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catena-Poly[[bis(nitrato-κO)copper(II)]-μ-1,4-bis(4,5-dihydro-1,3-oxazol-2-yl)-benzene-$\kappa^2 N:N'$]

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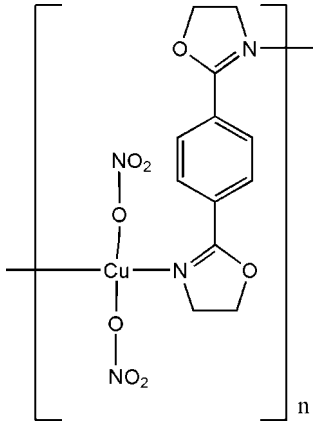
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.034; wR factor = 0.095; data-to-parameter ratio = 9.8.

In the title coordination polymer, $[Cu(NO_3)_2(C_{12}H_{12}N_2O_2)]_n$, the Cu^{II} ion, situated on an inversion center, is coordinated by two O atoms from two nitrate anions and two N atoms from two 1,4-bis(4,5-dihydro-1,3-oxazol-2-yl)benzene (L) ligands in a distorted square-planar geometry. Each L ligand also lies across an inversion center and bridges two Cu^{II} ions, forming a polymeric chain running along the [101] direction. The three O atoms of the nitrate group are disordered over two positions in a 3:2 ratio.

Related literature

For background to coordination polymers with organic ligands, see: Kitagawa *et al.* (2004). For related structures, see: Wang *et al.* (2008).



Experimental

Crystal data

$[Cu(NO_3)_2(C_{12}H_{12}N_2O_2)]$
M_r = 403.80
Triclinic, $P\overline{1}$
a = 6.5240 (8) Å
b = 7.5852 (8) Å
c = 8.3161 (8) Å
α = 90.393 (2)°
β = 103.556 (2)°
γ = 114.314 (2)°
V = 362.09 (7) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.56 mm^{-1}
T = 297 K
0.56 × 0.52 × 0.31 mm

Data collection

Bruker SMART 1000 diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.433, T_{max} = 0.616
2053 measured reflections
1392 independent reflections
1384 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.095
S = 1.08
1392 reflections
142 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu—N1	1.971 (2)	Cu—O3′	1.994 (6)
Cu—O2	2.005 (5)		

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT* and *SHELXTL* (Sheldrick, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2009); 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: XU5198).

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S1. Comment

The synthesis of metal coordination polymers has been a subject of intense research due to their interesting structural chemistry and potential applications in gas storage, separation, catalysis, magnetism, luminescence, and drug delivery (Kitagawa *et al.*, 2004). The Ag^{I} complexes containing 1,4-bis(4,5-dihydro-2-oxazolyl)benzene ligands has been reported, which show various two-dimensional networks (Wang *et al.*, 2008). The Cu···Cu distance separated by the bridging ligands is 9.289 (1) Å, while the ligands adopt the *anti* conformation in the structure. The 1-D chain of the title compound forms 3-D supramolecular structure which is interlinked by nitrate anions through C–H···O hydrogen bonds.

S2. Experimental

An aqueous solution (5.0 ml) of copper nitrate (1.0 mmol) was layered carefully over a methanolic solution (5.0 ml) of 1,4-bis(4,5-dihydro-2-oxazolyl)benzene (1.0 mmol) in a tube. Blue crystals were obtained after several weeks. These were washed with methanol and collected in 55.0% yield.

S3. Refinement

H atoms were constrained to ideal geometries, with C—H = 0.93 (phenyl) or 0.97 (methylene) Å and U_{iso}(H) = 1.2U_{eq}(C). The O atoms of the nitrate group are disordered over two positions in a 3:2 ratio in the structure.

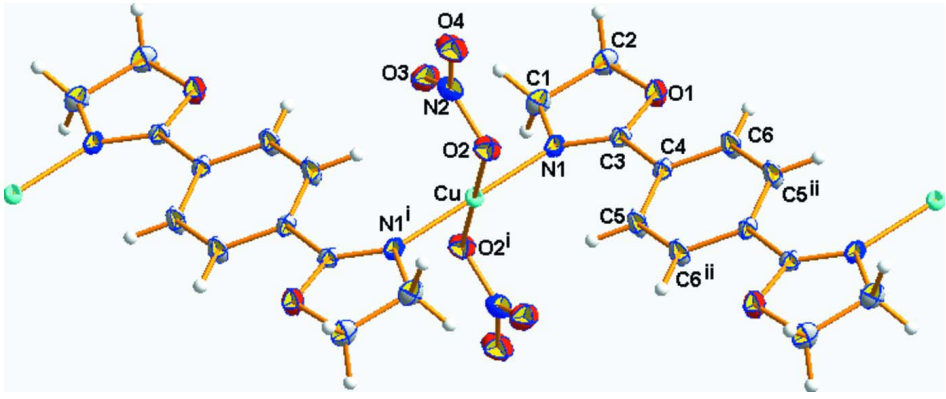

Figure 1

A portion of the chain structure. Ellipsoids are drawn at 30% probability level, and H atoms of spheres of arbitrary radius. Symmetry codes: (i) 1 - *x*, 1 - *y*, 1 - *z*; (ii) -*x*, 1 - *y*, -*z*. The disorder is not shown for clarity.

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Crystal data

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$\alpha = 90.393$ (2)°
$\beta = 103.556$ (2)°
$\gamma = 114.314$ (2)°
$V = 362.09$ (7) Å^3
$Z = 1$
$F(000) = 205$
$D_x = 1.852$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1976 reflections
$\theta = 2.5$–$26.0°$
$\mu = 1.56$ mm^{-1}
$T = 297$ K
Parallelepiped, blue
0.56 × 0.52 × 0.31 mm

Data collection

Bruker SMART 1000 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min} = 0.433$, $T_{max} = 0.616$
2053 measured reflections
1392 independent reflections
1384 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.5°$
$h = -8 \rightarrow 7$
$k = -8 \rightarrow 9$
$l = -7 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.095$
$S = 1.08$
1392 reflections
142 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0698P)^2 + 0.1776P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ 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)
Cu	0.5000	0.5000	0.5000	0.02820 (18)	
N1	0.5908 (3)	0.6368 (3)	0.3097 (2)	0.0301 (4)	
N2	0.5360 (5)	0.1919 (3)	0.3813 (3)	0.0423 (5)	

O1	0.6228 (3)	0.7793 (3)	0.0775 (2)	0.0392 (4)	
O2	0.6917 (12)	0.3558 (9)	0.4788 (8)	0.0408 (11)	0.60
O3	0.3378 (13)	0.1675 (8)	0.3452 (9)	0.0520 (14)	0.60
O4	0.6161 (11)	0.0764 (7)	0.3539 (7)	0.0586 (12)	0.60
O2′	0.719 (2)	0.3108 (16)	0.4449 (13)	0.050 (2)	0.40
O3′	0.3542 (17)	0.2391 (10)	0.3667 (12)	0.0364 (15)	0.40
O4′	0.4801 (17)	0.0347 (11)	0.2945 (10)	0.0634 (19)	0.40
C1	0.8447 (4)	0.7532 (4)	0.3336 (4)	0.0412 (6)	
H1A	0.9246	0.6695	0.3378	0.049*	
H1B	0.9119	0.8426	0.4353	0.049*	
C2	0.8593 (4)	0.8615 (4)	0.1836 (4)	0.0423 (6)	
H2A	0.9139	0.9999	0.2149	0.051*	
H2B	0.9643	0.8423	0.1273	0.051*	
C3	0.4874 (4)	0.6623 (3)	0.1666 (3)	0.0282 (4)	
C4	0.2358 (4)	0.5773 (3)	0.0837 (3)	0.0281 (4)	
C5	0.0729 (4)	0.4320 (4)	0.1458 (3)	0.0430 (6)	
H5A	0.1211	0.3858	0.2442	0.052*	
C6	0.1608 (4)	0.6452 (4)	−0.0632 (3)	0.0398 (6)	
H6A	0.2687	0.7432	−0.1060	0.048*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu	0.0260 (2)	0.0278 (2)	0.0279 (2)	0.01314 (17)	−0.00148 (15)	0.00318 (15)
N1	0.0231 (9)	0.0304 (10)	0.0319 (10)	0.0115 (8)	−0.0019 (7)	−0.0001 (7)
N2	0.0527 (16)	0.0355 (11)	0.0466 (13)	0.0223 (11)	0.0206 (11)	0.0115 (10)
O1	0.0270 (8)	0.0490 (10)	0.0338 (9)	0.0097 (7)	0.0056 (7)	0.0101 (8)
O2	0.036 (2)	0.038 (3)	0.050 (3)	0.0199 (18)	0.0077 (18)	0.005 (2)
O3	0.042 (3)	0.046 (4)	0.058 (3)	0.016 (3)	−0.0003 (19)	0.000 (3)
O4	0.088 (3)	0.049 (3)	0.062 (3)	0.045 (3)	0.031 (3)	0.013 (2)
O2′	0.042 (4)	0.056 (6)	0.055 (5)	0.028 (4)	0.005 (3)	0.009 (4)
O3′	0.035 (3)	0.025 (4)	0.044 (3)	0.012 (3)	0.000 (2)	−0.001 (3)
O4′	0.102 (6)	0.042 (3)	0.064 (5)	0.044 (4)	0.028 (4)	0.000 (3)
C1	0.0231 (11)	0.0453 (14)	0.0454 (14)	0.0103 (10)	−0.0007 (10)	0.0027 (11)
C2	0.0241 (11)	0.0472 (14)	0.0461 (14)	0.0084 (10)	0.0047 (10)	0.0041 (11)
C3	0.0254 (11)	0.0286 (10)	0.0288 (11)	0.0118 (8)	0.0036 (8)	0.0011 (8)
C4	0.0254 (10)	0.0317 (11)	0.0241 (10)	0.0122 (9)	0.0008 (8)	0.0013 (8)
C5	0.0308 (12)	0.0513 (15)	0.0354 (13)	0.0117 (11)	−0.0018 (10)	0.0199 (11)
C6	0.0272 (12)	0.0457 (14)	0.0354 (13)	0.0074 (10)	0.0028 (9)	0.0170 (11)

Geometric parameters (Å, º)

Cu—N1^{i}	1.971 (2)	O1—C3	1.337 (3)
Cu—N1	1.971 (2)	O1—C2	1.453 (3)
Cu—O2^{i}	2.005 (5)	C1—C2	1.498 (4)
Cu—O2	2.005 (5)	C1—H1A	0.9700
Cu—O3′^{i}	1.994 (6)	C1—H1B	0.9700
Cu—O3′	1.994 (6)	C2—H2A	0.9700

N1—C3	1.282 (3)	C2—H2B	0.9700
N1—C1	1.484 (3)	C3—C4	1.476 (3)
N2—O2′	1.152 (12)	C4—C5	1.383 (3)
N2—O3	1.190 (8)	C4—C6	1.390 (3)
N2—O4	1.234 (5)	C5—C6^{ii}	1.381 (4)
N2—O4′	1.258 (7)	C5—H5A	0.9300
N2—O2	1.340 (7)	C6—C5^{ii}	1.381 (4)
N2—O3′	1.354 (10)	C6—H6A	0.9300

N1^{i}—Cu—N1	180.0	O4—N2—O3′	150.9 (5)
N1^{i}—Cu—O3′^{i}	92.7 (3)	O4′—N2—O3′	112.3 (6)
N1—Cu—O3′^{i}	87.3 (3)	O2—N2—O3′	94.6 (4)
N1^{i}—Cu—O3′	87.3 (3)	C3—O1—C2	106.60 (19)
N1—Cu—O3′	92.7 (3)	N2—O2—Cu	103.0 (4)
O3′^{i}—Cu—O3′	180.000 (1)	N2—O3′—Cu	103.0 (5)
N1^{i}—Cu—O2^{i}	88.6 (2)	N1—C1—C2	103.7 (2)
N1—Cu—O2^{i}	91.4 (2)	N1—C1—H1A	111.0
O3′^{i}—Cu—O2^{i}	59.4 (3)	C2—C1—H1A	111.0
O3′—Cu—O2^{i}	120.6 (3)	N1—C1—H1B	111.0
N1^{i}—Cu—O2	91.4 (2)	C2—C1—H1B	111.0
N1—Cu—O2	88.6 (2)	H1A—C1—H1B	109.0
O3′^{i}—Cu—O2	120.6 (3)	O1—C2—C1	104.80 (19)
O3′—Cu—O2	59.4 (3)	O1—C2—H2A	110.8
O2^{i}—Cu—O2	180.000 (2)	C1—C2—H2A	110.8
C3—N1—C1	107.4 (2)	O1—C2—H2B	110.8
C3—N1—Cu	137.12 (16)	C1—C2—H2B	110.8
C1—N1—Cu	115.40 (16)	H2A—C2—H2B	108.9
O2′—N2—O3	139.9 (5)	N1—C3—O1	116.8 (2)
O2′—N2—O4	91.9 (5)	N1—C3—C4	128.7 (2)
O3—N2—O4	128.1 (4)	O1—C3—C4	114.5 (2)
O2′—N2—O4′	129.2 (6)	C5—C4—C6	119.0 (2)
O3—N2—O4′	90.1 (6)	C5—C4—C3	122.5 (2)
O4—N2—O4′	39.0 (4)	C6—C4—C3	118.5 (2)
O2′—N2—O2	23.8 (4)	C6^{ii}—C5—C4	120.6 (2)
O3—N2—O2	117.1 (4)	C6^{ii}—C5—H5A	119.7
O4—N2—O2	114.4 (4)	C4—C5—H5A	119.7
O4′—N2—O2	152.8 (6)	C5^{ii}—C6—C4	120.4 (2)
O2′—N2—O3′	117.1 (5)	C5^{ii}—C6—H6A	119.8
O3—N2—O3′	22.9 (3)	C4—C6—H6A	119.8

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