Journal of the Korean Chemical Society
2018, *Vol. 62, No. 5*
Printed in the Republic of Korea
https://doi.org/10.5012/jkcs.2018.62.5.1

SUPPORTING INFORMATION

1D-Coordination Polymer Formed by Structural Conversion of an Oxazolidine Ligand in Reaction with the Copper(II) Halides

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(Received May 20, 2018; Accepted July 12, 2018)

Crystal data

$C_{12}H_8CuN_2O_4$	Z = 1
M_r = 307.75	F(000) = 155.00
Triclinic, $P\bar{1}$	D_x = 1.873 Mg m^{-3}
a = 5.1544 (11) Å	Mo $K\alpha$ radiation, λ = 0.71075 Å
b = 7.619 (2) Å	Cell parameters from 673 reflections
c = 8.093 (3) Å	θ = 2.7–31.1°
α = 66.79 (3)°	μ = 2.01 mm^{-1}
β = 73.86 (2)°	T = 173 K
γ = 71.63 (2)°	Prism, purple
V = 272.87 (15) Å^3	0.12 × 0.11 × 0.03 mm

Data collection

Rigaku SCX mini diffractometer	1025 reflections with $F^2 > 2.0\sigma$ (F^2)
Detector resolution: 13.653 pixels mm^{-1}	R_{int} = 0.069
ω scans	θ_{max} = 31.9°, θ_{min} = 2.8°
Absorption correction: multi-scan CrysAlisPro 1.171.38.43 (Rigaku Oxford Diffraction, 2015) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	h = -7→7
T_{min} = 0.373, T_{max} = 0.941	k = -11→11
3276 measured reflections	l = -11→11
1662 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.090	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.263	H-atom parameters constrained
S = 1.02	$w = 1/[\sigma^2(F_o^2) + (0.1517P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
1662 reflections	$(\Delta/\sigma)_{max} < 0.001$
88 parameters	$\Delta\rangle_{max}$ = 2.16 e Å^{-3}
0 restraints	$\Delta\rangle_{min}$ = −1.56 e Å^{-3}
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

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

	x	y	z	U_{iso}*/U_{eq}
Cu1	1.0000	0.5000	0.5000	0.0334 (4)
O2	0.7135 (8)	0.6328 (7)	0.3485 (6)	0.0331 (10)
O3	0.2697 (9)	0.7986 (7)	0.3608 (7)	0.0380 (11)
N1	0.7365 (10)	0.6319 (8)	0.6657 (8)	0.0328 (12)
C1	0.5030 (12)	0.7395 (9)	0.6012 (9)	0.0309 (13)
C2	0.4863 (12)	0.7250 (9)	0.4235 (9)	0.0319 (14)
C4	0.2927 (12)	0.8526 (10)	0.6949 (10)	0.0350 (15)
H4	0.1264	0.9280	0.6488	0.042*
C5	0.3355 (14)	0.8506 (11)	0.8563 (11)	0.0415 (16)
H5	0.1986	0.9283	0.9214	0.050*
C6	0.5738 (15)	0.7376 (12)	0.9242 (11)	0.0433 (17)
H6	0.6026	0.7321	1.0373	0.052*
C7	0.7714 (13)	0.6313 (10)	0.8204 (10)	0.0355 (14)
H7	0.9395	0.5548	0.8637	0.043*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0154 (5)	0.0391 (7)	0.0488 (8)	0.0058 (4)	-0.0121 (4)	-0.0230 (6)
O2	0.0165 (18)	0.037 (2)	0.045 (3)	0.0055 (16)	-0.0126 (17)	-0.018 (2)
O3	0.0199 (19)	0.040 (3)	0.055 (3)	0.0052 (18)	-0.0150 (19)	-0.021 (2)
N1	0.017 (2)	0.039 (3)	0.045 (3)	0.000 (2)	-0.007 (2)	-0.020 (2)
C1	0.017 (2)	0.026 (3)	0.049 (4)	-0.002 (2)	-0.007 (2)	-0.014 (3)
C2	0.018 (2)	0.030 (3)	0.046 (4)	0.000 (2)	-0.011 (2)	-0.011 (3)
C4	0.017 (2)	0.029 (3)	0.052 (4)	0.000 (2)	-0.005 (2)	-0.011 (3)
C5	0.030 (3)	0.041 (4)	0.052 (4)	-0.007 (3)	0.003 (3)	-0.023 (3)
C6	0.032 (3)	0.053 (5)	0.049 (4)	-0.010 (3)	-0.002 (3)	-0.025 (4)
C7	0.024 (3)	0.038 (4)	0.043 (4)	-0.005 (2)	-0.007 (2)	-0.012 (3)

Geometric parameters (Å, º)

Cu1—O2^i	1.948 (4)	C1—C2	1.513 (10)
Cu1—O2	1.948 (4)	C4—C5	1.377 (11)
Cu1—N1	1.960 (5)	C4—H4	0.9500
Cu1—N1^i	1.960 (5)	C5—C6	1.374 (11)
O2—C2	1.287 (8)	C5—H5	0.9500
O3—C2	1.231 (7)	C6—C7	1.392 (10)
N1—C7	1.312 (9)	C6—H6	0.9500

N1—C1	1.335 (8)	C7—H7	0.9500
C1—C4	1.401 (9)		
$O2^{i}$—Cu1—O2	180.0	O3—C2—C1	120.7 (5)
$O2^{i}$—Cu1—N1	96.6 (2)	O2—C2—C1	114.3 (5)
O2—Cu1—N1	83.4 (2)	C5—C4—C1	117.7 (6)
$O2^{i}$—Cu1—$N1^{i}$	83.4 (2)	C5—C4—H4	121.2
O2—Cu1—$N1^{i}$	96.6 (2)	C1—C4—H4	121.2
N1—Cu1—$N1^{i}$	180.0	C6—C5—C4	120.8 (6)
C2—O2—Cu1	114.7 (4)	C6—C5—H5	119.6
C7—N1—C1	119.6 (6)	C4—C5—H5	119.6
C7—N1—Cu1	127.8 (4)	C5—C6—C7	117.2 (7)
C1—N1—Cu1	112.5 (5)	C5—C6—H6	121.4
N1—C1—C4	121.6 (6)	C7—C6—H6	121.4
N1—C1—C2	114.4 (5)	N1—C7—C6	123.1 (6)
C4—C1—C2	124.0 (6)	N1—C7—H7	118.4
O3—C2—O2	125.1 (6)	C6—C7—H7	118.4
C7—N1—C1—C4	0.0 (10)	C4—C1—C2—O2	172.1 (6)
Cu1—N1—C1—C4	-177.1 (5)	N1—C1—C4—C5	0.5 (10)
C7—N1—C1—C2	-179.1 (6)	C2—C1—C4—C5	179.5 (6)
Cu1—N1—C1—C2	3.8 (7)	C1—C4—C5—C6	-1.5 (11)
Cu1—O2—C2—O3	-171.1 (5)	C4—C5—C6—C7	2.0 (11)
Cu1—O2—C2—C1	9.4 (7)	C1—N1—C7—C6	0.5 (11)
N1—C1—C2—O3	171.6 (6)	Cu1—N1—C7—C6	177.1 (5)
C4—C1—C2—O3	-7.5 (10)	C5—C6—C7—N1	-1.5 (11)
N1—C1—C2—O2	-8.9 (9)		

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

Crystal data

$C_{12}H_8CuN_2O_4$	$Z = 1$
$M_r = 307.75$	$F(000) = 155.00$
Triclinic, $P\bar{1}$	$D_x = 1.893$ Mg m^{-3}
$a = 5.1553$ (4) Å	Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
$b = 7.5399$ (14) Å	Cell parameters from 2933 reflections
$c = 8.0711$ (12) Å	$\theta = 2.8$–$28.0°$
$\alpha = 66.927$ (16)°	$\mu = 2.03$ mm^{-1}
$\beta = 73.928$ (10)°	$T = 93$ K
$\gamma = 71.883$ (11)°	Prism, purple
$V = 269.98$ (8) Å^3	0.18 × 0.09 × 0.09 mm

Data collection

Rigaku XtaLAB P200 diffractometer	$R_{int} = 0.350$
Detector resolution: 5.811 pixels mm^{-1}	$\theta_{max} = 28.3°$, $\theta_{min} = 2.8°$
ω scans	$h = -6 \rightarrow 6$
4641 measured reflections	$k = -9 \rightarrow 9$
1167 independent reflections	$l = -10 \rightarrow 10$
1068 reflections with $F^2 > 2.0\sigma(F^2)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.119$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.290$	H-atom parameters constrained
$S = 1.15$	$w = 1/[\sigma^2(F_o^2) + (0.2P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
1167 reflections	$(\Delta/\sigma)_{max} < 0.001$
88 parameters	$\Delta\rangle_{max} = 2.26$ e Å^{-3}
0 restraints	$\Delta\rangle_{min} = -2.39$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

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

	x	y	z	U_{iso}*/U_{eq}
Cu1	1.0000	0.5000	0.5000	0.0200 (6)
O2	0.7089 (10)	0.6356 (7)	0.3504 (8)	0.0221 (11)
O3	0.2690 (11)	0.8009 (8)	0.3654 (8)	0.0259 (12)
N1	0.7360 (12)	0.6325 (9)	0.6676 (8)	0.0200 (12)
C1	0.5024 (15)	0.7405 (11)	0.6054 (10)	0.0209 (14)
C2	0.4863 (16)	0.7269 (10)	0.4243 (10)	0.0224 (15)
C3	0.2958 (16)	0.8505 (11)	0.6974 (13)	0.0271 (17)
H3	0.1286	0.9243	0.6522	0.032*
C4	0.3412 (15)	0.8499 (11)	0.8625 (12)	0.0253 (16)
H4	0.2045	0.9274	0.9285	0.030*
C5	0.5803 (17)	0.7386 (12)	0.9282 (11)	0.0277 (17)
H5	0.6097	0.7345	1.0409	0.033*
C6	0.7792 (15)	0.6316 (11)	0.8246 (11)	0.0227 (15)
H6	0.9489	0.5564	0.8659	0.027*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0156 (8)	0.0243 (8)	0.0267 (8)	0.0021 (5)	-0.0067 (5)	-0.0185 (6)
O2	0.015 (2)	0.026 (3)	0.031 (3)	0.002 (2)	-0.009 (2)	-0.018 (2)
O3	0.020 (3)	0.032 (3)	0.034 (3)	-0.002 (2)	-0.009 (2)	-0.019 (2)
N1	0.014 (3)	0.027 (3)	0.023 (3)	-0.002 (2)	-0.001 (2)	-0.017 (2)
C1	0.018 (3)	0.023 (3)	0.025 (4)	-0.002 (3)	-0.004 (3)	-0.014 (3)
C2	0.025 (4)	0.021 (3)	0.027 (4)	-0.006 (3)	-0.003 (3)	-0.015 (3)
C3	0.019 (3)	0.022 (3)	0.046 (5)	0.000 (3)	-0.008 (3)	-0.019 (3)
C4	0.021 (4)	0.023 (3)	0.038 (4)	-0.004 (3)	-0.002 (3)	-0.020 (3)
C5	0.030 (4)	0.036 (4)	0.024 (4)	-0.010 (3)	0.000 (3)	-0.017 (3)
C6	0.023 (4)	0.022 (3)	0.031 (4)	-0.001 (3)	-0.004 (3)	-0.022 (3)

Geometric parameters (Å, º)

Cu1—O2^{i}	1.959 (5)	C1—C2	1.531 (10)
Cu1—O2	1.959 (5)	C3—C4	1.413 (12)
Cu1—N1	1.968 (6)	C3—H3	0.9500
Cu1—N1^{i}	1.968 (6)	C4—C5	1.369 (12)
O2—C2	1.264 (10)	C4—H4	0.9500
O3—C2	1.221 (10)	C5—C6	1.393 (11)
N1—C1	1.331 (10)	C5—H5	0.9500
N1—C6	1.343 (10)	C6—H6	0.9500
C1—C3	1.367 (12)		
O2^{i}—Cu1—O2	180.0	O3—C2—C1	119.3 (6)
O2^{i}—Cu1—N1	97.4 (2)	O2—C2—C1	114.3 (6)
O2—Cu1—N1	82.6 (2)	C1—C3—C4	117.3 (7)
O2^{i}—Cu1—N1^{i}	82.6 (2)	C1—C3—H3	121.4
O2—Cu1—N1^{i}	97.4 (2)	C4—C3—H3	121.4
N1—Cu1—N1^{i}	180.0 (3)	C5—C4—C3	120.6 (7)
C2—O2—Cu1	115.5 (5)	C5—C4—H4	119.7
C1—N1—C6	120.2 (6)	C3—C4—H4	119.7
C1—N1—Cu1	113.1 (5)	C4—C5—C6	117.9 (7)
C6—N1—Cu1	126.6 (5)	C4—C5—H5	121.0
N1—C1—C3	122.6 (7)	C6—C5—H5	121.0
N1—C1—C2	113.7 (6)	N1—C6—C5	121.4 (7)
C3—C1—C2	123.7 (7)	N1—C6—H6	119.3
O3—C2—O2	126.4 (7)	C5—C6—H6	119.3
C6—N1—C1—C3	-1.4 (11)	C3—C1—C2—O2	172.7 (6)
Cu1—N1—C1—C3	-177.5 (6)	N1—C1—C3—C4	1.5 (11)
C6—N1—C1—C2	179.5 (6)	C2—C1—C3—C4	-179.5 (6)
Cu1—N1—C1—C2	3.4 (7)	C1—C3—C4—C5	-1.7 (11)
Cu1—O2—C2—O3	-170.7 (6)	C3—C4—C5—C6	1.9 (11)
Cu1—O2—C2—C1	8.9 (7)	C1—N1—C6—C5	1.6 (11)
N1—C1—C2—O3	171.4 (6)	Cu1—N1—C6—C5	177.1 (5)
C3—C1—C2—O3	-7.6 (11)	C4—C5—C6—N1	-1.8 (10)
N1—C1—C2—O2	-8.2 (9)		

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