Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[chlorido(1,10-phenanthroline)copper(II)]-μ-{2-[(1*S*,3*S*)-3-acetyl-2,2-dimethylcyclobutyl]acetato}]

Shi-ying Ma[a]* and Yan-fei Li[b]

[a]Department of Chemistry and Environmental Sciences, Taishan University, 271021 Taian, Shandong, People's Republic of China, and [b]Department of Materials and Chemistry Engineering, Taishan University, 271021 Taian, Shandong, People's Republic of China
Correspondence e-mail: mashy910@163.com

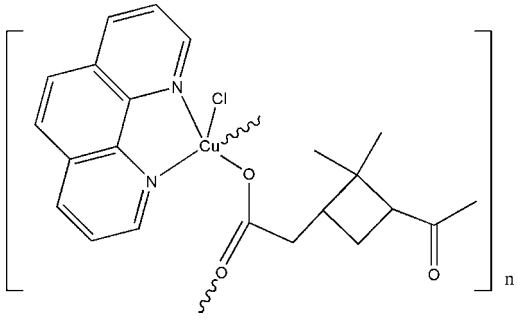
Received 27 October 2011; accepted 15 November 2011

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.036; wR factor = 0.097; data-to-parameter ratio = 13.8.

The title compound, $[Cu(C_{10}H_{15}O_3)Cl(C_{12}H_8N_2)]_n$, is a one-dimensional coordination polymer. The Cu^{II} atom is coordinated by a chloride ion, two N atoms from the 1,10-phenanthroline ligand, and a monodentate carboxylate O atom from the pinononate anion, forming a CuN_2ClO approximate square plane. A symmetry-generated pinononate O atom completes a square-based pyramidal geometry for the copper ion. The bridging 2-(3-acetyl-2,2-dimethylcyclobutyl)-acetate anion leads to chains in the crystal propagating in [001]. Adjacent 1,10-phenanthroline rings form a dihedral angle of 39.4 (2)°.

Related literature

For related structures, see: Che *et al.* (2006); Lalancette *et al.* (1999); Vanderhoff *et al.* (1986).



Experimental

Crystal data

$[Cu(C_{10}H_{15}O_3)Cl(C_{12}H_8N_2)]$
M_r = 462.41
Monoclinic, $P2_1/c$
a = 14.6143 (11) Å
b = 14.4920 (12) Å
c = 9.8419 (8) Å
β = 98.208 (1)°
V = 2063.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.21 mm^{-1}
T = 273 K
0.20 × 0.18 × 0.16 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Siemens, 1996)
T_{min} = 0.793, T_{max} = 0.829
10533 measured reflections
3647 independent reflections
2924 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.097
S = 1.03
3647 reflections
265 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1	1.937 (2)	Cu1—Cl1	2.2610 (8)
Cu1—N2	2.030 (2)	Cu1—O2^{i}	2.305 (2)
Cu1—N1	2.050 (2)		

Symmetry code: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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*.

This project was supported by the Postgraduate Foundation of Taishan University (No·Y07–2-14).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6482).

References

Che, G.-B., Xu, Z.-L. & Liu, C.-B. (2006). *Acta Cryst.* E**62**, m1695–m1696.
Lalancette, R. A., Thompson, H. W. & Brunskill, A. P. J. (1999). *Acta Cryst.* C**55**, 1908–1911.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1996). *SMART*, *SAINT* and *SADABS*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Vanderhoff, P. A., Thompson, H. W. & Lalancette, R. A. (1986). *Acta Cryst.* C**42**, 1766–1769.

supporting information

Acta Cryst. (2011). E**67**, m1789 [https://doi.org/10.1107/S1600536811048586]

catena-Poly[[chlorido(1,10-phenanthroline)copper(II)]-μ-{2-[(1*S*,3*S*)-3-acetyl-2,2-dimethylcyclobutyl]acetato}]

Shi-ying Ma and Yan-fei Li

S1. Comment

In the structural investigation of pinonate complexes, it has been found that the pinonic acid functions as a monodenate ligand (Lalancette *et al.*, 1999). We sythesized the pinonic acid that obtained from α-pinene oxidated by potassium permangate. In the present paper, we describe the crystal stucture of the title compound.The polymer molecule contains CuN_2O_2Cl square-based pyramids (Fig.1). The Cu(II) atom exists in a distorted square pyramidal enviroment,defined by two carboxyl O atoms from two monodentate pinonate ligand,two N atoms from 1,10-phenanthroline ligand and one Cl^- anion.

S2. Experimental

Pinonic acid is synthesized from α-pinene oxidated by potassium permangate.The pinonic acid (0.5 mmol)and NaOH (0.5 mmol) were dissolved in methanol (5 ml). A methanolic solution (5 ml) of $CuCl_2.H_2O$ (0.25 mmol) and 1,10-phenanthroline (0.25 mmol) was slowly droped to the solution of the pinonic acid with stirring.The result solution was flitered and allowed to stand in air at room temperature for seven days,yielding blue blocks of (I).

S3. Refinement

All H atoms were initially located in a difference Fourier map and were placed in geometrically idealized positions, with C—H = 0.93 - 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C).

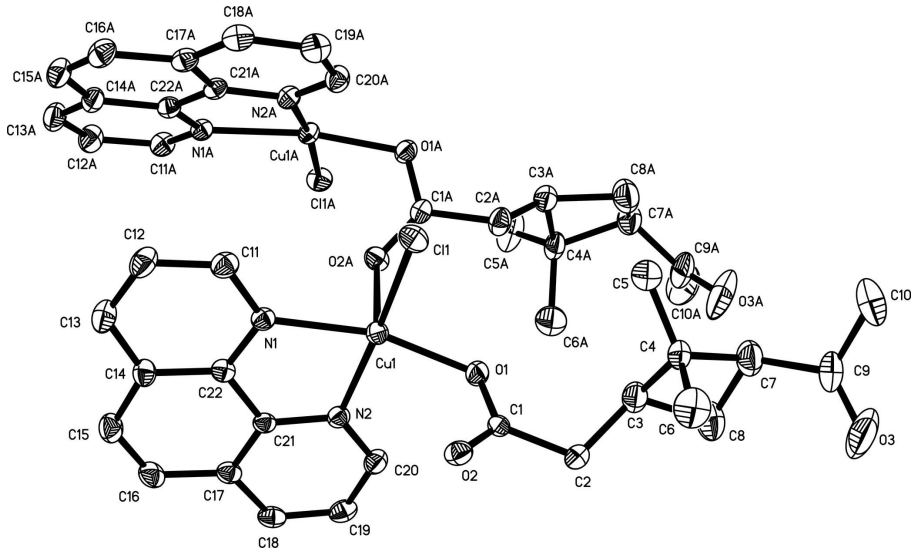


Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

***catena*-Poly[[chlorido(1,10-phenanthroline)copper(II)]-μ- {2-[(1*S*,3*S*)-3-acetyl-2,2-dimethylcyclobutyl]acetato}]**

Crystal data

$[Cu(C_{10}H_{15}O_3)Cl(C_{12}H_8N_2)]$
$M_r = 462.41$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 14.6143$ (11) Å
$b = 14.4920$ (12) Å
$c = 9.8419$ (8) Å
$\beta = 98.208$ (1)°
$V = 2063.1$ (3) Å^3
$Z = 4$
$F(000) = 956$
$D_x = 1.489$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3334 reflections
$\theta = 2.5$–25.1°
$\mu = 1.21$ mm^{-1}
$T = 273$ K
Block, blue
0.20 × 0.18 × 0.16 mm

Data collection

Siemens SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Siemens, 1996)
$T_{min} = 0.793$, $T_{max} = 0.829$
10533 measured reflections
3647 independent reflections
2924 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 25.1°$, $\theta_{min} = 1.4°$
$h = -15 \rightarrow 17$
$k = -17 \rightarrow 14$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.097$
$S = 1.03$
3647 reflections
265 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

$w = 1/[\sigma^2(F_o^2) + (0.0467P)^2 + 1.5378P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.67$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.38042 (2)	0.23582 (2)	0.56377 (4)	0.02863 (13)
Cl1	0.34460 (5)	0.08697 (5)	0.51189 (8)	0.0398 (2)
O1	0.26729 (14)	0.25754 (14)	0.6401 (2)	0.0347 (5)
O2	0.33639 (14)	0.21019 (14)	0.8438 (2)	0.0355 (5)
O3	−0.1289 (3)	0.1493 (3)	0.8971 (5)	0.1157 (15)
N1	0.51618 (16)	0.22377 (16)	0.5353 (2)	0.0289 (5)
N2	0.42648 (16)	0.36312 (16)	0.6269 (2)	0.0295 (5)
C1	0.26816 (19)	0.24062 (19)	0.7671 (3)	0.0279 (6)
C2	0.1786 (2)	0.2630 (2)	0.8208 (3)	0.0397 (8)
H2A	0.1808	0.2364	0.9116	0.048*
H2B	0.1739	0.3294	0.8298	0.048*
C3	0.0939 (2)	0.2285 (2)	0.7320 (4)	0.0461 (8)
H3	0.0985	0.2437	0.6362	0.055*
C4	0.0640 (2)	0.1255 (3)	0.7399 (3)	0.0435 (8)
C5	0.0936 (3)	0.0622 (3)	0.6319 (5)	0.0767 (14)
H5A	0.1598	0.0615	0.6401	0.115*
H5B	0.0683	0.0842	0.5423	0.115*
H5C	0.0714	0.0010	0.6447	0.115*
C6	0.0917 (3)	0.0859 (3)	0.8825 (4)	0.0663 (11)
H6A	0.0653	0.0256	0.8872	0.099*
H6B	0.0695	0.1255	0.9489	0.099*
H6C	0.1578	0.0817	0.9016	0.099*
C7	−0.0376 (2)	0.1627 (3)	0.7195 (4)	0.0574 (10)
H7	−0.0622	0.1633	0.6214	0.069*
C8	−0.0020 (3)	0.2584 (3)	0.7638 (5)	0.0651 (11)
H8A	−0.0037	0.2718	0.8600	0.078*
H8B	−0.0299	0.3079	0.7057	0.078*
C9	−0.1054 (3)	0.1142 (3)	0.7988 (5)	0.0697 (12)
C10	−0.1413 (3)	0.0230 (4)	0.7437 (6)	0.0972 (18)
H10A	−0.1668	−0.0102	0.8139	0.146*

H10B	−0.0916	−0.0121	0.7153	0.146*
H10C	−0.1884	0.0326	0.6665	0.146*
C11	0.5589 (2)	0.1529 (2)	0.4869 (3)	0.0375 (7)
H11	0.5255	0.0995	0.4619	0.045*
C12	0.6521 (2)	0.1559 (2)	0.4722 (4)	0.0451 (8)
H12	0.6801	0.1048	0.4383	0.054*
C13	0.7023 (2)	0.2334 (2)	0.5073 (4)	0.0458 (8)
H13	0.7645	0.2358	0.4968	0.055*
C14	0.6600 (2)	0.3100 (2)	0.5596 (3)	0.0357 (7)
C15	0.7052 (2)	0.3956 (2)	0.5989 (3)	0.0435 (8)
H15	0.7678	0.4019	0.5929	0.052*
C16	0.6593 (2)	0.4668 (2)	0.6442 (3)	0.0411 (8)
H16	0.6907	0.5214	0.6695	0.049*
C17	0.5629 (2)	0.4600 (2)	0.6541 (3)	0.0330 (7)
C18	0.5098 (2)	0.5331 (2)	0.6977 (3)	0.0370 (7)
H18	0.5367	0.5901	0.7208	0.044*
C19	0.4190 (2)	0.5183 (2)	0.7050 (3)	0.0406 (8)
H19	0.3831	0.5656	0.7336	0.049*
C20	0.3791 (2)	0.4324 (2)	0.6697 (3)	0.0367 (7)
H20	0.3169	0.4236	0.6765	0.044*
C21	0.51761 (19)	0.37713 (19)	0.6199 (3)	0.0275 (6)
C22	0.56575 (19)	0.3011 (2)	0.5705 (3)	0.0295 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0292 (2)	0.0275 (2)	0.0297 (2)	−0.00360 (15)	0.00622 (14)	−0.00034 (15)
Cl1	0.0446 (5)	0.0285 (4)	0.0455 (5)	−0.0070 (3)	0.0040 (4)	−0.0003 (3)
O1	0.0312 (11)	0.0448 (13)	0.0287 (11)	−0.0034 (9)	0.0060 (9)	0.0014 (9)
O2	0.0377 (12)	0.0373 (12)	0.0309 (12)	0.0077 (9)	0.0032 (9)	−0.0031 (9)
O3	0.109 (3)	0.110 (3)	0.152 (4)	−0.012 (2)	0.098 (3)	−0.022 (3)
N1	0.0325 (13)	0.0249 (13)	0.0299 (13)	−0.0009 (10)	0.0064 (10)	−0.0007 (10)
N2	0.0319 (13)	0.0291 (13)	0.0285 (13)	−0.0023 (11)	0.0074 (10)	−0.0016 (10)
C1	0.0291 (15)	0.0235 (15)	0.0319 (16)	−0.0071 (12)	0.0071 (13)	−0.0064 (12)
C2	0.0345 (17)	0.051 (2)	0.0347 (18)	−0.0008 (15)	0.0101 (13)	−0.0085 (15)
C3	0.0356 (18)	0.060 (2)	0.044 (2)	−0.0002 (16)	0.0080 (15)	0.0042 (17)
C4	0.0289 (17)	0.058 (2)	0.045 (2)	−0.0049 (15)	0.0095 (14)	−0.0051 (17)
C5	0.058 (3)	0.095 (3)	0.082 (3)	−0.023 (2)	0.026 (2)	−0.043 (3)
C6	0.067 (3)	0.061 (3)	0.071 (3)	0.004 (2)	0.012 (2)	0.010 (2)
C7	0.0360 (19)	0.075 (3)	0.061 (2)	−0.0026 (19)	0.0078 (17)	0.004 (2)
C8	0.042 (2)	0.066 (3)	0.088 (3)	0.0026 (19)	0.011 (2)	0.007 (2)
C9	0.039 (2)	0.090 (3)	0.085 (3)	−0.013 (2)	0.026 (2)	−0.003 (3)
C10	0.065 (3)	0.107 (4)	0.122 (5)	−0.044 (3)	0.023 (3)	−0.006 (3)
C11	0.0436 (18)	0.0303 (17)	0.0400 (18)	−0.0009 (14)	0.0106 (14)	−0.0020 (14)
C12	0.0455 (19)	0.0368 (19)	0.057 (2)	0.0080 (16)	0.0200 (17)	−0.0022 (16)
C13	0.0365 (18)	0.045 (2)	0.059 (2)	0.0019 (16)	0.0186 (16)	0.0034 (17)
C14	0.0311 (16)	0.0359 (17)	0.0411 (18)	−0.0034 (14)	0.0089 (13)	0.0024 (14)
C15	0.0353 (18)	0.045 (2)	0.052 (2)	−0.0086 (15)	0.0119 (15)	0.0008 (16)

C16	0.0419 (18)	0.0379 (19)	0.0434 (19)	−0.0153 (15)	0.0062 (15)	−0.0018 (15)
C17	0.0392 (17)	0.0322 (17)	0.0272 (16)	−0.0054 (13)	0.0040 (13)	0.0002 (13)
C18	0.050 (2)	0.0267 (16)	0.0332 (17)	−0.0053 (14)	0.0038 (14)	−0.0042 (13)
C19	0.052 (2)	0.0323 (18)	0.0387 (19)	0.0045 (15)	0.0121 (15)	−0.0070 (14)
C20	0.0362 (17)	0.0362 (18)	0.0396 (18)	0.0023 (14)	0.0118 (14)	−0.0026 (14)
C21	0.0322 (15)	0.0284 (15)	0.0221 (15)	−0.0039 (12)	0.0044 (11)	−0.0008 (12)
C22	0.0325 (15)	0.0269 (15)	0.0289 (15)	−0.0020 (13)	0.0041 (12)	0.0011 (12)

Geometric parameters (Å, º)

Cu1—O1	1.937 (2)	C7—C9	1.519 (5)
Cu1—N2	2.030 (2)	C7—C8	1.523 (6)
Cu1—N1	2.050 (2)	C7—H7	0.9800
Cu1—Cl1	2.2610 (8)	C8—H8A	0.9700
Cu1—O2^{i}	2.305 (2)	C8—H8B	0.9700
O1—C1	1.272 (4)	C9—C10	1.496 (7)
O2—C1	1.242 (3)	C10—H10A	0.9600
O2—Cu1^{ii}	2.305 (2)	C10—H10B	0.9600
O3—C9	1.186 (5)	C10—H10C	0.9600
N1—C11	1.326 (4)	C11—C12	1.391 (4)
N1—C22	1.352 (4)	C11—H11	0.9300
N2—C20	1.322 (4)	C12—C13	1.360 (5)
N2—C21	1.359 (3)	C12—H12	0.9300
C1—C2	1.514 (4)	C13—C14	1.403 (4)
C2—C3	1.496 (5)	C13—H13	0.9300
C2—H2A	0.9700	C14—C22	1.403 (4)
C2—H2B	0.9700	C14—C15	1.431 (4)
C3—C8	1.541 (5)	C15—C16	1.342 (5)
C3—C4	1.559 (5)	C15—H15	0.9300
C3—H3	0.9800	C16—C17	1.430 (4)
C4—C5	1.513 (5)	C16—H16	0.9300
C4—C6	1.517 (5)	C17—C21	1.390 (4)
C4—C7	1.566 (5)	C17—C18	1.414 (4)
C5—H5A	0.9600	C18—C19	1.357 (4)
C5—H5B	0.9600	C18—H18	0.9300
C5—H5C	0.9600	C19—C20	1.398 (4)
C6—H6A	0.9600	C19—H19	0.9300
C6—H6B	0.9600	C20—H20	0.9300
C6—H6C	0.9600	C21—C22	1.430 (4)
O1—Cu1—N2	89.87 (9)	C9—C7—H7	109.7
O1—Cu1—N1	164.36 (9)	C8—C7—H7	109.7
N2—Cu1—N1	80.45 (9)	C4—C7—H7	109.7
O1—Cu1—Cl1	93.42 (6)	C7—C8—C3	88.2 (3)
N2—Cu1—Cl1	172.71 (7)	C7—C8—H8A	113.9
N1—Cu1—Cl1	94.89 (7)	C3—C8—H8A	113.9
O1—Cu1—O2^{i}	99.78 (8)	C7—C8—H8B	113.9
N2—Cu1—O2^{i}	90.84 (8)	C3—C8—H8B	113.9

N1—Cu1—O2^{i}	92.67 (8)	H8A—C8—H8B	111.1
Cl1—Cu1—O2^{i}	95.00 (6)	O3—C9—C10	123.2 (4)
C1—O1—Cu1	117.42 (18)	O3—C9—C7	120.5 (4)
C1—O2—Cu1^{ii}	122.84 (18)	C10—C9—C7	116.3 (4)
C11—N1—C22	118.1 (2)	C9—C10—H10A	109.5
C11—N1—Cu1	129.0 (2)	C9—C10—H10B	109.5
C22—N1—Cu1	112.83 (18)	H10A—C10—H10B	109.5
C20—N2—C21	117.7 (3)	C9—C10—H10C	109.5
C20—N2—Cu1	128.4 (2)	H10A—C10—H10C	109.5
C21—N2—Cu1	113.88 (18)	H10B—C10—H10C	109.5
O2—C1—O1	124.1 (3)	N1—C11—C12	122.1 (3)
O2—C1—C2	121.5 (3)	N1—C11—H11	118.9
O1—C1—C2	114.4 (3)	C12—C11—H11	118.9
C3—C2—C1	114.2 (3)	C13—C12—C11	120.0 (3)
C3—C2—H2A	108.7	C13—C12—H12	120.0
C1—C2—H2A	108.7	C11—C12—H12	120.0
C3—C2—H2B	108.7	C12—C13—C14	119.9 (3)
C1—C2—H2B	108.7	C12—C13—H13	120.1
H2A—C2—H2B	107.6	C14—C13—H13	120.1
C2—C3—C8	119.2 (3)	C22—C14—C13	116.3 (3)
C2—C3—C4	120.3 (3)	C22—C14—C15	118.6 (3)
C8—C3—C4	89.5 (3)	C13—C14—C15	125.0 (3)
C2—C3—H3	108.8	C16—C15—C14	121.6 (3)
C8—C3—H3	108.8	C16—C15—H15	119.2
C4—C3—H3	108.8	C14—C15—H15	119.2
C5—C4—C6	110.8 (4)	C15—C16—C17	120.9 (3)
C5—C4—C3	115.8 (3)	C15—C16—H16	119.6
C6—C4—C3	111.6 (3)	C17—C16—H16	119.6
C5—C4—C7	118.6 (3)	C21—C17—C18	117.2 (3)
C6—C4—C7	111.8 (3)	C21—C17—C16	118.9 (3)
C3—C4—C7	86.1 (3)	C18—C17—C16	123.9 (3)
C4—C5—H5A	109.5	C19—C18—C17	118.8 (3)
C4—C5—H5B	109.5	C19—C18—H18	120.6
H5A—C5—H5B	109.5	C17—C18—H18	120.6
C4—C5—H5C	109.5	C18—C19—C20	120.3 (3)
H5A—C5—H5C	109.5	C18—C19—H19	119.9
H5B—C5—H5C	109.5	C20—C19—H19	119.9
C4—C6—H6A	109.5	N2—C20—C19	122.4 (3)
C4—C6—H6B	109.5	N2—C20—H20	118.8
H6A—C6—H6B	109.5	C19—C20—H20	118.8
C4—C6—H6C	109.5	N2—C21—C17	123.6 (3)
H6A—C6—H6C	109.5	N2—C21—C22	115.8 (2)
H6B—C6—H6C	109.5	C17—C21—C22	120.6 (3)
C9—C7—C8	119.7 (4)	N1—C22—C14	123.6 (3)
C9—C7—C4	116.8 (3)	N1—C22—C21	117.0 (2)
C8—C7—C4	89.8 (3)	C14—C22—C21	119.4 (3)
N2—Cu1—O1—C1	−84.8 (2)	C4—C3—C8—C7	−19.2 (3)

N1—Cu1—O1—C1	−33.3 (4)	C8—C7—C9—O3	−1.9 (7)
Cl1—Cu1—O1—C1	88.70 (19)	C4—C7—C9—O3	104.6 (5)
O2^{i}—Cu1—O1—C1	−175.62 (19)	C8—C7—C9—C10	176.5 (4)
O1—Cu1—N1—C11	128.7 (3)	C4—C7—C9—C10	−76.9 (5)
N2—Cu1—N1—C11	−178.8 (3)	C22—N1—C11—C12	0.3 (4)
Cl1—Cu1—N1—C11	6.8 (3)	Cu1—N1—C11—C12	179.2 (2)
O2^{i}—Cu1—N1—C11	−88.4 (3)	N1—C11—C12—C13	−0.4 (5)
O1—Cu1—N1—C22	−52.3 (4)	C11—C12—C13—C14	0.6 (5)
N2—Cu1—N1—C22	0.14 (19)	C12—C13—C14—C22	−0.8 (5)
Cl1—Cu1—N1—C22	−174.20 (18)	C12—C13—C14—C15	−179.4 (3)
O2^{i}—Cu1—N1—C22	90.55 (19)	C22—C14—C15—C16	−0.6 (5)
O1—Cu1—N2—C20	−13.9 (3)	C13—C14—C15—C16	177.9 (3)
N1—Cu1—N2—C20	178.4 (3)	C14—C15—C16—C17	−0.4 (5)
Cl1—Cu1—N2—C20	−130.9 (5)	C15—C16—C17—C21	1.9 (5)
O2^{i}—Cu1—N2—C20	85.9 (3)	C15—C16—C17—C18	−178.3 (3)
O1—Cu1—N2—C21	167.71 (19)	C21—C17—C18—C19	0.7 (4)
N1—Cu1—N2—C21	0.05 (19)	C16—C17—C18—C19	−179.1 (3)
Cl1—Cu1—N2—C21	50.7 (6)	C17—C18—C19—C20	−0.1 (5)
O2^{i}—Cu1—N2—C21	−92.51 (19)	C21—N2—C20—C19	1.1 (4)
Cu1^{ii}—O2—C1—O1	137.8 (2)	Cu1—N2—C20—C19	−177.3 (2)
Cu1^{ii}—O2—C1—C2	−40.6 (3)	C18—C19—C20—N2	−0.8 (5)
Cu1—O1—C1—O2	−0.9 (4)	C20—N2—C21—C17	−0.5 (4)
Cu1—O1—C1—C2	177.59 (19)	Cu1—N2—C21—C17	178.1 (2)
O2—C1—C2—C3	−134.8 (3)	C20—N2—C21—C22	−178.8 (3)
O1—C1—C2—C3	46.7 (4)	Cu1—N2—C21—C22	−0.2 (3)
C1—C2—C3—C8	−171.3 (3)	C18—C17—C21—N2	−0.4 (4)
C1—C2—C3—C4	80.3 (4)	C16—C17—C21—N2	179.4 (3)
C2—C3—C4—C5	−97.2 (4)	C18—C17—C21—C22	177.9 (3)
C8—C3—C4—C5	138.7 (4)	C16—C17—C21—C22	−2.4 (4)
C2—C3—C4—C6	30.8 (4)	C11—N1—C22—C14	−0.6 (4)
C8—C3—C4—C6	−93.2 (3)	Cu1—N1—C22—C14	−179.6 (2)
C2—C3—C4—C7	142.8 (3)	C11—N1—C22—C21	178.8 (3)
C8—C3—C4—C7	18.7 (3)	Cu1—N1—C22—C21	−0.3 (3)
C5—C4—C7—C9	100.1 (5)	C13—C14—C22—N1	0.8 (5)
C6—C4—C7—C9	−30.8 (5)	C15—C14—C22—N1	179.5 (3)
C3—C4—C7—C9	−142.6 (4)	C13—C14—C22—C21	−178.5 (3)
C5—C4—C7—C8	−136.3 (4)	C15—C14—C22—C21	0.2 (4)
C6—C4—C7—C8	92.8 (4)	N2—C21—C22—N1	0.4 (4)
C3—C4—C7—C8	−19.0 (3)	C17—C21—C22—N1	−178.0 (3)
C9—C7—C8—C3	140.3 (4)	N2—C21—C22—C14	179.7 (3)
C4—C7—C8—C3	19.2 (3)	C17—C21—C22—C14	1.4 (4)
C2—C3—C8—C7	−144.2 (3)		

Symmetry codes: (i) x, $-y+1/2$, $z-1/2$; (ii) x, $-y+1/2$, $z+1/2$.