	C14—C18	1.383 (3)
C3—C4	1.381 (3)	C14—C15	1.385 (3)
C3—H3	0.9300	C15—C16	1.381 (3)
C4—C5	1.384 (3)	C15—H15	0.9300
C4—C6	1.509 (3)	C16—C17	1.373 (3)
C5—N1	1.354 (2)	C16—H16	0.9300
C5—H5	0.9300	C17—N2	1.351 (2)
C6—O1	1.412 (2)	C17—H17	0.9300
C6—H6A	0.9700	C18—N2	1.334 (2)
C6—H6B	0.9700	C18—H18	0.9300
C7—O1	1.380 (2)	Cu1—N2^{i}	2.0153 (16)
C7—C12	1.383 (3)	Cu1—N2^{ii}	2.0153 (16)
C7—C8	1.386 (3)	Cu1—N1	2.0669 (16)
C8—C9	1.389 (3)	Cu1—N1^{iii}	2.0669 (16)
C8—H8	0.9300	Cu1—O3	2.5460 (15)
C9—C10	1.383 (3)	N2—Cu1^{iv}	2.0153 (16)
C9—H9	0.9300	N3—O4	1.226 (7)
C10—O2	1.380 (2)	N3—O5	1.229 (2)
C10—C11	1.382 (3)	N3—O4'	1.253 (8)
C11—C12	1.389 (3)	N3—O3	1.259 (2)
C11—H11	0.9300	O4—O4'	0.773 (8)
C12—H12	0.9300		
N1—C1—C2	122.43 (18)	H13A—C13—H13B	108.7
N1—C1—H1	118.8	C18—C14—C15	117.88 (17)
C2—C1—H1	118.8	C18—C14—C13	118.12 (17)
C1—C2—C3	119.7 (2)	C15—C14—C13	124.00 (18)
C1—C2—H2	120.1	C16—C15—C14	118.58 (19)
C3—C2—H2	120.1	C16—C15—H15	120.7
C2—C3—C4	118.72 (18)	C14—C15—H15	120.7
C2—C3—H3	120.6	C17—C16—C15	120.29 (18)
C4—C3—H3	120.6	C17—C16—H16	119.9
C3—C4—C5	118.58 (17)	C15—C16—H16	119.9
C3—C4—C6	122.69 (17)	N2—C17—C16	121.55 (17)
C5—C4—C6	118.65 (18)	N2—C17—H17	119.2
N1—C5—C4	123.05 (19)	C16—C17—H17	119.2
N1—C5—H5	118.5	N2—C18—C14	123.85 (17)
C4—C5—H5	118.5	N2—C18—H18	118.1
O1—C6—C4	107.81 (17)	C14—C18—H18	118.1
O1—C6—H6A	110.1	N2^{i}—Cu1—N2^{ii}	180.000 (1)
C4—C6—H6A	110.1	N2^{i}—Cu1—N1	89.35 (6)

O1—C6—H6B	110.1	$N2^{ii}$—Cu1—N1	90.65 (6)
C4—C6—H6B	110.1	$N2^{i}$—Cu1—$N1^{iii}$	90.65 (6)
H6A—C6—H6B	108.5	$N2^{ii}$—Cu1—$N1^{iii}$	89.35 (6)
O1—C7—C12	124.94 (18)	N1—Cu1—$N1^{iii}$	180.000 (1)
O1—C7—C8	115.08 (18)	$N2^{i}$—Cu1—O3	86.22 (6)
C12—C7—C8	119.98 (17)	$N2^{ii}$—Cu1—O3	93.78 (6)
C7—C8—C9	120.21 (19)	N1—Cu1—O3	92.59 (6)
C7—C8—H8	119.9	$N1^{iii}$—Cu1—O3	87.41 (6)
C9—C8—H8	119.9	C1—N1—C5	117.48 (16)
C10—C9—C8	119.67 (18)	C1—N1—Cu1	118.31 (12)
C10—C9—H9	120.2	C5—N1—Cu1	123.96 (13)
C8—C9—H9	120.2	C18—N2—C17	117.81 (16)
O2—C10—C11	114.98 (18)	C18—N2—$Cu1^{iv}$	118.98 (12)
O2—C10—C9	124.83 (18)	C17—N2—$Cu1^{iv}$	123.21 (13)
C11—C10—C9	120.18 (17)	O4—N3—O5	118.1 (5)
C10—C11—C12	120.20 (19)	O4—N3—O4'	36.3 (4)
C10—C11—H11	119.9	O5—N3—O4'	118.6 (4)
C12—C11—H11	119.9	O4—N3—O3	119.1 (5)
C7—C12—C11	119.76 (19)	O5—N3—O3	120.22 (18)
C7—C12—H12	120.1	O4'—N3—O3	117.2 (5)
C11—C12—H12	120.1	C7—O1—C6	117.53 (16)
O2—C13—C14	106.10 (16)	C10—O2—C13	117.89 (16)
O2—C13—H13A	110.5	N3—O3—Cu1	134.44 (13)
C14—C13—H13A	110.5	O4'—O4—N3	73.8 (10)
O2—C13—H13B	110.5	O4—O4'—N3	69.9 (10)
C14—C13—H13B	110.5		

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

Fig. 1

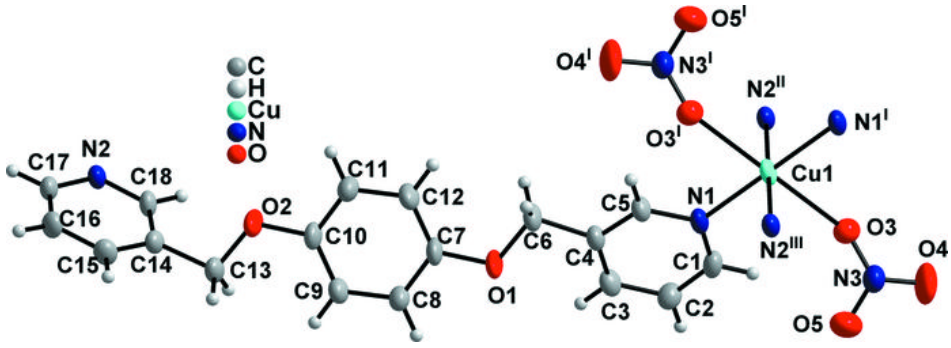
C
H
Cu
N
O
O5I
O4I
N3I
N2II
N1I
O3I
Cu1
C17
N2
C18
C16
C15
C14
C13
O2
C11
C12
C10
C7
C9
C8
O1
C6
C5
N1
C4
C1
C3
C2
O3
O4
N3
O5
N2III

Fig. 2