Acta Crystallographica Section E **Structure Reports** Online

ISSN 1600-5368

## Bis[(E)-4-bromo-2-(methoxyiminomethyl)phenolato- $\kappa^2 N_i O^1$ [copper(II)

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Received 5 November 2009; accepted 12 November 2009

Key indicators: single-crystal X-ray study; T = 298 K; mean  $\sigma$ (C–C) = 0.006 Å; R factor = 0.032; wR factor = 0.053; data-to-parameter ratio = 13.1.

In the title centrosymmetric mononuclear copper(II) complex, [Cu(C<sub>8</sub>H<sub>7</sub>BrNO<sub>2</sub>)<sub>2</sub>], the Cu<sup>II</sup> atom, lying on an inversion centre, is four-coordinated in a *trans*-CuN<sub>2</sub>O<sub>2</sub> square-planar geometry by two phenolate O atoms and two oxime N atoms from two symmetry-related N,O-bidentate oxime-type ligands. Intermolecular  $C-H \cdots O$  hydrogen bonds link neighbouring molecules into a one-dimensional supramolecular structure with an  $R_2^2(14)$  ring motif. This structure is further stabilized by  $\pi$ - $\pi$  stacking interactions between adjacent benzene rings [centroid–centroid distance = 3.862(1) Å].

### **Related literature**

For general background to oxime compounds, see: Chaudhuri (2003); Dong et al. (2007a, 2008). For related structures, see: Dong et al. (2007b, 2009). For the ligand synthesis, see: Wang et al. (2008); Zhao et al. (2009).



### **Experimental**

Crystal data  $[Cu(C_8H_7BrNO_2)_2]$  $M_r = 521.65$ Monoclinic, C2/c a = 24.691 (3) Å b = 3.8623 (5) Å c = 20.260 (2) Å  $\beta = 117.453 (2)^{\circ}$ 

V = 1714.4 (3) Å <sup>3</sup>
Z = 4
Mo $K\alpha$ radiation
$\mu = 5.96 \text{ mm}^{-1}$
T = 298  K
$0.40\times0.12\times0.11$ mm

# metal-organic compounds

#### Data collection

Siemens SMART 1000 CCD	3981 measured reflections
diffractometer	1521 independent reflections
Absorption correction: multi-scan	1128 reflections with $I > 2\sigma(I)$
(SADABS; Sheldrick, 1996)	$R_{\rm int} = 0.040$
$T_{\min} = 0.199, \ T_{\max} = 0.560$	

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$	116 parameters
$wR(F^2) = 0.053$	H-atom parameters constrained
S = 1.04	$\Delta \rho_{\rm max} = 0.54 \text{ e } \text{\AA}^{-3}$
1521 reflections	$\Delta \rho_{\rm min} = -0.40 \text{ e } \text{\AA}^{-3}$

#### Table 1

Selected bond lengths (Å).

Cu1-O2	1.910 (2)	Cu1-N1	2.000 (3)

### Table 2

Hydrogen-bond geometry (Å, °).

$D - H \cdot \cdot \cdot A$	$D-\mathrm{H}$	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$C1-H1C\cdotsO1^{i}$	0.96	2.52	3.328 (5)	142

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

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) and Mercury (Macrae et al., 2006); software used to prepare material for publication: SHELXTL.

This work was supported by the Foundation of the Education Department of Gansu Province (0904-11) and the 'Jing Lan' Talent Engineering Funds of Lanzhou Jiaotong University, which are gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2253).

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supplementary materials

Acta Cryst. (2009). E65, m1599 [doi:10.1107/S1600536809047989]

## Bis[(*E*)-4-bromo-2-(methoxyiminomethyl)phenolato- $\kappa^2 N, O^1$ ]copper(II)

### L.-Q. Chai, J. Yao and S.-S. Gong

### Comment

Oximes are a traditional class of chelating ligands widely used in coordination and analytical chemistry and extraction metallurgy (Chaudhuri, 2003; Dong *et al.*, 2007a,b, 2008, 2009). We report here the title mononuclear copper(II) complex with an oxime-type ligand.

The molecular structure of the title compound is shown in Fig. 1. The  $Cu^{II}$  ion, lying on an inversion centre is four-coordinated in a *trans*- $CuN_2O_2$  square-planar geometry, with two phenolate O atoms and two oxime N atoms from two N,Obidentate oxime-type ligands. Bond lengths and angles are within normal ranges (Table 1). The Cu—O and Cu—N bond lengths are 1.910 (2) Å and 2.000 (3) Å, respectively, which are slightly longer than those observed in a similar Schiff base copper(II) complex [the mean bond lengths of Cu—O and Cu—N are 1.894 (2) and 1.990 (3) Å] (Dong *et al.*, 2009).

In the crystal structure, intermolecular C1—H1C···O1 hydrogen bonds link neighbouring molecules into a one-dimensional supramolecular structure, with an  $R_2^2(14)$  ring motif (Table 2 and Fig. 2). The one-dimensional structure is further stabilized by weak  $\pi$ - $\pi$  stacking interactions between the adjacent benzene rings [centroid–centroid distance = 3.862 (1) Å] (Fig. 2).

### Experimental

(*E*)-5-Bromo-2-hydroxybenzaldehyde *O*-methyl oxime (H*L*) was synthesized according to an analogous method in literature (Wang *et al.*, 2008; Zhao *et al.*, 2009). A blue solution of copper(II) acetate monohydrate (1.7 mg, 0.008 mmol) in methanol (4 ml) was added dropwise to a solution of H*L* (4.1 mg, 0.016 mmol) in methanol (5 ml) at room temperature. The colour of the mixing solution turned to yellow immediately then turned to brown slowly. The mixture was allowed to stand at room temperature for several days. With evaporating of the solvent, dark-brown needle-like single crystals suitable for X-ray crystallographic analysis were obtained (yield 49.3%). IR: v(C=N) 1607, v(Ar—O) 1243, v(Cu—N) 447, v(Cu—O) 422 cm<sup>-1</sup>. Analysis, calculated for C<sub>16</sub>H<sub>14</sub>Br<sub>2</sub>CuN<sub>2</sub>O<sub>4</sub>: C 39.30, H 3.32, Cu 11.51, N 5.13%; found: C 39.21, H 3.39, Cu 11.64, N 4.85%.

### Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.96 (CH<sub>3</sub>) and 0.93 Å (CH) and with  $U_{iso}(H) = 1.2(1.5 \text{ for methyl})U_{eq}(C)$ .

Figures



Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted. [Symmetry code: (i) 1-x, 1-y, 1-z.]

Fig. 2. Packing diagram for the title compound, showing the one-dimensional supramolecular structure formed by intermolecular C—H···O hydrogen bonds (dashed lines) and  $\pi$ - $\pi$  stacking interactions (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry code: (ii) x, 1+y, z.]

### Bis[(*E*)-4-bromo-2-(methoxyiminomethyl)phenolato- $\kappa^2 N$ , $O^1$ ]copper(II)

Crystal data

[Cu(C<sub>8</sub>H<sub>7</sub>BrNO<sub>2</sub>)<sub>2</sub>]  $M_r = 521.65$ Monoclinic, C2/c Hall symbol: -C 2yc a = 24.691 (3) Å b = 3.8623 (5) Å c = 20.260 (2) Å  $\beta = 117.453$  (2)° V = 1714.4 (3) Å<sup>3</sup> Z = 4

### Data collection

Siemens SMART 1000 CCD diffractometer	1521 independent reflections
Radiation source: fine-focus sealed tube	1128 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\rm int} = 0.040$
<i>T</i> = 298 K	$\theta_{\text{max}} = 25.0^{\circ}$
$\phi$ and $\omega$ scans	$\theta_{\min} = 1.9^{\circ}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -21 \rightarrow 28$
$T_{\min} = 0.199, T_{\max} = 0.560$	$k = -4 \rightarrow 4$
3981 measured reflections	$l = -24 \rightarrow 23$

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

 $F_{000} = 1020$   $D_{\rm x} = 2.021 \text{ Mg m}^{-3}$ Mo K\alpha radiation, \lambda = 0.71073 Å Cell parameters from 1233 reflections  $\theta = 2.2-23.4^{\circ}$   $\mu = 5.96 \text{ mm}^{-1}$  T = 298 KNeedle-like, dark-brown  $0.40 \times 0.12 \times 0.11 \text{ mm}$ 

$R[F^2 > 2\sigma(F^2)] = 0.032$	H-atom parameters constrained
$wR(F^2) = 0.053$	$w = 1/[\sigma^2(F_0^2) + (0.0126P)^2]$ where $P = (F_0^2 + 2F_c^2)/3$
<i>S</i> = 1.04	$(\Delta/\sigma)_{max} < 0.001$
1521 reflections	$\Delta \rho_{max} = 0.54 \text{ e } \text{\AA}^{-3}$
116 parameters	$\Delta \rho_{min} = -0.40 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters  $(\hat{A}^2)$ 

	x	У	Ζ	$U_{\rm iso}*/U_{\rm eq}$
Cu1	0.5000	0.5000	0.5000	0.0478 (2)
Br1	0.169435 (18)	0.60817 (11)	0.35138 (2)	0.04703 (16)
N1	0.46014 (14)	0.4521 (8)	0.56593 (15)	0.0359 (8)
01	0.48859 (12)	0.2994 (7)	0.63799 (13)	0.0454 (7)
O2	0.43631 (11)	0.8108 (7)	0.43906 (13)	0.0459 (8)
C1	0.54119 (19)	0.4966 (11)	0.6868 (2)	0.0563 (13)
H1A	0.5672	0.5306	0.6638	0.084*
H1B	0.5632	0.3737	0.7328	0.084*
H1C	0.5284	0.7173	0.6964	0.084*
C2	0.40218 (17)	0.4722 (9)	0.54291 (19)	0.0353 (10)
H2	0.3870	0.3956	0.5747	0.042*
C3	0.35910 (16)	0.6052 (9)	0.47123 (18)	0.0303 (9)
C4	0.37870 (17)	0.7699 (10)	0.42340 (19)	0.0337 (10)
C5	0.33223 (17)	0.9004 (10)	0.35507 (19)	0.0357 (10)
H5	0.3434	1.0184	0.3232	0.043*
C6	0.27127 (17)	0.8574 (9)	0.33473 (19)	0.0358 (10)
H6	0.2418	0.9423	0.2894	0.043*
C7	0.25404 (16)	0.6861 (9)	0.3825 (2)	0.0308 (9)
C8	0.29692 (16)	0.5679 (9)	0.45035 (19)	0.0323 (9)
H8	0.2847	0.4628	0.4826	0.039*

Atomic displacement parameters  $(\text{\AA}^2)$ 

	$U^{11}$	$U^{22}$	U <sup>33</sup>	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.0365 (4)	0.0708 (6)	0.0413 (4)	0.0207 (4)	0.0224 (4)	0.0218 (4)
Br1	0.0330 (3)	0.0476 (3)	0.0530 (3)	-0.0031 (2)	0.0134 (2)	-0.0005 (2)
N1	0.035 (2)	0.044 (2)	0.0273 (18)	0.0067 (17)	0.0131 (15)	0.0089 (15)
O1	0.0378 (17)	0.057 (2)	0.0334 (15)	0.0074 (14)	0.0095 (13)	0.0140 (14)
O2	0.0311 (17)	0.064 (2)	0.0454 (16)	0.0148 (15)	0.0198 (13)	0.0245 (14)
C1	0.057 (3)	0.060 (3)	0.037 (2)	0.003 (2)	0.009 (2)	-0.001 (2)
C2	0.038 (3)	0.036 (3)	0.036 (2)	0.001 (2)	0.020 (2)	0.0039 (18)
C3	0.034 (2)	0.032 (2)	0.026 (2)	0.0051 (19)	0.0140 (18)	0.0016 (19)
C4	0.034 (2)	0.037 (2)	0.030 (2)	0.007 (2)	0.015 (2)	0.0004 (19)
C5	0.043 (3)	0.036 (2)	0.033 (2)	0.008 (2)	0.0216 (19)	0.004 (2)
C6	0.036 (3)	0.038 (3)	0.027 (2)	0.009 (2)	0.0097 (19)	0.003 (2)

# supplementary materials

Geometric parameters (Å. $^9$ )           Cul-O2         1.910 (2)         C2-H2         0.9300           Cul-N1         2.000 (3)         C3-C8         1.399 (5)           Brl-C7         1.907 (4)         C3-C4         1.418 (5)           NI-C1         1.287 (4)         C4-C5         1.422 (5)           NI-C1         1.424 (3)         C5-C6         1.375 (5)           Ol-C1         1.435 (4)         C5-H5         0.9300           O2-C4         1.316 (4)         C6-C7         1.91 (5)           C1-H1A         0.9600         C6-H6         0.9300           C2-C3         1.442 (5)         U         U           O2'-Cul-O2         180.000 (2)         C3-C2-H12         17.7           O2'-Cul-N1         9.127 (11)         C4-C3-C2         121.5 (3)           O2'-Cul-N1         8.73 (11)         C4-C3-C2         124.3 (3)           O2'-Cul-N1         8.873 (11)         C4-C3-C3         124.1 (3)           NI-Cd-I-N1 <sup>4</sup> 180.000 (1)         02-C4-C5         119.3 (3)           C2-NI-O1         109.7 (5)         C3-C4-C5         119.6 (3)           C3-Cul-N1         124.0 (2)         C6-C5-C4         122.0 (4)           O1	C7 C8	0.031 (2) 0.039 (2)	0.024 (2) 0.032 (2)	0.036 (2) 0.034 (2)	0.0008 (18) 0.000 (2)	0.0148 (19) 0.0224 (19)	-0.0039 (18) 0.0001 (19)
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Geometric parar	neters (Å, °)					
Cui - Ni       2000 (3)       C3 - C8       1.399 (5)         BrI-C7       1.907 (4)       C3 - C4       1.418 (5)         NI-C2       1.287 (4)       C4 - C5       1.422 (5)         NI-O1       1.424 (3)       C5 - C6       1.375 (5)         Ol-C1       1.435 (4)       C5 - C6       1.375 (5)         O2-C4       1.316 (4)       C6 - C7       1.391 (5)         C1-H1A       0.9600       C6 - H6       0.9300         C1-H1B       0.9600       C6 - H8       0.9300         C2-C3       1.442 (5)       0.22-C4       1.370 (5)         C2-C3       1.442 (5)       0.22-C4       1.77         O2 <sup>1</sup> -Cul-O2       180.000 (2)       C3 - C2 - H2       117.7         O2 <sup>1</sup> -Cul-N1       9.127 (11)       C8 - C3 - C2       121.5 (3)         O2 <sup>1</sup> -Cul-N1 <sup>1</sup> 88.73 (11)       C4 - C3       124.1 (3)         NI-Cul-N1 <sup>14</sup> 9.127 (11)       0.2 - C4 - C3       124.1 (3)         NI-Cul-N1 <sup>1</sup> 180.000 (1)       0.2 - C4 - C5       119.3 (3)         C2-NI-Cul       109.7 (3)       C3 - C4 - C5       116.6 (3)         C2-NI-Cul       124.0 (2)       C6 - C5 - H5       119.0         O1-Cul-N1 <sup>16</sup> <t< td=""><td>Cu12</td><td></td><td>1 910 (2)</td><td>С2—Н2</td><td></td><td>0.930</td><td>0</td></t<>	Cu12		1 910 (2)	С2—Н2		0.930	0
$ \begin{array}{c} \text{Ch} -\text{Ch} & 2.500 (3) & \text{Ch} -\text{Ch} & 1.438 (4) \\ \text{NI} - \text{C2} & 1.287 (4) & \text{C4} - \text{C5} & 1.422 (5) \\ \text{NI} - \text{OI} & 1.424 (3) & \text{C5} - \text{C6} & 1.375 (5) \\ \text{OI} - \text{C1} & 1.435 (4) & \text{C5} - \text{H5} & 0.9300 \\ \text{OI} - \text{C1} & 1.435 (4) & \text{C6} - \text{C7} & 1.391 (5) \\ \text{CI} - \text{HIA} & 0.9600 & \text{C6} - \text{H6} & 0.9300 \\ \text{CI} - \text{HIB} & 0.9600 & \text{C7} - \text{C8} & 1.370 (5) \\ \text{CI} - \text{HIC} & 0.9600 & \text{C8} - \text{H8} & 0.9300 \\ \text{C2} - \text{C3} & 1.442 (5) & & & & & & & & & & & & & & & & & & &$	Cu1—02		2,000(3)	C2—112		1 390	) (5)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Br1—C7		1.907(4)	C3-C4		1.575	S (5)
$\begin{split} & \text{NI-Ol} & 1.424 (3) & \text{CS} - \text{C6} & 1.375 (5) \\ & \text{OI-C1} & 1.435 (4) & \text{CS} - \text{HS} & 0.9300 \\ & \text{O2-C4} & 1.316 (4) & \text{C6} - \text{C7} & 1.391 (5) \\ & \text{C1-H1A} & 0.9600 & \text{C6} - \text{If6} & 0.9300 \\ & \text{C1-H1B} & 0.9600 & \text{C7} - \text{C8} & 1.370 (5) \\ & \text{C1-H1C} & 0.9600 & \text{C8} - \text{H8} & 0.9300 \\ & \text{C1-H1C} & 0.9600 & \text{C8} - \text{H8} & 0.9300 \\ & \text{C2} - \text{C3} & 1.442 (5) \\ & \text{O2}^{\perp} - \text{Cu} - \text{O2} & 180000 (2) & \text{C3} - \text{C2} - \text{H2} & 117.7 \\ & \text{O2}^{\perp} - \text{Cu} - \text{O1} & 91.27 (11) & \text{C8} - \text{C3} - \text{C4} & 120.8 (3) \\ & \text{O2} - \text{Cu} - \text{N1} & 91.27 (11) & \text{C8} - \text{C3} - \text{C2} & 117.7 (3) \\ & \text{O2}^{\perp} - \text{Cu} - \text{N1} & 88.73 (11) & \text{C4} - \text{C3} - \text{C2} & 117.7 (3) \\ & \text{O2}^{\perp} - \text{Cu} - \text{N1} & 88.73 (11) & \text{C4} - \text{C3} - \text{C2} & 119.3 (3) \\ & \text{O2} - \text{Cu} - \text{N1}^{\perp} & 91.27 (11) & \text{O2} - \text{C4} - \text{C3} & 124.1 (3) \\ & \text{N1} - \text{Cu} - \text{N1}^{\perp} & 91.27 (11) & \text{O2} - \text{C4} - \text{C5} & 119.3 (3) \\ & \text{C2} - \text{N1} - \text{O1} & 109.7 (3) & \text{C3} - \text{C4} - \text{C5} & 119.3 (3) \\ & \text{C2} - \text{N1} - \text{O1} & 109.7 (3) & \text{C3} - \text{C4} - \text{C5} & 119.3 (3) \\ & \text{C2} - \text{N1} - \text{O1} & 124.0 (2) & \text{C6} - \text{C5} - \text{H5} & 119.0 \\ & \text{N1} - \text{O1} - \text{C1} & 124.0 (2) & \text{C6} - \text{C5} - \text{H5} & 119.0 \\ & \text{O1} - \text{C1} - \text{H1A} & 109.5 & \text{C5} - \text{C6} - \text{H6} & 120.2 \\ & \text{O1} - \text{C1} - \text{H1A} & 109.5 & \text{C7} - \text{C6} - \text{H6} & 120.2 \\ & \text{O1} - \text{C1} - \text{H1B} & 109.5 & \text{C7} - \text{C6} - \text{H6} & 120.2 \\ & \text{H1A} - \text{C1} - \text{H1B} & 109.5 & \text{C7} - \text{C6} - \text{H6} & 120.2 \\ & \text{H1A} - \text{C1} - \text{H1B} & 109.5 & \text{C7} - \text{C6} - \text{H6} & 120.2 \\ & \text{H1A} - \text{C1} - \text{H1C} & 109.5 & \text{C7} - \text{C6} - \text{H6} & 120.2 \\ & \text{H1A} - \text{C1} - \text{H1C} & 109.5 & \text{C7} - \text{C8} - \text{C8} & 120.0 \\ & \text{O1} - \text{C1} - \text{H1B} & 109.5 & \text{C7} - \text{C8} - \text{C8} & 120.0 \\ & \text{O2}^{\perp} - \text{C1} - \text{N1} & 190.0 (3) \\ & \text{H1B} - \text{C1} - \text{H1C} & 109.5 & \text{C8} - \text{C7} - \text{C8} & 120.0 \\ & \text{O1} - \text{C1} - \text{H1B} & 109.5 & \text{C8} - \text{C7} - \text{C8} & 120.0 \\ & \text{O2}^{\perp} - \text{C1} - \text{N1} & 130.0 (3) & \text{C2} - \text{C4} - \text{C5} & 178.1 \\ & 190.0 (3) \\ & \text{H1} - \text{C1} - H1$	N1—C2		1.287 (4)	C4—C5		1.422	2 (5)
$01-C1$ $1.435$ (4) $CS-H5$ $0.9300$ $02-C4$ $1.316$ (4) $C6-C7$ $1.391$ (5) $C1-H1A$ $0.9600$ $C6-H6$ $0.9300$ $C1-H1B$ $0.9600$ $C8-H8$ $0.9300$ $C2-C3$ $1.442$ (5) $0.9500$ $C8-H8$ $0.9300$ $02^1-Cu1-02$ $180.000$ (2) $C3-C2-H2$ $117.7$ $02^1-Cu1-N1$ $91.27$ (11) $C8-C3-C4$ $120.8$ (3) $02^2-Cu1-N1$ $88.73$ (11) $C4-C3-C2$ $121.5$ (3) $02^2-Cu1-N1^1$ $88.73$ (11) $C4-C3-C2$ $121.5$ (3) $02^2-Cu1-N1^1$ $88.73$ (11) $02-C4-C5$ $119.3$ (3) $02-Cu1-N1^1$ $180.000$ (1) $02-C4-C5$ $119.6$ (3) $02-N1-Cu1$ $192.0$ (2) $C6-C5-H5$ $119.0$ (3) $(2-N1-O1)$ $192.0$ (2) $C6-C5-H5$ $119.0$ (3) $(2-N1-O1)$ $192.0$ (2) $C6-C5-H5$ $119.0$ (3) $(2-N1-O1)$ $104.0$ (2) $C6-C5-H5$ $119.0$ (3) $(2-N1-O1)$ $102.0$ (3) $122.0$ (4) $01-C1$ $(1-N1-C$	N1-01		1.424 (3)	C5—C6		1.375	5 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	01—C1		1.435 (4)	С5—Н5		0.930	00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2—C4		1.316 (4)	C6—C7		1.391	(5)
C1—H1B         0.9600         C7—C8         1.370 (5)           C1—H1C         0.9600         C8—H8         0.9300           C2—C3         1.442 (5)	C1—H1A		0.9600	С6—Н6		0.930	00
C1-H1C0.9600C8-H80.9300 $C2-C3$ 1.442 (5)117.7 $O2^{i}-Cul-O2$ 180.000 (2)C3-C2-H2117.7 (3) $O2^{i}-Cul-N1$ 91.27 (11)C8-C3-C4120.8 (3) $O2-Cul-N1$ 88.73 (11)C4-C3-C2121.5 (3) $O2^{i}-Cul-N1^{i}$ 88.73 (11)C4-C3-C2124.1 (3) $O2^{i}-Cul-N1^{i}$ 91.27 (11)02-C4-C3124.1 (3) $O2^{i}-Cul-N1^{i}$ 91.27 (11)02-C4-C5119.3 (3) $O2-Cul-N1^{i}$ 19.0 (1)02-C4-C5119.3 (3) $O2-N1-Cul-N1^{i}$ 180.000 (1)02-C4-C5119.0 (3) $O1-N1-Cul-N1^{i}$ 124.0 (2)C6-C5-H5119.0 $O1-N1-Cul$ 124.0 (2)C6-C5-H5119.0 $O1-N1-Cul$ 109.7 (3)C4-C5-H5119.0 $O1-O1-H1C$ 109.5C5-C6-H6120.2 $O1-C1-H1B$ 109.5C5-C6-H6120.2 $O1-C1-H1B$ 109.5C6-C7-Brl19.0 (3) $O1-C1-H1C$ 109.5C6-C7-Brl19.0 (3) $O1-C1-H1C$ 109.5C6-C7-Brl19.0 (3) $O1-C1-H1C$ 109.5C7-C8-C312.0 (1) $O1-C1-H1C$ 109.5C7-C8-C312.0 (1) $O1-C1-H1C$ 109.5C7-C8-C312.0 (1) $O1-C1-H1C$ 109.5C7-C8-C315.(5) $O2-Cul-N1-C2$ 31.5 (3)C2-C4-C515.(5) $O2-Cul-N1-C2$ 31.5 (3)C2-C4-C5178.1 (3) $O2-Cul-N1-C2$ 31.5 (3)C2-C4-C5-C6178.2 (3) $O2-Cul-N1-C2$ </td <td>C1—H1B</td> <td></td> <td>0.9600</td> <td>С7—С8</td> <td></td> <td>1.370</td> <td>0 (5)</td>	C1—H1B		0.9600	С7—С8		1.370	0 (5)
C2-C3       1.442 (5) $O2^{i}-Cul-O2$ 180.000 (2)       C3-C2-H2       117.7 $O2^{i}-Cul-N1$ 91.27 (1)       C8-C3-C4       120.8 (3) $O2-Cul-N1$ 88.73 (1)       C4-C3-C2       117.7 (3) $O2^{i}-Cul-N1$ 88.73 (1)       C4-C3-C2       121.5 (3) $O2-Cul-N1^{i}$ 91.27 (1) $O2-C4-C3$ 124.1 (3) $O2-Cul-N1^{i}$ 180.000 (1) $O2-C4-C5$ 119.3 (3) $O2-N1-O1$ 109.7 (3)       C3-C4-C5       116.6 (3) $O2-N1-O1$ 109.7 (3)       C3-C4-C5       119.0 $O1-N1-Cul$ 124.0 (2)       C6-C5-H5       119.0 $O1-O1-Cl$ 110.4 (3)       C4-C5-H5       119.0 $O1-O1-H1A$ 109.5       C5-C6-H6       120.2 $O1-C1-H1B$ 109.5       C7-C6-H6       120.2 $O1-C1-H1B$ 109.5       C7-C6-H6       120.9 (4) $O1-C1-H1B$ 109.5       C7-C6-H6       120.9 (4) $O1-C1-H1C$ 109.5       C7-C6-H3       120.0 (3) $H1A-C1-H1C$ 109.5       C7-C8-C3       120.1 (3) $O1-C1-H1C$ 109.5       C7-	C1—H1C		0.9600	С8—Н8		0.930	00
$O2^{i}-Cu1-O2$ 180.000 (2) $C3-C2-H2$ 117.7 $O2^{i}-Cu1-N1$ 91.27 (11) $C8-C3-C4$ 120.8 (3) $O2^{-}-Cu1-N1$ 88.73 (11) $C8-C3-C2$ 117.7 (3) $O2^{i}-Cu1-N1^{i}$ 88.73 (11) $C4-C3-C2$ 121.5 (3) $O2-Cu1-N1^{i}$ 91.27 (11) $O2-C4-C3$ 124.1 (3) $O2-Cu1-N1^{i}$ 91.27 (11) $O2-C4-C3$ 124.1 (3) $O2-Cu1-N1^{i}$ 180.000 (1) $O2-C4-C3$ 119.3 (3) $C2-N1-O1$ 199.7 (3) $C3-C4-C5$ 119.3 (3) $C2-N1-Cu1$ 124.0 (2) $C6-C5-C4$ 122.0 (4) $O1-N1-Cu1$ 124.0 (2) $C6-C5-H5$ 119.0 $N1-O1-C1$ 110.4 (3) $C4-C5-H5$ 119.0 $O1-C1-H1A$ 199.5 $C5-C6-H6$ 120.2 $O1-C1-H1A$ 109.5 $C5-C6-H6$ 120.2 $O1-C1-H1B$ 109.5 $C8-C7-C6$ 120.9 (4) $O1-C1-H1B$ 109.5 $C6-C7-Br1$ 119.0 (3) $H1A-C1-H1C$ 109.5 $C6-C7-Br1$ 119.0 (3) $H1A-C1-H1C$ 109.5 $C7-C8-H8$ 120.0 $O1-C2-H1C$ 109.5 $C7-C8-H8$ 120.0 $N1-C2-C3$ 124.5 (3) $C7-C8-H8$ 120.0 $N1-C2-H1C$ 109.5 $C7-C8-H8$ 120.0 $N1-C2-C4$ 13.2 (3) $C8-C3-C4-C2$ 17.9 (3) $O2^{i}-Cu1-N1-O1$ 13.2 (3) $C2-C3-C4-C5$ 1.5 (5) $O2-Cu1-N1-O1$ 13.2 (3) $C2-C3-C4-C5$ 1.5 (5) $O2-Cu1-N1-O1$ 13.3 (3) $O2-Cu-C5-C6$ 17.8 1 (3) $O2^{i}-Cu1-N1-O1$	C2—C3		1.442 (5)				
$O2^{i}-Cul-Nl$ $91.27$ (1) $C8-C3-C4$ $120.8$ (3) $O2-Uul-Nl$ $88.73$ (1) $C8-C3-C2$ $117.7$ (3) $O2^{i}-Cul-Nl^{i}$ $88.73$ (1) $C4-C3-C2$ $121.5$ (3) $O2-Cul-Nl^{i}$ $91.27$ (1) $O2-C4-C3$ $124.1$ (3) $O2-Cul-Nl^{i}$ $91.27$ (1) $O2-C4-C5$ $119.3$ (3) $C2-Nl-O1$ $199.7$ (3) $C3-C4-C5$ $116.6$ (3) $C2-Nl-Cul$ $124.0$ (2) $C6-C5-H5$ $119.0$ $O1-O1-C1$ $104.4$ (2) $C6-C5-H5$ $119.0$ $O1-O1-C1$ $110.4$ (3) $C4-C5-H5$ $119.0$ $O1-O1-H1L$ $124.5$ (2) $C5-C6-C7$ $119.5$ (3) $O1-C1-H1B$ $109.5$ $C5-C6-H6$ $120.2$ $O1-C1-H1B$ $109.5$ $C8-C7-Brl$ $120.0$ (3) $H1A-C1-H1C$ $109.5$ $C8-C7-Brl$ $119.0$ (3) $H1A-C1-H1C$ $109.5$ $C7-C8-H8$ $120.0$ $O1-C1-H1C$ $109.5$ $C7-C8-H8$ $120.0$ $O1-C2-H1C$ $109.5$	O2 <sup>i</sup> —Cu1—O2		180.000 (2)	C3—C2	—Н2	117.7	,
$02-Cul-Nl$ $88.73$ (1) $C8-C3-C2$ $117.7$ (3) $02^{\perp}-Cul-Nl^{\perp}$ $88.73$ (1) $C4-C3-C2$ $121.5$ (3) $02-Cul-Nl^{\perp}$ $91.27$ (11) $02-C4-C3$ $124.1$ (3) $01-Cul-Nl^{\perp}$ $180.000$ (1) $02-C4-C5$ $119.3$ (3) $C2-Nl-Ol$ $109.7$ (3) $C3-C4-C5$ $116.6$ (3) $C2-Nl-Cul$ $124.0$ (2) $C6-C5-C4$ $122.0$ (4) $01-Nl-Cul$ $124.1$ (2) $C6-C5-H5$ $119.0$ $Nl-Ol-Cl$ $110.4$ (3) $C4-C5-H5$ $119.0$ $01-Nl-Cul$ $120.2$ $C6-C5-H5$ $120.2$ $01-Cl-H1A$ $109.5$ $C5-C6-C7$ $119.5$ (3) $01-Cl-H1B$ $109.5$ $C8-C7-C6$ $120.2$ $H1A-Cl-H1B$ $109.5$ $C6-C7-Brl$ $120.0$ (3) $01-Cl-H1C$ $109.5$ $C6-C7-Brl$ $120.0$ (3) $N1-C2-C3$ $124.5$ (3) $C7-C8-H8$ $120.0$ $N1-C2-H2$ $117.7$ $C3-C8-C3$ $120.1$ (3) $N1-C2-H1C$ $109.5$ $C6-C7-Brl$ $119.0$ (3) $N1-C2-H1C$	O2 <sup>i</sup> —Cu1—N1		91.27 (11)	C8—C3	—C4	120.8	8 (3)
$O2^{i}-Cu1-N1^{i}$ $88.73$ (1) $C4-C3-C2$ $121.5$ (3) $O2-Cu1-N1^{i}$ $91.27$ (1) $O2-C4-C3$ $124.1$ (3) $N1-Cu1-N1^{i}$ $180.000$ (1) $O2-C4-C5$ $119.3$ (3) $C2-N1-O1$ $109.7$ (3) $C3-C4-C5$ $116.6$ (3) $C2-N1-Cu1$ $109.7$ (3) $C3-C4-C5$ $116.6$ (3) $C2-N1-Cu1$ $124.0$ (2) $C6-C5-C4$ $122.0$ (4) $O1-N1-Cu1$ $124.1$ (2) $C6-C5-H5$ $119.0$ $N1-O1-C1$ $110.4$ (3) $C4-C5-H5$ $119.0$ $O1-C1-H1A$ $109.5$ $C5-C6-C7$ $119.5$ (3) $O1-C1-H1B$ $109.5$ $C5-C6-H6$ $120.2$ $O1-C1-H1B$ $109.5$ $C8-C7-C6$ $120.9$ (4) $O1-C1-H1C$ $109.5$ $C8-C7-Brl$ $119.0$ (3) $I1A-C1-H1C$ $109.5$ $C7-C8-C3$ $120.1$ (3) $O1-C1-H1C$ $109.5$ $C7-C8-C3$ $120.1$ (3) $N1-C2-C3$ $124.5$ (3) $C7-C8-H8$ $120.0$ $N1-C2-H2$ $117.7$ $C3-C8-H8$ $120.0$ $O2^{i}-Cu1-N1-C2$ $-148.5$ (3) $C2-C3-C4-O2$ $-179.3$ (3) $O2-Cu1-N1-C2$ $31.5$ (3) $C2-C3-C4-C5$ $1.5$ (5) $O2-Cu1-N1-O1$ $132.0$ $C3-C4-C5-C6$ $718.1$ (3) $O2^{i}-Cu1-N1-O1$ $133.0$ (3) $O2-C4-C5-C6$ $718.1$ (3) $O2^{i}-U1-N1-O1$ $133.0$ (3) $C2-C3-C4-C5$ $1.5$ (5) $O2^{i}-U1-N1-O1$ $63.0$ (3) $C3-C4-C5-C6$ $718.1$ (3) $O2^{i}-U1-N1-O1$ $63.0$ (3) $C3-C4-C5-C6$ $718.1$ (3)	O2—Cu1—N1		88.73 (11)	C8—C3	—C2	117.7	(3)
$O2-Cu_{II}-NI^{i}$ $91.27(11)$ $O2-C4-C3$ $124.1(3)$ $NI-Cu_{I}-NI^{i}$ $180.000(1)$ $O2-C4-C5$ $119.3(3)$ $C2-NI-O1$ $109.7(3)$ $C3-C4-C5$ $116.6(3)$ $C2-NI-Cu_{I}$ $124.0(2)$ $C6-C5-C4$ $122.0(4)$ $O1-NI-Cu_{I}$ $124.1(2)$ $C6-C5-H5$ $119.0$ $NI-O1-C1$ $110.4(3)$ $C4-C5-H5$ $119.0$ $C4-O2-Cu_{I}$ $123.8(2)$ $C5-C6-C7$ $119.5(3)$ $O1-C1-H1A$ $109.5$ $C5-C6-H6$ $120.2$ $O1-C1-H1B$ $109.5$ $C8-C7-C6$ $120.9(4)$ $O1-C1-H1B$ $109.5$ $C8-C7-BrI$ $119.0(3)$ $O1-C1-H1C$ $109.5$ $C8-C7-BrI$ $119.0(3)$ $I1A-C1-H1C$ $109.5$ $C7-C8-H8$ $120.0(3)$ $I1A-C1-H1C$ $109.5$ $C7-C8-H8$ $120.0(3)$ $I1A-C2-H1C$ $109.5$ $C7-C8-H8$ $120.0(3)$ $I1A-C1-H1C$ $109.5$ $C7-C8-H8$ $120.0(3)$ $I1A-C1-H1C$ $109.5$ $C7-C8-H8$ $120.0(3)$ $I1A-C2-H1$ $109.5$ $C7-C8-H8$ $120.0(3)$ $O1-C1-H1C$ $109.5$ $C7-C8-H8$ $120.0(3)$ $O2-Cu_{1}-N1-C2$ $-148.5(3)$ $C8-C3-C4-O2$ $-179.3(3)$ $O2-Cu_{1}-N1-C2$ $-148.5(3)$ $C8-C3-C4-C5$ $-5(5)$ $O2-Cu_{1}-N1-O1$ $-132.0(3)$ $C2-C4-C5-C6$ $-178.1(3)$ $O2-Cu_{1}-N1-O1$ $-138.8(3)$ $C4-C5-C6-C7$ $10.0(6)$ $O1-C1-O2-C4$ $-38.8(3)$ $C4-C5-C6-C7-Br1$ $-176.9(3)$ $O1-N1-O2-C3$	O2 <sup>i</sup> —Cu1—N1 <sup>i</sup>		88.73 (11)	C4—C3	—C2	121.5	5 (3)
N1-Cu1-N1 <sup>i</sup> 180.000 (1)02-C4-C5119.3 (3)C2-N1-O1109.7 (3)C3-C4-C5116.6 (3)C2-N1-Cu1124.0 (2)C6-C5-C4122.0 (4)O1-N1-Cu1124.1 (2)C6-C5-H5119.0N1-O1-C1110.4 (3)C4-C5-H5119.0C4-O2-Cu1123.8 (2)C5-C6-C7119.5 (3)O1-C1-H1A109.5C5-C6-H6120.2O1-C1-H1B109.5C8-C7-C6120.9 (4)O1-C1-H1C109.5C8-C7-Brl120.0 (3)H1A-C1-H1C109.5C8-C7-Brl120.0 (3)H1B-C1-H1C109.5C7-C8-H8120.0N1-C2-C3124.5 (3)C7-C8-H8120.0N1-C2-H2117.7C3-C8-H8120.0O2-Cu1-N1-C231.5 (3)C2-C3-C4-O2-179.3 (3)O2-Cu1-N1-O113.2 (3)C8-C3-C4-C51.5 (5)O2-Cu1-N1-O113.3 0 (3)O2-C4-C5-C6178.2 (3)C2-N1-O1-C1-133.0 (3)C3-C4-C5-C6-2.6 (5)N1-C2-C3-178.3 (3)C3-C4-C5-C6-2.6 (5)N1-C1-O2-C4-38.8 (3)C4-C5-C6-C71.0 (6)N1-C1-O2-C4-38.8 (3)C4-C5-C6-C71.0 (6)N1-C2-C3-C8171.7 (3)Br1-C7-C8-C3-2.8 (5)N1-C2-C3-C8171.7 (3)Br1-C7-C8-C3-2.8 (5)N1-C2-C3-C4-48.6 (6)C4-C3-C8-C71.1 (5)	O2—Cu1—N1 <sup>i</sup>		91.27 (11)	O2—C4	—C3	124.1	(3)
C2-NI-O1109.7 (3)C3-C4-C5116.6 (3)C2-NI-Cul124.0 (2)C6-C5-C4122.0 (4)O1-NI-Cul124.1 (2)C6-C5-H5119.0NI-O1-C1110.4 (3)C4-C5-H5119.0C4-O2-Cul123.8 (2)C5-C6-C7119.5 (3)O1-C1-H1A109.5C5-C6-H6120.2O1-C1-H1B109.5C7-C6-H6120.9O1-C1-H1C109.5C8-C7-C6120.9 (4)O1-C1-H1C109.5C6-C7-Br1120.0 (3)H1A-C1-H1C109.5C6-C7-Br119.0 (3)H1B-C1-H1C109.5C7-C8-H8120.0N1-C2-C3124.5 (3)C7-C8-H8120.0O2 <sup>1</sup> -Cul-N1-C2-148.5 (3)C8-C3-C4-O2-179.3 (3)O22-Cul-N1-C2-148.5 (3)C2-C3-C4-O21.1 (6)O2 <sup>1</sup> -Cul-N1-C113.2 (3)C8-C3-C4-C51.5 (5)O2-Cul-N1-O113.2 (3)C2-C3-C4-C51.5 (5)O2-Cul-N1-O113.2 (3)C3-C4-C5-C678.2 (3)Cul-N1-O1-C1-133.0 (3)O2-C4-C5-C678.2 (3)Cul-N1-O1-C163.0 (3)C3-C4-C5-C6-2.6 (5)N1-Cul-O2-C4-38.8 (3)C4-C5-C6-C71.0 (6)N1 <sup>1</sup> -Cul-O2-C4-178.3 (3)C5-C6-C7-C81.8 (5)O1-N1-C2-C3-178.3 (3)C5-C6-C7-C81.8 (5)O1-N1-C2-C3-178.3 (3)C5-C6-C7-C83.8 (5)O1-N1-C2-C3-178.3 (3)C5-C6-C7-C81.9 (3)N1-C2-C3-C8171.7 (3)Br1-C7-C8-C3-2.8 (5)N1-C2-C3	N1—Cu1—N1 <sup>i</sup>		180.000 (1)	O2—C4	—C5	119.3	(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2—N1—O1		109.7 (3)	C3—C4	—C5	116.6	(3)
$O1-N1-Cu1$ $124.1 (2)$ $C6-C5-H5$ $119.0$ $N1-O1-C1$ $110.4 (3)$ $C4-C5-H5$ $119.0$ $C4-O2-Cu1$ $123.8 (2)$ $C5-C6-C7$ $119.5 (3)$ $O1-C1-H1A$ $109.5$ $C5-C6-H6$ $120.2$ $O1-C1-H1B$ $109.5$ $C7-C6-H6$ $120.9 (4)$ $O1-C1-H1B$ $109.5$ $C8-C7-C6$ $120.9 (4)$ $O1-C1-H1C$ $109.5$ $C8-C7-Br1$ $120.0 (3)$ $H1A-C1-H1C$ $109.5$ $C6-C7-Br1$ $119.0 (3)$ $H1A-C1-H1C$ $109.5$ $C7-C8-C3$ $120.1 (3)$ $N1-C2-C3$ $124.5 (3)$ $C7-C8-H8$ $120.0$ $N1-C2-H2$ $117.7$ $C3-C8-H8$ $120.0$ $O2^{i}-Cu1-N1-C2$ $-148.5 (3)$ $C8-C3-C4-O2$ $-179.3 (3)$ $O2^{-Cu1-N1-C2}$ $31.5 (3)$ $C2-C3-C4-C5$ $1.5 (5)$ $O2-Cu1-N1-O1$ $13.2 (3)$ $C8-C3-C4-C5$ $1.5 (5)$ $O2^{-Cu1-N1-O1}$ $-166.8 (3)$ $C2-C3-C4-C5$ $-178.1 (3)$ $C2-N1-O1-C1$ $-133.0 (3)$ $O2-C4-C5-C6$ $-2.6 (5)$ $N1-Cu-O2-C4$ $411.2 (3)$ $C5-C6-C7-Br1$ $-176.9 (3)$ $O1-N1-C2-C3$ $-178.3 (6)$ $C4-C3-C8-C7$ $1.1 (5)$	C2—N1—Cu1		124.0 (2)	C6—C5	—C4	122.0	0 (4)
N1O1C1110.4 (3)C4C5H5119.0C4O2Cu1123.8 (2)C5C6C7119.5 (3)O1C1H1A109.5C5C6H6120.2O1C1H1B109.5C7C6H6120.2H1AC1H1B109.5C8C7C6120.9 (4)O1C1H1C109.5C8C7Br1120.0 (3)H1AC1H1C109.5C6C7Br1119.0 (3)H1BC1H1C109.5C7C8C3120.1 (3)N1C2C3124.5 (3)C7C8H8120.0N1C2H2117.7C3C8H8120.0O2 <sup>i</sup> -Cu1-N1-C2-148.5 (3)C8C3C4O2-179.3 (3)O2 <sup>ci</sup> -Cu1-N1-C231.5 (3)C2C3C4O21.1 (6)O2 <sup>i</sup> -Cu1-N1-O113.2 (3)C8C3C4C51.5 (5)O2Cu1-N1-O1-166.8 (3)C2C3C4C5-178.1 (3)C2N1-O1-C1-133.0 (3)O2C4C5C6178.2 (3)Cu1-N1-O2-C4414.2 (3)C5C6-C71.0 (6)N1-C2-C3-178.3 (3)C5C6-C7R81.8 (5)O1-N1-C2-C3-178.3 (3)C5C6-C7R81.8 (5)O1-N1-C2-C3-178.3 (3)C5C6-C7R81.8 (5)O1-N1-C2-C3-178.3 (3)C5C6-C7R81.8 (5)O1-N1-C2-C3-143.5 (5)C6C7R81.75.9 (3)N1-C2-C3-C4-66.6C4C3C8-C71.1 (5)	O1—N1—Cu1		124.1 (2)	C6—C5	—Н5	119.0	)
$C4-02-Cul$ 123.8 (2) $C5-C6-C7$ 119.5 (3) $O1-C1-H1A$ 109.5 $C5-C6-H6$ 120.2 $O1-C1-H1B$ 109.5 $C7-C6-H6$ 120.9 (4) $O1-C1-H1B$ 109.5 $C8-C7-C6$ 120.9 (4) $O1-C1-H1C$ 109.5 $C8-C7-Br1$ 120.0 (3) $H1A-C1-H1C$ 109.5 $C6-C7-Br1$ 19.0 (3) $H1B-C1-H1C$ 109.5 $C7-C8-C3$ 120.1 (3) $N1-C2-C3$ 124.5 (3) $C7-C8-H8$ 120.0 $N1-C2-H2$ 117.7 $C3-C8-H8$ 120.0 $O2^i-Cu1-N1-C2$ -148.5 (3) $C8-C3-C4-O2$ -179.3 (3) $O2^-Cu1-N1-C2$ 31.5 (3) $C2-C3-C4-O2$ 1.1 (6) $O2^i-Cu1-N1-O1$ 13.2 (3) $C8-C3-C4-C5$ 1.5 (5) $O2-Cu1-N1-O1$ -166.8 (3) $C2-C3-C4-C5$ -178.1 (3) $C2-N1-O1-C1$ -33.0 (3) $O2-C4-C5-C6$ 178.2 (3) $Cu-N1-O1-C1$ 63.0 (3) $C3-C4-C5-C6$ 1.8 (5) $N1-C2-C3$ -178.3 (3) $C5-C6-C7-C8$ 1.8 (5) $N1-C2-C3$ -178.3 (3) $C5-C6-C7-C8-C3$ -2.8 (5) $N1-C2-C3-C4$ -178.3 (3) $C5-C6-C7-C8-C3$ -2.8 (5) $N1-C2-C3-C4$ -143.5 (5) $C6-C7-C8-C3$ -2.8 (5) $N1-C2-C3-C4$ -143.6 (5) $C4-C3-C8-C7$ 1.1 (5)	N1-01-C1		110.4 (3)	C4—C5	—Н5	119.0	)
$O1-C1-H1A$ $109.5$ $C5-C6-H6$ $120.2$ $O1-C1-H1B$ $109.5$ $C7-C6-H6$ $120.9$ (4) $O1-C1-H1B$ $109.5$ $C8-C7-C6$ $120.9$ (4) $O1-C1-H1C$ $109.5$ $C8-C7-Br1$ $120.0$ (3) $H1A-C1-H1C$ $109.5$ $C6-C7-Br1$ $119.0$ (3) $H1B-C1-H1C$ $109.5$ $C7-C8-C3$ $120.1$ (3) $N1-C2-C3$ $124.5$ (3) $C7-C8-H8$ $120.0$ $N1-C2-H2$ $117.7$ $C3-C8-H8$ $120.0$ $O2^i-Cu1-N1-C2$ $-148.5$ (3) $C8-C3-C4-O2$ $-179.3$ (3) $O2-Cu1-N1-C2$ $31.5$ (3) $C2-C3-C4-O2$ $1.1$ (6) $O2^i-Cu1-N1-O1$ $13.2$ (3) $C8-C3-C4-C5$ $1.5$ (5) $O2-Cu1-N1-O1$ $-166.8$ (3) $C2-C3-C4-C5$ $-178.1$ (3) $C2-N1-O1-C1$ $-133.0$ (3) $O2-C4-C5-C6$ $-2.6$ (5) $N1-Cu1-O2-C4$ $-38.8$ (3) $C4-C5-C6-C7$ $1.0$ (6) $N1^i-Cu1-O2-C4$ $-143.5$ (3) $C5-C6-C7-C8$ $1.8$ (5) $O1-N1-C2-C3$ $-178.3$ (3) $C5-C6-C7-C8-C3$ $-2.8$ (5) $N1-C2-C3-C4$ $-178.3$ (3) $C5-C6-C7-C8-C3$ $-2.8$ (5) $N1-C2-C3-C4$ $-143.5$ $C6-C7-C8-C3$ $-2.8$ (5) $N1-C2-C3-C4$ $-8.6$ (6) $C4-C3-C8-C7$ $1.1$ (5)	C4—O2—Cu1		123.8 (2)	C5—C6	—C7	119.5	5 (3)
$O1C1H1B$ $109.5$ $C7C6H6$ $120.2$ $H1AC1H1B$ $109.5$ $C8C7C6$ $120.9$ (4) $O1C1H1C$ $109.5$ $C8C7Br1$ $120.0$ (3) $H1AC1H1C$ $109.5$ $C6C7Br1$ $119.0$ (3) $H1BC1H1C$ $109.5$ $C7C8C3$ $120.1$ (3) $N1C2C3$ $124.5$ (3) $C7C8H8$ $120.0$ $N1C2H2$ $117.7$ $C3C8H8$ $120.0$ $O2^iCu1N1C2$ $-148.5$ (3) $C8C3C4O2$ $-179.3$ (3) $O2Cu1N1C2$ $-148.5$ (3) $C2C3C4O2$ $1.1$ (6) $O2^iCu1N1C2$ $31.5$ (3) $C2C3C4C5$ $1.5$ (5) $O2Cu1N1O1$ $13.2$ (3) $C2C3C4C5$ $-178.1$ (3) $C2N1O1C1$ $-166.8$ (3) $C2C3C4C5$ $-178.1$ (3) $C2N1O1C1$ $-133.0$ (3) $O2C4C5C6$ $-72.6$ (5) $N1Cu1O2C4$ $-38.8$ (3) $C4C5C6C7$ $1.0$ (6) $N1^iCu1O2C4$ $141.2$ (3) $C5C6C7Br1$ $-176.9$ (3) $O1N1C2C3$ $-178.3$ (3) $C5C6C7Br1$ $-176.9$ (3) $O1N1C2C3$ $-14.3$ (5) $C6C7C8C3$ $-2.8$ (5) $N1C2C3C4$ $-8.6$ (6) $C4C3C8C7$ $1.1$ (5)	01—C1—H1A		109.5	C5—C6	—Н6	120.2	2
HIA-CI-HIB109.5 $C8-C7-C6$ $120.9 (4)$ OI-CI-HIC109.5 $C8-C7-Brl$ $120.0 (3)$ HIA-CI-HIC109.5 $C6-C7-Brl$ $119.0 (3)$ HIB-CI-HIC109.5 $C7-C8-C3$ $120.1 (3)$ NI-C2-C3 $124.5 (3)$ $C7-C8-H8$ $120.0$ NI-C2-H2117.7 $C3-C8-H8$ $120.0$ $O2^i-Cul-NI-C2$ $-148.5 (3)$ $C8-C3-C4-O2$ $-179.3 (3)$ $O2-Cul-NI-C2$ $31.5 (3)$ $C2-C3-C4-O2$ $1.1 (6)$ $O2^i-Cul-NI-C1$ $13.2 (3)$ $C8-C3-C4-C5$ $1.5 (5)$ $O2-Cul-NI-O1$ $13.2 (3)$ $C2-C3-C4-C5$ $-178.1 (3)$ $C2-NI-O1-C1$ $-166.8 (3)$ $C2-C3-C4-C5$ $-178.1 (3)$ $C2-NI-O1-C1$ $-133.0 (3)$ $O2-C4-C5-C6$ $-2.6 (5)$ $NI-Cu1-O2-C4$ $41.2 (3)$ $C5-C6-C7-C8$ $1.8 (5)$ $O1-NI-C2-C3$ $-178.3 (3)$ $C5-C6-C7-C8-C3$ $-2.8 (5)$ $NI-C2-C3-C8$ $171.7 (3)$ $Br1-C7-C8-C3$ $75.9 (3)$ $NI-C2-C3-C4$ $-8.6 (6)$ $C4-C3-C8-C7$ $1.1 (5)$	O1—C1—H1B		109.5	C7—C6	—H6	120.2	
O1C1H1C109.5 $C8C7Br1$ 120.0 (3)H1AC1H1C109.5 $C6C7Br1$ 119.0 (3)H1BC1H1C109.5 $C7C8C3$ 120.1 (3)N1C2C3124.5 (3) $C7C8H8$ 120.0N1C2H2117.7 $C3C8H8$ 120.0 $O2^iCu1N1C2$ -148.5 (3) $C8C3C4O2$ -179.3 (3) $O2^Cu1N1C2$ 31.5 (3) $C2C3C4O2$ 1.1 (6) $O2^iCu1N1C1$ 13.2 (3) $C8C3C4C5$ 1.5 (5) $O2Cu1N1O1$ -166.8 (3) $C2C3C4C5$ -178.1 (3) $C2N1O1C1$ -133.0 (3) $O2C4C5C6$ 178.2 (3) $Cu1N1-O1C1$ 63.0 (3) $C3C4C5C6$ -2.6 (5) $N1Cu1-O2C4$ -38.8 (3) $C4C5C6C7$ 1.0 (6) $N1^iCu1-O2C4$ 141.2 (3) $C5C6C7Br1$ -176.9 (3) $O1N1C2C3$ -178.3 (3) $C5C6C7Br1$ -176.9 (3) $O1-N1C2C3C8$ 171.7 (3) $Br1C7C8C3$ -2.8 (5) $N1C2C3C4$ -8.6 (6) $C4C3C8C7$ 1.1 (5)	H1A—C1—H1B		109.5	C8—C7	—C6	120.9	9 (4)
HIA-CI-HIC109.5 $C6-C7-Br1$ 119.0 (3)HIB-CI-HIC109.5 $C7-C8-C3$ 120.1 (3)NI-C2-C3124.5 (3) $C7-C8-H8$ 120.0NI-C2-H2117.7 $C3-C8-H8$ 120.0 $O2^{i}-Cul-N1-C2$ -148.5 (3) $C8-C3-C4-O2$ -179.3 (3) $O2-Cul-N1-C2$ 31.5 (3) $C2-C3-C4-O2$ 1.1 (6) $O2^{i}-Cul-N1-O1$ 13.2 (3) $C8-C3-C4-C5$ 1.5 (5) $O2-Cul-N1-O1$ -166.8 (3) $C2-C3-C4-C5$ -178.1 (3) $C2-N1-O1-C1$ -133.0 (3) $O2-C4-C5-C6$ 178.2 (3) $Cul-N1-O2-C4$ -38.8 (3) $C4-C5-C6-C7$ 1.0 (6) $N1^{i}-Cul-O2-C4$ 141.2 (3) $C5-C6-C7-C8$ 1.8 (5) $O1-N1-C2-C3$ -178.3 (3) $C5-C6-C7-C8-C3$ -2.8 (5) $N1-C2-C3-C8$ 171.7 (3) $Br1-C7-C8-C3$ 175.9 (3) $N1-C2-C3-C4$ -8.6 (6) $C4-C3-C8-C7$ 1.1 (5)	Ol—Cl—HlC		109.5	C8—C7	—Brl	120.0	0 (3)
HIB-C1-HIC109.5 $C7-C8-C3$ 120.1 (3)N1-C2-C3124.5 (3) $C7-C8-H8$ 120.0N1-C2-H2117.7 $C3-C8-H8$ 120.0 $O2^i-Cu1-N1-C2$ -148.5 (3) $C8-C3-C4-O2$ -179.3 (3) $O2-Cu1-N1-C2$ 31.5 (3) $C2-C3-C4-O2$ 1.1 (6) $O2^i-Cu1-N1-O1$ 13.2 (3) $C8-C3-C4-C5$ 1.5 (5) $O2-Cu1-N1-O1$ -166.8 (3) $C2-C3-C4-C5$ -178.1 (3) $O2-Cu1-N1-O1$ -166.8 (3) $O2-C4-C5-C6$ 178.2 (3) $O2-Cu1-N1-O1-C1$ -133.0 (3) $O2-C4-C5-C6$ 178.2 (3) $O2-N1-O1-C1$ -38.8 (3) $C4-C5-C6-C7$ 1.0 (6) $N1^i-Cu1-O2-C4$ 141.2 (3) $C5-C6-C7-C8$ 1.8 (5) $O1-N1-C2-C3$ -178.3 (3) $C5-C6-C7-Br1$ -176.9 (3) $O1-N1-C2-C3-C8$ 171.7 (3) $Br1-C7-C8-C3$ -2.8 (5) $N1-C2-C3-C4$ -8.6 (6) $C4-C3-C8-C7$ 1.1 (5)	HIA-CI-HIC		109.5	C6—C7	—Brl	119.0	(3)
N1C2C3124.5 (3)C7C8H8120.0N1C2H2117.7C3C8H8120.0 $O2^{i}$ Cu1N1C2-148.5 (3)C8C3C4O2-179.3 (3) $O2$ Cu1N1C231.5 (3)C2C3C4O21.1 (6) $O2^{i}$ Cu1N1-O113.2 (3)C8C3C4O21.1 (6) $O2^{i}$ Cu1N1-O1-166.8 (3)C2C3C4C51.5 (5) $O2$ Cu1N1-O1-166.8 (3)C2C3C4C5-178.1 (3) $C2$ N1-O1C1-133.0 (3)O2C4C5C6178.2 (3)Cu1N1-O1C163.0 (3)C3C4C5C6-2.6 (5)N1Cu1-O2C4141.2 (3)C5C6C7C81.8 (5)O1N1-C2C3-178.3 (3)C5C6C7Br1-176.9 (3)Cu1N1-C2C3-14.3 (5)C6C7C8C3-2.8 (5)N1C2C3C8171.7 (3)Br1C7C8C3175.9 (3)N1C2C3C4-8.6 (6)C4C3C8C71.1 (5)	HIB-CI-HIC		109.5	C/-C8	C3	120.1	(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N1 = C2 = C3 N1 = C2 = H2		124.3 (3)	C7—C8	—по —ня	120.0	)
$02 = Cu1 = N1 = C2$ $1.0.0 (s)$ $0.0 cs^{-1} + 0.2$ $1.0.0 (s)$ $02 = Cu1 = N1 = C2$ $31.5 (3)$ $C2 = C3 = C4 = C2$ $1.1 (6)$ $02^{i} = Cu1 = N1 = O1$ $13.2 (3)$ $C8 = C3 = C4 = C5$ $1.5 (5)$ $02 = Cu1 = N1 = O1$ $-166.8 (3)$ $C2 = C3 = C4 = C5$ $-178.1 (3)$ $02 = Cu1 = N1 = O1$ $-166.8 (3)$ $C2 = C3 = C4 = C5$ $-178.1 (3)$ $02 = Cu1 = N1 = O1$ $-166.8 (3)$ $02 = C4 = C5 = C6$ $178.2 (3)$ $C2 = N1 = O1 = C1$ $-133.0 (3)$ $02 = C4 = C5 = C6$ $-2.6 (5)$ $N1 = Cu1 = O2 = C4$ $-38.8 (3)$ $C4 = C5 = C6 = C7$ $1.0 (6)$ $N1^{i} = Cu1 = O2 = C4$ $141.2 (3)$ $C5 = C6 = C7 = C8$ $1.8 (5)$ $01 = N1 = C2 = C3$ $-178.3 (3)$ $C5 = C6 = C7 = C8$ $1.8 (5)$ $01 = N1 = C2 = C3$ $-178.3 (3)$ $C5 = C6 = C7 = C8$ $1.76.9 (3)$ $Cu1 = N1 = C2 = C3$ $-14.3 (5)$ $C6 = C7 = C8 = C3$ $-2.8 (5)$ $N1 = C2 = C3 = C8$ $171.7 (3)$ $Br1 = C7 = C8 = C3$ $175.9 (3)$ $N1 = C2 = C3 = C4$ $-8.6 (6)$ $C4 = C3 = C8 = C7$ $1.1 (5)$	$M^{-}C_{2}$ $M^{-}M^{-}$	C2	-1485(3)	C3—C3	-110	-179	3 (3)
$O2^{i}$ Gui - Mi + $O2^{i}$ $D13(0)^{i}$ $C2^{i}$ CS + $C1^{i}$ $O2^{i}$ $D11(0)^{i}$ $O2^{i}$ - Cul - N1 - O113.2 (3) $C8$ - C3 - C4 - C51.5 (5) $O2$ - Cul - N1 - O1-166.8 (3) $C2$ - C3 - C4 - C5-178.1 (3) $C2$ - N1 - O1 - C1-133.0 (3) $O2$ - C4 - C5 - C6178.2 (3) $Cul$ - N1 - O1 - C163.0 (3) $C3$ - C4 - C5 - C6-2.6 (5)N1 - Cul - O2 - C4-38.8 (3)C4 - C5 - C6 - C71.0 (6)N1^{i} - Cul - O2 - C4141.2 (3)C5 - C6 - C7 - C81.8 (5)O1 - N1 - C2 - C3-178.3 (3)C5 - C6 - C7 - Brl-176.9 (3)Cul - N1 - C2 - C3-14.3 (5)C6 - C7 - C8 - C3-2.8 (5)N1 - C2 - C3 - C8171.7 (3)Brl - C7 - C8 - C3175.9 (3)N1 - C2 - C3 - C4-8.6 (6)C4 - C3 - C8 - C71.1 (5)	02 - Cu1 - N1 - 02 - Cu1 - Cu1 - 02 - Cu1 - Cu1 - 02 - Cu1 - Cu1 - CU1 -	C2	31.5 (3)	C2-C3	-C4-02	11(	5) 5)
$O_2 = Cu1 = N1 = O1$ $I_1J_2(5)^{-1}$ $CO^{-1}CS^{-1}CS^{-1}CS^{-1}CS^{-1}CS^{-1}S^{-1$	$O2^{i}$ Cu1 N1	01	132(3)	C8-C3	-C4-C5	1.5 (4	5)
$C2-C4-C3$ $178.1 (3)$ $C2-N1-O1-C1$ $-133.0 (3)$ $O2-C4-C5-C6$ $178.2 (3)$ $Cu1-N1-O1-C1$ $63.0 (3)$ $C3-C4-C5-C6$ $-2.6 (5)$ $N1-Cu1-O2-C4$ $-38.8 (3)$ $C4-C5-C6-C7$ $1.0 (6)$ $N1^i-Cu1-O2-C4$ $141.2 (3)$ $C5-C6-C7-C8$ $1.8 (5)$ $O1-N1-C2-C3$ $-178.3 (3)$ $C5-C6-C7-Br1$ $-176.9 (3)$ $Cu1-N1-C2-C3$ $-14.3 (5)$ $C6-C7-C8-C3$ $-2.8 (5)$ $N1-C2-C3-C8$ $171.7 (3)$ $Br1-C7-C8-C3$ $175.9 (3)$ $N1-C2-C3-C4$ $-8.6 (6)$ $C4-C3-C8-C7$ $1.1 (5)$	$O_2 = Cu_1 = N_1 = 0$	01	-166.8(3)		$C_1 C_2$	-178	1 (3)
Cu1-N1-O1-C1 $63.0(3)$ $C3-C4-C5-C6$ $-2.6(5)$ N1-Cu1-O2-C4 $-38.8(3)$ $C4-C5-C6-C7$ $1.0(6)$ N1 <sup>i</sup> -Cu1-O2-C4 $141.2(3)$ $C5-C6-C7-C8$ $1.8(5)$ O1-N1-C2-C3 $-178.3(3)$ $C5-C6-C7-Br1$ $-176.9(3)$ Cu1-N1-C2-C3 $-14.3(5)$ $C6-C7-C8-C3$ $-2.8(5)$ N1-C2-C3-C8 $171.7(3)$ $Br1-C7-C8-C3$ $175.9(3)$ N1-C2-C3-C4 $-8.6(6)$ $C4-C3-C8-C7$ $1.1(5)$	$C_2 = C_1 = N_1 = C_2$	1	-133.0(3)	02-03	—C4—C5 —C5—C6	178 2	(3)
N1—Cu1—O2—C4 $-38.8 (3)$ C4—C5—C6—C7 $1.0 (6)$ N1 <sup>i</sup> —Cu1—O2—C4141.2 (3)C5—C6—C7—C8 $1.8 (5)$ O1—N1—C2—C3 $-178.3 (3)$ C5—C6—C7—Br1 $-176.9 (3)$ Cu1—N1—C2—C3 $-14.3 (5)$ C6—C7—C8—C3 $-2.8 (5)$ N1—C2—C3—C8 $171.7 (3)$ Br1—C7—C8—C3 $175.9 (3)$ N1—C2—C3—C4 $-8.6 (6)$ C4—C3—C8—C7 $1.1 (5)$	Cu1—N1—01—	C1	63 0 (3)	C3—C4		-2.6	(5)
N1 <sup>i</sup> -Cu1-O2-C4       141.2 (3)       C5-C6-C7-C8       1.8 (5)         O1-N1-C2-C3       -178.3 (3)       C5-C6-C7-Br1       -176.9 (3)         Cu1-N1-C2-C3       -14.3 (5)       C6-C7-C8-C3       -2.8 (5)         N1-C2-C3-C8       171.7 (3)       Br1-C7-C8-C3       175.9 (3)         N1-C2-C3-C4       -8.6 (6)       C4-C3-C8-C7       1.1 (5)	N1—Cu1—O2—	C4	-38.8 (3)	C4—C5		1.0 (6	5)
N1 - C2 - C3       -178.3 (3)       C5 - C6 - C7 - Br1       -176.9 (3)         Cu1 - N1 - C2 - C3       -14.3 (5)       C6 - C7 - C8 - C3       -2.8 (5)         N1 - C2 - C3 - C8       171.7 (3)       Br1 - C7 - C8 - C3       175.9 (3)         N1 - C2 - C3 - C4       -8.6 (6)       C4 - C3 - C8 - C7       1.1 (5)	$N1^{i}$ $Cu1$ $O2$	-C4	141.2 (3)	C5—C6		186	5)
Cu1-N1-C2-C3 $-14.3 (5)$ C6-C7-C8-C3 $-2.8 (5)$ N1-C2-C3-C8171.7 (3)Br1-C7-C8-C3175.9 (3)N1-C2-C3-C4 $-8.6 (6)$ C4-C3-C8-C71.1 (5)	01 - N1 - C2 - C2	3	-1783(3)	C5_C6	$-C7-Br^{1}$	-176	9(3)
N1-C2-C3-C8     171.7 (3)     Br1-C7-C8-C3     175.9 (3)       N1-C2-C3-C4     -8.6 (6)     C4-C3-C8-C7     1.1 (5)	$C_{11} = N_1 = C_2 = C_2$	C3	-143(5)	C6	- <u>C8</u> - <u>C3</u>	-2 8	(5)
N1-C2-C3-C4 -8.6 (6) C4-C3-C8-C7 1.1 (5)	N1-C2-C3-C	8	171.7 (3)	Br1—C	7	175 9	(3)
	N1-C2-C3-C	4	-8.6 (6)	C4—C3	C7	1.1 (5	5)

# supplementary materials

Cu1—O2—C4—C3	29.8 (5)	C2—C3—C8—C7	-	-179.2 (3)			
Cu1—O2—C4—C5	-151.0 (3)						
Symmetry codes: (i) $-x+1, -y+1, -z+1$ .							
Hydrogen-bond geometry (Å, °)							
D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	D—H···A			
C1—H1C···O1 <sup>ii</sup>	0.96	2.52	3.328 (5)	142			
Symmetry codes: (ii) $x, y+1, z$ .							

Fig. 1



