metal-organic compounds

Acta Crystallographica Section E Structure Reports Online

ISSN 1600-5368

catena-Poly[[[bis(2-methyl-1*H*-imidazole- κN^3)copper(II)]- μ -biphenyl-2,2'dicarboxylato- $\kappa^2 O:O'$] dihydrate]

Liang Wang,* Xiu-Ying Li, Yang Liu and Jian Wang

Department of Chemistry, Jilin Normal University, Siping 136000, People's Republic of China

Correspondence e-mail: liangwangjl@yahoo.com.cn

Received 24 September 2007; accepted 26 September 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ (C–C) = 0.005 Å; R factor = 0.043; wR factor = 0.101; data-to-parameter ratio = 17.7.

In the title compound, $\{[Cu(C_{14}H_8O_4)(C_4H_6N_2)_2]\cdot 2H_2O\}_n$, each Cu^{II} atom is four-coordinated by two N atoms from two 2-methyl-1*H*-imidazole (mi) ligands and two O atoms from two biphenyl-2,2'-dicarboxylate (dpdc) anions in a distorted square-planar coordination environment. Each dpdc ligand bridges two neighboring Cu^{II} atoms in a bis-mono-dentate mode, forming a zigzag chain along the *b* axis. These chains are decorated with mi ligands alternately on the two sides. O-H···O and N-H···O hydrogen bonds involving the water molecules link the chains together, forming a supra-molecular structure.

Related literature

For related literature, see: Chen & Liu (2002); De (2007); Lehn (1990).



Experimental

Crystal data [Cu(C₁₄H₈O₄)(C₄H₆N₂)₂]·2H₂O $M_r = 503.99$ Monoclinic, $P2_1/n$ a = 8.7554 (18) Å b = 17.940 (4) Å c = 16.116 (3) Å $\beta = 104.65$ (3)°

 $V = 2449.0 (9) \text{ Å}^{3}$ Z = 4Mo K\alpha radiation $\mu = 0.94 \text{ mm}^{-1}$ T = 293 (2) K $0.33 \times 0.25 \times 0.19 \text{ mm}$

Data collection

```
Rigaku R-AXIS RAPID
diffractometer
Absorption correction: multi-scan
(ABSCOR; Higashi, 1995)
T_{\rm min} = 0.731, T_{\rm max} = 0.836
```

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$	H atoms treated by a mixture of
$wR(F^2) = 0.101$	independent and constrained
S = 1.03	refinement
5578 reflections	$\Delta \rho_{\rm max} = 0.47 \ {\rm e} \ {\rm \AA}^{-3}$
316 parameters	$\Delta \rho_{\rm min} = -0.32 \text{ e} \text{ Å}^{-3}$
12 restraints	

23229 measured reflections

 $R_{\rm int} = 0.056$

5578 independent reflections

4004 reflections with $I > 2\sigma(I)$

Table 1

Selected geometric parameters (Å, °).

Cu1—N1	1.994 (2)	$\begin{array}{c} Cu1\!-\!O2\\ Cu1\!-\!O4^i \end{array}$	1.9488 (17)
Cu1—N3	1.960 (2)		2.0005 (18)
D2-Cu1-N3	165.28 (8)	$\begin{array}{c} O2{-}Cu1{-}O4^i\\ N3{-}Cu1{-}O4^i\\ N1{-}Cu1{-}O4^i \end{array}$	89.39 (8)
D2-Cu1-N1	91.99 (9)		90.88 (9)
N3-Cu1-N1	90.72 (9)		168.31 (8)
······	. 1 1 . 3		

Symmetry code: (i) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$.

Table 2 Hydrogen-bond geometry (Å. Second second

Η	yd	rogen-	bond	geometry	(A,	°).	
---	----	--------	------	----------	-----	-----	--

$D - H \cdots A$	D-H	$H \cdots A$	$D \cdot \cdot \cdot A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$O1W - HW12 \cdots O2W^{ii}$	0.840 (17)	1.94 (2)	2.757 (4)	163 (3)
$O1W - HW11 \cdots O2W^{iii}$	0.837 (17)	2.02 (2)	2.846 (4)	169 (3)
$O2W - HW21 \cdots O1$	0.842 (17)	1.922 (18)	2.761 (3)	174 (4)
O2W−HW22···O3	0.859 (18)	1.884 (18)	2.738 (3)	173 (4)
$N2-H2\cdots O4^{iv}$	0.86	1.98	2.814 (3)	164
$N4-H4A\cdotsO1W$	0.86	1.90	2.738 (4)	163
Symmetry codes: (ii) -x + 1, -y + 1, -z + 2.	$-x - \frac{1}{2}, y - \frac{1}{2},$	$-z + \frac{3}{2};$ (iii)	$x - \frac{1}{2}, -y +$	$\frac{1}{2}, z + \frac{1}{2};$ (iv)

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

The authors thank Jilin Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2473).

References

- Chen, X. M. & Liu, G. F. (2002). Chem. Eur. J. 8, 4811-4817.
- De, G. (2007). Acta Cryst. E63, m1748-m1749.
- Higashi, T. (1995). ABSCOR. Rigaku Corporation, Tokyo, Japan.
- Lehn, J. M. (1990). Angew. Chem. Int. Ed. Engl. 29, 1304-1305.
- Rigaku (1998). PROCESS-AUTO. Rigaku Corporation, Tokyo, Japan.
- Sheldrick, G. M. (1990). SHELXTL-Plus. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.

Acta Cryst. (2007). E63, m2636 [doi:10.1107/S160053680704723X]

catena-Poly[[[bis(2-methyl-1*H*-imidazole- κN^3)copper(II)]- μ -biphenyl-2,2'-dicarboxylato- $\kappa^2 O:O'$] dihydrate]

L. Wang, X.-Y. Li, Y. Liu and J. Wang

Comment

Helical or chain structures have received much attention in coordination chemistry (Chen & Liu, 2002). An appropriate bidentate carboxylate could be useful in the formation of helical chains in the presence of secondary ligands (Lehn, 1990). 2,2'-Diphenyldicarboxylic acid (H₂dpdc) is a benzoic acid-based ligand, where the two phenyl rings can freely twist to meet the requirements of the coordination geometries of metal ions in the assembly process. We selected H₂dpdc as a bridging ligand and 2-methyl-1*H*-imidazole (mi) as a secondary ligand, generating a new zigzag chain coordination polymer, $[Cu(dpdc)(mi)_2]$ ²H₂O, (I), which is reported here.

Selected bond lengths and angles are listed in Table 1. In the title compound, each Cu^{II} atom is four-coordinated by two N atoms from two mi ligands, and two O atoms from two dpdc ligands in a square-planar coordination environment (Fig. 1). The Cu—O distances vary from 1.9488 (17) to 2.0005 (18) Å (Table 1), and the Cu1—N3 and Cu1—N1 distances are 1.960 (2) and 1.994 (2) Å, respectively. Each dpdc ligand bridges two neighboring Cu^{II} atoms in a bis-monodentate mode, forming a zigzag chain along the *b* axis (Fig. 2). The chain is decorated with mi ligands alternately at two sides. Furthermore, the O—H…O and N—H…O hydrogen bonds (Table 2) link the chains together, resulting in a supramolecular structure.

Experimental

A mixture of $CuCl_2 2H_2O(0.5 \text{ mmol})$, $H_2dpdc(0.5 \text{ mmol})$, mi (0.5 mmol), and $H_2O(500 \text{ mmol})$ was adjusted to pH=5.8 by addition of aqueous NaOH solution, and heated at 458 K for 2 d. After the mixture was slowly cooled to room temperature, blue crystals of (I) were obtained (yield 27%).

Refinement

C- and N-bound H atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93–0.96 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(\text{carrier})$. The water H-atoms were located in a difference Fourier map, and were refined with distance restraints of O–H = 0.85 Å The U^{ij} components of atom O1 were approximated to isotropic behaviour.

Figures



Fig. 1. The structure of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (i) 1/2 - x, y - 1/2, 3/1 - z.



Fig. 2. View of the chain structure in the title compound.

catena-Poly[[[bis(2-methyl-1*H*-imidazole- κN^3)copper(II)]- μ -biphenyl-2,2'-dicarboxylato- $\kappa^2 O:O'$] dihydrate]

 $D_{\rm x} = 1.367 \text{ Mg m}^{-3}$ Mo *K* α radiation $\lambda = 0.71073 \text{ Å}$

 $0.33 \times 0.25 \times 0.19 \text{ mm}$

Cell parameters from 17307 reflections

 $F_{000} = 1044$

 $\theta = 3.0-27.5^{\circ}$ $\mu = 0.94 \text{ mm}^{-1}$ T = 293 (2) KBlock, blue

Crystal data
$[Cu(C_{14}H_8O_4)(C_4H_6N_2)_2] \cdot 2H_2O$
$M_r = 503.99$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
<i>a</i> = 8.7554 (18) Å
<i>b</i> = 17.940 (4) Å
c = 16.116 (3) Å
$\beta = 104.65 \ (3)^{\circ}$
$V = 2449.0 (9) \text{ Å}^3$
Z = 4

Data collection

Rigaku R-AXIS RAPID diffractometer	5578 independent reflections
Radiation source: rotating anode	4004 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\rm int} = 0.056$
Detector resolution: 10.0 pixels mm ⁻¹	$\theta_{\text{max}} = 27.5^{\circ}$
T = 293(2) K	$\theta_{\min} = 3.0^{\circ}$
ω scans	$h = -11 \rightarrow 11$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	<i>k</i> = −23→23
$T_{\min} = 0.731, T_{\max} = 0.836$	$l = -20 \rightarrow 20$
23229 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.101$	$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 1.0153P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{\rm max} = 0.001$
5578 reflections	$\Delta \rho_{\rm max} = 0.47 \ {\rm e} \ {\rm \AA}^{-3}$

316 parameters

 $\Delta \rho_{min} = -0.32 \text{ e } \text{\AA}^{-3}$

12 restraints

Extinction correction: none

Primary atom site location: structure-invariant direct methods

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.

	x	У	z	$U_{\rm iso}$ */ $U_{\rm eq}$
C1	-0.0628 (3)	0.14907 (16)	0.89714 (17)	0.0417 (6)
C2	0.0462 (4)	0.09492 (19)	0.9508 (2)	0.0650 (9)
H2A	-0.0049	0.0716	0.9902	0.097*
H2B	0.1394	0.1203	0.9822	0.097*
H2C	0.0748	0.0576	0.9147	0.097*
C3	-0.2843 (4)	0.2071 (2)	0.8369 (2)	0.0628 (9)
Н3	-0.3902	0.2207	0.8210	0.075*
C4	-0.1646 (3)	0.23935 (19)	0.81210 (19)	0.0527 (8)
H4	-0.1740	0.2799	0.7752	0.063*
C5	0.1416 (4)	0.29497 (18)	1.00860 (19)	0.0521 (7)
Н5	0.0352	0.3051	0.9852	0.063*
C6	0.2215 (4)	0.3096 (2)	1.0897 (2)	0.0588 (8)
H6	0.1819	0.3315	1.1322	0.071*
C7	0.3821 (3)	0.25763 (16)	1.02174 (17)	0.0444 (6)
C8	0.5277 (4)	0.2251 (2)	1.0070 (2)	0.0699 (10)
H8A	0.5976	0.2116	1.0610	0.105*
H8B	0.5784	0.2609	0.9788	0.105*
H8C	0.5017	0.1815	0.9717	0.105*
С9	0.3097 (3)	0.34777 (15)	0.78098 (17)	0.0381 (6)
C10	0.4314 (3)	0.40035 (15)	0.76376 (17)	0.0397 (6)
C11	0.5341 (4)	0.37354 (18)	0.7172 (2)	0.0581 (8)
H11	0.5226	0.3250	0.6964	0.070*
C12	0.6531 (4)	0.4179 (2)	0.7015 (2)	0.0695 (11)
H12	0.7201	0.3994	0.6699	0.083*
C13	0.6715 (4)	0.4893 (2)	0.7328 (2)	0.0679 (10)
H13	0.7528	0.5189	0.7236	0.081*
C14	0.5691 (4)	0.51740 (18)	0.7781 (2)	0.0558 (8)
H14	0.5817	0.5662	0.7981	0.067*
C15	0.4473 (3)	0.47388 (15)	0.79433 (17)	0.0398 (6)

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

C16	0.3490 (3)	0.50494 (15)	0.84949 (17)	0.0409 (6)
C17	0.3339 (4)	0.46496 (17)	0.92179 (19)	0.0540 (8)
H17	0.3793	0.4179	0.9322	0.065*
C18	0.2531 (5)	0.4938 (2)	0.9781 (2)	0.0700 (10)
H18	0.2425	0.4659	1.0249	0.084*
C19	0.1889 (5)	0.5637 (2)	0.9645 (2)	0.0805 (12)
H19	0.1351	0.5834	1.0024	0.097*
C20	0.2040 (5)	0.60497 (19)	0.8946 (2)	0.0682 (10)
H20	0.1615	0.6527	0.8863	0.082*
C21	0.2815 (3)	0.57618 (15)	0.83676 (17)	0.0429 (6)
C22	0.2822 (3)	0.62358 (15)	0.75948 (18)	0.0414 (6)
N1	0.2424 (3)	0.26251 (13)	0.96545 (14)	0.0411 (5)
N2	0.3718 (3)	0.28605 (15)	1.09724 (15)	0.0528 (6)
H2	0.4479	0.2889	1.1429	0.063*
N3	-0.0259 (2)	0.20308 (13)	0.84973 (13)	0.0394 (5)
N4	-0.2186 (3)	0.15028 (15)	0.89015 (16)	0.0530 (6)
H4A	-0.2689	0.1201	0.9152	0.064*
01	0.1663 (2)	0.36111 (11)	0.75780 (13)	0.0527 (5)
O2	0.3644 (2)	0.28816 (10)	0.82080 (11)	0.0399 (4)
O1W	-0.3240 (3)	0.03831 (16)	0.9770 (2)	0.0705 (7)
O3	0.2146 (3)	0.60283 (11)	0.68615 (13)	0.0564 (5)
O2W	0.0770 (3)	0.46838 (15)	0.63200 (15)	0.0693 (7)
O4	0.3503 (2)	0.68677 (10)	0.77385 (11)	0.0412 (4)
Cu1	0.18444 (3)	0.234302 (17)	0.841723 (19)	0.03370 (10)
HW11	-0.343 (4)	0.040 (2)	1.0252 (14)	0.092 (15)*
HW12	-0.387 (3)	0.0107 (17)	0.9426 (16)	0.067 (12)*
HW21	0.098 (4)	0.4360 (15)	0.6711 (19)	0.085 (13)*
HW22	0.117 (5)	0.5101 (13)	0.653 (2)	0.104 (16)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0451 (15)	0.0391 (15)	0.0404 (15)	-0.0007 (12)	0.0100 (12)	-0.0022 (12)
C2	0.064 (2)	0.056 (2)	0.074 (2)	0.0047 (17)	0.0160 (18)	0.0243 (18)
C3	0.0450 (17)	0.091 (3)	0.055 (2)	0.0161 (17)	0.0183 (15)	0.0137 (18)
C4	0.0500 (16)	0.065 (2)	0.0435 (16)	0.0158 (15)	0.0132 (13)	0.0115 (15)
C5	0.0534 (17)	0.0579 (19)	0.0472 (18)	0.0024 (15)	0.0166 (14)	-0.0099 (15)
C6	0.065 (2)	0.069 (2)	0.0455 (18)	-0.0003 (17)	0.0192 (16)	-0.0166 (16)
C7	0.0541 (16)	0.0437 (16)	0.0335 (14)	0.0004 (13)	0.0075 (12)	-0.0014 (12)
C8	0.0571 (19)	0.095 (3)	0.052 (2)	0.0228 (19)	0.0043 (16)	-0.0044 (19)
C9	0.0462 (15)	0.0306 (14)	0.0399 (15)	0.0026 (12)	0.0150 (12)	-0.0013 (11)
C10	0.0447 (14)	0.0344 (14)	0.0419 (15)	0.0066 (12)	0.0144 (12)	0.0114 (12)
C11	0.071 (2)	0.0449 (18)	0.067 (2)	0.0132 (16)	0.0320 (18)	0.0109 (15)
C12	0.071 (2)	0.071 (3)	0.083 (3)	0.0221 (19)	0.049 (2)	0.032 (2)
C13	0.0544 (19)	0.062 (2)	0.095 (3)	0.0034 (17)	0.0333 (19)	0.034 (2)
C14	0.0557 (18)	0.0437 (17)	0.068 (2)	-0.0022 (15)	0.0153 (16)	0.0164 (15)
C15	0.0432 (14)	0.0341 (14)	0.0411 (15)	0.0018 (12)	0.0086 (12)	0.0127 (12)
C16	0.0511 (15)	0.0342 (15)	0.0371 (14)	-0.0044 (12)	0.0106 (12)	0.0030 (11)

C17	0.076 (2)	0.0389 (17)	0.0474 (17)	-0.0025 (15)	0.0164 (16)	0.0080 (13)
C18	0.109 (3)	0.057 (2)	0.053 (2)	-0.001 (2)	0.039 (2)	0.0134 (16)
C19	0.132 (4)	0.057 (2)	0.074 (3)	0.013 (2)	0.065 (3)	0.0047 (19)
C20	0.106 (3)	0.0456 (19)	0.066 (2)	0.0128 (19)	0.045 (2)	0.0068 (16)
C21	0.0554 (16)	0.0351 (15)	0.0404 (15)	-0.0004 (13)	0.0163 (13)	0.0064 (12)
C22	0.0495 (15)	0.0342 (15)	0.0425 (16)	0.0069 (12)	0.0153 (13)	0.0036 (12)
N1	0.0453 (12)	0.0425 (13)	0.0351 (12)	-0.0010 (11)	0.0092 (10)	-0.0045 (10)
N2	0.0574 (15)	0.0622 (17)	0.0339 (13)	-0.0017 (13)	0.0027 (11)	-0.0090 (11)
N3	0.0407 (12)	0.0406 (13)	0.0352 (12)	0.0008 (10)	0.0066 (10)	0.0047 (10)
N4	0.0478 (14)	0.0635 (17)	0.0538 (15)	-0.0040 (13)	0.0239 (12)	0.0033 (13)
01	0.0491 (8)	0.0475 (9)	0.0609 (9)	0.0017 (7)	0.0128 (7)	0.0060 (7)
O2	0.0460 (10)	0.0300 (9)	0.0425 (11)	-0.0002 (8)	0.0090 (8)	0.0062 (8)
O1W	0.0589 (15)	0.0783 (19)	0.0736 (18)	-0.0173 (13)	0.0155 (14)	0.0119 (15)
O3	0.0795 (15)	0.0430 (12)	0.0420 (12)	-0.0114 (11)	0.0065 (11)	0.0007 (9)
O2W	0.0917 (18)	0.0457 (15)	0.0552 (14)	-0.0042 (13)	-0.0099 (13)	0.0049 (12)
O4	0.0513 (11)	0.0327 (10)	0.0383 (10)	-0.0024 (8)	0.0089 (8)	0.0039 (8)
Cu1	0.03913 (17)	0.02943 (16)	0.03139 (16)	0.00027 (14)	0.00683 (12)	0.00007 (14)

Geometric parameters (Å, °)

C1—N3	1.324 (3)	C12—H12	0.93
C1—N4	1.340 (3)	C13—C14	1.386 (5)
C1—C2	1.478 (4)	С13—Н13	0.93
C2—H2A	0.96	C14—C15	1.399 (4)
C2—H2B	0.96	C14—H14	0.93
C2—H2C	0.96	C15—C16	1.493 (4)
C3—C4	1.344 (4)	C16—C21	1.401 (4)
C3—N4	1.363 (4)	C16—C17	1.403 (4)
С3—Н3	0.93	C17—C18	1.384 (4)
C4—N3	1.376 (3)	С17—Н17	0.93
C4—H4	0.93	C18—C19	1.369 (5)
C5—C6	1.343 (4)	C18—H18	0.93
C5—N1	1.383 (4)	C19—C20	1.383 (4)
С5—Н5	0.93	С19—Н19	0.93
C6—N2	1.357 (4)	C20—C21	1.384 (4)
С6—Н6	0.93	С20—Н20	0.93
C7—N1	1.328 (4)	C21—C22	1.509 (4)
C7—N2	1.343 (3)	C22—O3	1.238 (3)
С7—С8	1.475 (4)	C22—O4	1.274 (3)
C8—H8A	0.96	Cu1—N1	1.994 (2)
C8—H8B	0.96	N2—H2	0.86
C8—H8C	0.96	Cu1—N3	1.960 (2)
C9—O1	1.240 (3)	N4—H4A	0.86
C9—O2	1.276 (3)	Cu1—O2	1.9488 (17)
C9—C10	1.500 (4)	O1W—HW11	0.837 (17)
C10-C11	1.395 (4)	O1W—HW12	0.840 (17)
C10-C15	1.403 (4)	O2W—HW21	0.842 (17)
C11—C12	1.384 (5)	O2W—HW22	0.859 (18)
C11—H11	0.93	O4—Cu1 ⁱ	2.0005 (18)

N3-C1-N4 109.4 (2) C15-C14-H14 119.3 N3-C1-C2 127.1 (3) C14-C15-C16 119.0 (3) C1-C2 123.6 (3) C14-C15-C16 122.6 (2) C1-C2-H2A 109.5 C10-C15-C16 122.6 (2) C1-C2-H2B 109.5 C12-C16-C15 122.6 (2) C1-C2-H2C 109.5 C18-C17-C16 121.6 (3) H2A-C2-H2C 109.5 C18-C17-H17 119.2 C4-C3-H3 127.1 C19-C18-C17 119.7 (3) H2B-C2-H12C 109.5 (3) C16-C17-H17 119.2 C4-C3-H3 127.1 C19-C18-H18 120.1 C3-C4-H3 127.1 C19-C18-H18 120.1 C3-C4-H4 125.3 C18-C19-H19 120.0 C6-C5-H1 109.3 (3) C20-C19-H19 120.0 C6-C5-H5 125.4 C19-C20-C12 120.9 (3) N1-C5-H5 125.4 C19-C20-H20 119.5 C5-C6-H6 126.8 C20-C21-C2 120.2 (3) N1-C7-N2 109.4 (3)	C12—C13	1.371 (5)	Cu1—O4 ⁱⁱ	2.0005 (18)
N3-C1-C2 127.1 (3) C14-C15-C10 118.2 (3) N4-C1-C2 123.6 (3) C14-C15-C16 122.6 (2) C1-C2-H2A 109.5 C10-C15-C16 122.6 (2) C1-C2-H2B 109.5 C1-C16-C15 129.6 (3) H2A-C2-H2C 109.5 C18-C17-C16 121.6 (3) H2B-C2-H2C 109.5 C18-C17-C16 121.6 (3) H2B-C2-H2C 109.5 C18-C17-H17 119.2 C4-C3-N4 105.8 (3) C16-C17-H17 119.7 (3) N4-C3-H3 127.1 C19-C18-C17 119.7 (3) C3-C4-N3 109.5 (3) C17-C16-H18 120.1 C3-C4-N3 109.5 (3) C17-C16-H18 120.1 C3-C4-N4 125.3 C18-C19-C20 120.0 (3) C4-C3-N1 109.3 (3) C20-C19-H19 120.0 C6-C5-N1 109.3 (3) C21-C20-C21 120.9 (3) C5-C6-N2 106.3 (3) C21-C20-H20 119.5 C5-C6-N2 106.3 (3) C21-C20-H20 119.5 C5-C6-N2 106.3 (3) C32-C2-C21 120.8 (3) N1-C7-N2	N3—C1—N4	109.4 (2)	C15—C14—H14	119.3
N4-ClC2 123.6 (3) Cl4-Cl5-Cl6 119.0 (3) ClC2-H2A 109.5 Cl0-Cl5-Cl6 122.6 (2) H2A-C2-H2B 109.5 ClCl-Cl6 122.6 (2) H2A-C2-H2B 109.5 ClCl-Cl5 129.6 (3) H2A-C2-H2C 109.5 Cl8-Cl7-Cl6 121.6 (3) H2A-C2-H2C 109.5 Cl8-Cl7-H17 119.2 C4-C3-H3 127.1 Cl9-Cl8-Cl7 119.7 (3) N4-C3-H3 127.1 Cl9-Cl8-H18 120.1 C3-C4-H4 125.3 Cl8-Cl9-H19 120.0 (3) C6-C5-N1 109.3 (3) C20-Cl9-H19 120.0 (3) C6-C5-H5 125.4 Cl9-C20-C21 120.9 (3) N1-C5-H5 125.4 Cl9-C20-H20 119.5 C5-C6-H6 126.8 C20-C21-Cl6 120.2 (3) N1-C7-N2 109.4 (3) Cl6-C2-L-C1 123.0 (2) N1-C7-C8 126.9 (3) O3-C22-O4 122.0 (2) N2-C7-C8 123.7 (3) O3-C22-O4 122.0 (2) N1-C7-C8 <td< td=""><td>N3—C1—C2</td><td>127.1 (3)</td><td>C14—C15—C10</td><td>118.2 (3)</td></td<>	N3—C1—C2	127.1 (3)	C14—C15—C10	118.2 (3)
C1-C2-H2A 109.5 C10-C15-C16 122.6 (2) C1-C2-H2B 109.5 C21-C16-C17 117.6 (2) H2A-C2-H2B 109.5 C17-C16-C15 122.6 (2) C1-C2-H2C 109.5 C18-C17-C16 121.6 (3) H2A-C2-H2C 109.5 C18-C17-H17 119.2 C4-C3-N4 105.8 (3) C16-C17-H17 119.2 C4-C3-H3 127.1 C19-C18-H18 120.1 C3-C4-N3 109.5 (3) C17-C18-H18 120.1 C3-C4-H4 125.3 C18-C19-H19 120.0 C6-C5-N1 109.3 (3) C20-C19-H19 120.0 C6-C5-H5 125.4 C19-C20-H20 119.5 C5-C6-N2 106.3 (3) C21-C20-H20 119.5 C5-C6-N2 106.3 (3) C21-C22 16.8 (3) N1-C7-N2 109.4 (3) C16-C21-C22 12.8 (3) N1-C7-R8 126.9 (3) O3-C22-C1 12.2 (3) N1-C7-R8 126.9 (3) O3-C22-C21 12.2 (3) C7-C8-H8B 109.5	N4—C1—C2	123.6 (3)	C14—C15—C16	119.0 (3)
CI-C2-H2B 109.5 $C2I-C16-C17$ 117.6 (2) $H2A-C2-H2B$ 109.5 $C2I-C16-C15$ 122.6 (2) $C1-C2-H2C$ 109.5 $C17-C16-C15$ 129.6 (3) $H2A-C2-H2C$ 109.5 $C18-C17-C16$ 121.6 (3) $H2B-C2-H2C$ 109.5 $C18-C17-H17$ 119.2 $C4-C3-M4$ 105.8 (3) $C16-C17-H17$ 119.2 $C4-C3-M3$ 109.5 (3) $C17-C18-H18$ 120.1 $C3-C4-H4$ 125.3 $C18-C19-H19$ 120.0 $C6-C5-H1$ 109.3 (3) $C21-C20-H19$ 120.0 $C6-C5-H5$ 125.4 $C19-C20-C21$ 120.9 (6) $NI-C5-H5$ 125.4 $C19-C20-H19$ 120.0 $C5-C6-H6$ 126.8 $C20-C21-C16$ 120.2 (3) $N1-C7-N2$ 109.4 (3) $C16-C1-C22-C22$ 116.8 (3) $N1-C7-N2$ 109.4 (3) $C16-C21-C22$ 120.0 (2) $N2-C5-H6$ 126.8 C20-C21-C12 120.0 (2) $N2-C5-H6$ 126.8 C20-C21-C12 116.8 (2)	C1—C2—H2A	109.5	C10-C15-C16	122.6 (2)
H2A-C2-H2B 109.5 C21-C16-C15 122.6 (2) C1-C2-H2C 109.5 C17-C16-C15 121.6 (3) H2A-C2-H2C 109.5 C18-C17-C16 121.6 (3) H2B-C2-H2C 109.5 C18-C17-H17 119.2 C4-C3-H4 105.8 (3) C16-C17-H17 119.7 (3) N4-C3-H3 127.1 C19-C18-H18 120.1 C3-C4-H4 125.3 C18-C17-H19 120.0 C6-C5-H1 109.3 (3) C20-C19-H19 120.0 C6-C5-H1 109.3 (3) C20-C19-H19 120.0 C6-C5-H5 125.4 C19-C20-H20 119.5 C5-C6-H2 106.3 (3) C21-C20-H20 119.5 C5-C6-H5 126.8 C20-C21-C16 120.2 (3) N2-C6-H6 126.8 C20-C21-C16 120.2 (3) N2-C7-R2 109.4 (3) C16-C21-C22 116.8 (3) N1-C7-R2 126.9 (3) 03-C22-O4 122.0 (2) N2-C7-R4 126.9 (3) 03-C22-C21 121.2 (3) C7-C8-H8B 109.5 C7-N1-C3 108.8 (3) RA-C8-H8C 109.5	C1—C2—H2B	109.5	C21—C16—C17	117.6 (2)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H2A—C2—H2B	109.5	C21—C16—C15	122.6 (2)
H2A-C2-H2C 109.5 $C18-C17-C16$ 121.6 (3) $H2B-C2-H2C$ 109.5 $C18-C17-H17$ 119.2 $C4-C3-H4$ 105.8 (3) $C16-C17-H17$ 119.7 (3) $N4-C3-H3$ 127.1 $C19-C18-H18$ 120.1 $C3-C4-H4$ 125.3 $C18-C19-C20$ 120.0 (3) $N3-C4-H4$ 125.3 $C18-C19-H19$ 120.0 $C6-C5-H1$ 109.3 (3) C20-C19-H19 120.0 $C6-C5-H1$ 109.3 (3) C20-C19-H19 120.9 (3) $N1-C5-H5$ 125.4 C19-C20-H20 119.5 $C5-C6-H2$ 106.3 (3) C21-C20-H20 119.5 $C5-C6-H2$ 106.3 (3) C16-C21-C22 118.6 (3) $N1-C7-N2$ 109.4 (3) C16-C21-C22 118.6 (3) $N1-C7-R8$ 123.7 (3) 03-C22-O4 122.0 (2) $N2-C6-H8$ 109.5 C7-N1-C1 128.57 (19) $N1-C7-R8$ 123.7 (3) 03-C22-C21 116.6 (2) $C7-C8-H8A$ 109.5 C7-N1-C4 106.2 (2) $N1-C7-R8$ 123.7 (3) C5-N1-C4 125.17 (19)	C1—C2—H2C	109.5	C17—C16—C15	119.6 (3)
H2B-C2-H2C 109.5 C18-C17-H17 119.2 C4-C3-N4 105.8 (3) C16-C17-H17 119.7 (3) N4-C3-H3 127.1 C19-C18-C17 119.7 (3) N4-C3-H3 127.1 C19-C18-H18 120.1 C3-C4-N3 109.5 (3) C17-C18-H18 120.0 C6-C5-N1 109.3 (3) C20-C19-H19 120.0 C6-C5-N1 109.3 (3) C20-C19-H19 120.0 C6-C5-H5 125.4 C19-C20-C21 129.9 (3) N1-C5-H5 125.4 C19-C20-H20 119.5 C5-C6-N2 106.3 (3) C21-C20-H20 119.5 C5-C6-H6 126.8 C20-C21-C16 120.2 (3) N1-C7-C8 126.9 (3) O3-C22-C21 116.8 (3) N1-C7-C8 126.9 (3) O3-C22-C21 116.8 (2) C7-C8-H8A 109.5 C7-N1-C5 106.2 (2) N2-C6-H8A 109.5 C7-N1-C41 125.17 (19) C7-C8-H8B 109.5 C7-N1-C41 125.17 (19) C7-C8-H8C 109.5 C7-N2-C6 108.8 (3) NBA-C8-H8C 109.5 <	H2A—C2—H2C	109.5	C18—C17—C16	121.6 (3)
C4-C3-N4 105.8 (3) $C16-C17-H17$ 119.2 $C4-C3-H3$ 127.1 $C19-C18-C17$ 119.7 (3) $N4-C3-H3$ 109.5 (3) $C17-C18-H18$ 120.1 $C3-C4-H3$ 109.5 (3) $C17-C18-H18$ 120.1 $C3-C4-H4$ 125.3 $C18-C19-C20$ 120.0 (3) $N3-C4-H4$ 125.3 $C18-C19-H19$ 120.0 $C6-C5-H1$ 109.3 (3) $C20-C19-H19$ 120.0 $C6-C5-H5$ 125.4 $C19-C20-H20$ 119.5 $C5-C6-N2$ 106.3 (3) $C21-C20-H20$ 119.5 $C5-C6-H6$ 126.8 $C20-C21-C22$ 16.8 (3) $N1-C7-X2$ 109.4 (3) $C16-C21-C22$ 123.0 (2) $N-C7-C8$ 123.7 (3) $O3-C22-C41$ 121.2 (3) $C7-C8-H8A$ 109.5 $C7-N1-C5$ 106.2 (2) $N=A-C8-H8B$ 109.5 $C7-N1-C5$ 106.2 (2) $N=A-C8-H8C$ 109.5 $C7-N1-C5$ 106.2 (2) $N=A-C8-H8C$ 109.5 $C7-N1-C1$ 125.6 (2)	H2B—C2—H2C	109.5	С18—С17—Н17	119.2
C4-C3-H3 127.1 $C19-C18-C17$ $119.7 (3)$ $N4-C3-H3$ 127.1 $C19-C18-H18$ 120.1 $C3-C4-N3$ 109.5 (3) $C17-C18-H18$ 120.1 $C3-C4-H4$ 125.3 $C18-C19-C20$ 120.0 (3) $N3-C4-H4$ 125.3 $C18-C19-H19$ 120.0 $C6-C5-N1$ 109.3 (3) $C20-C19-H19$ 120.0 $C6-C5-H5$ 125.4 $C19-C20-C21$ 120.9 (3) $N1-C5-H5$ 125.4 $C19-C20-H20$ 119.5 $C5-C6-N2$ 106.3 (3) $C21-C20-H20$ 119.5 $C5-C6-H6$ 126.8 $C20-C21-C12$ 123.0 (2) $N1-C7-N2$ 109.4 (3) $C16-C21-C22$ 123.0 (2) $N1-C7-C8$ 126.9 (3) $O3-C22-C4$ 122.0 (2) $N2-C6-H8$ 109.5 $C7-N1-C5$ 106.2 (2) $N8-C8-H8B$ 109.5 $C7-N1-C11$ 128.57 (19) $C7-C8-H8A$ 109.5 $C7-N2-H2$ 125.6 $O1-C9-O2$ 122.4 (2) $C6-N2-H2$ 125.6	C4—C3—N4	105.8 (3)	С16—С17—Н17	119.2
N4—C3—H3 127.1 C19—C18—H18 120.1 C3—C4—N3 109.5 (3) C17—C18—H18 120.1 C3—C4—H4 125.3 C18—C19—C20 120.0 (3) N3—C4—H4 125.3 C18—C19—H19 120.0 C6—C5—N1 109.3 (3) C20—C19—H19 120.9 (3) N1—C5—H5 125.4 C19—C20—H20 119.5 C5—C6—N2 106.3 (3) C21—C20—H20 119.5 C5—C6—H6 126.8 C20—C21—C16 120.2 (3) N1—C7—N2 109.4 (3) C16—C21—C22 116.8 (3) N1—C7—N2 109.4 (3) C16—C21—C22 123.0 (2) N1—C7—C8 126.9 (3) O3—C22—C4 122.0 (2) N2—C7—C8 123.7 (3) O3—C22—C1 116.8 (2) C7—C8—H8B 109.5 C7—N1—CS 106.2 (2) H8—C8—H8E 109.5 C7—N1—Cul 128.57 (19) C7—C8—H8B 109.5 C7—N1—Cul 125.6 O1—C9—O2 122.4 (2) C6—N2—H2 125.6 O1—C9—O1 122.4 (2)	С4—С3—Н3	127.1	C19—C18—C17	119.7 (3)
C3-C4-N3 109.5 (3) C17-C18-H18 120.1 C3-C4-H4 125.3 C18-C19-C20 120.0 (3) N3-C4-H4 125.3 C18-C19-C20 120.0 C6-C5-N1 109.3 (3) C20-C19-H19 120.0 C6-C5-H5 125.4 C19-C20-C21 120.9 (3) N1-C5-H5 125.4 C19-C20-H20 119.5 C5-C6-N2 106.3 (3) C21-C20-H20 119.5 C5-C6-H6 126.8 C20-C21-C16 120.2 (3) N2-C6-H6 126.8 C20-C21-C16 120.2 (3) N1-C7-N2 109.4 (3) C16-C21-C22 13.0 (2) N1-C7-C8 123.7 (3) 03-C22-O4 122.0 (2) N2-C7-C8 123.7 (3) 03-C22-C21 16.8 (2) C7-C8-H8A 109.5 C7-N1-C5 106.2 (2) H8A-C8-H8C 109.5 C7-N1-C1 128.57 (19) C7-C8-H8B 109.5 C7-N2-C6 108.8 (3) H8B-C8-H8C 109.5 C7-N2-H2 125.6 O1-C9-C10 122.4 (2)	N4—C3—H3	127.1	С19—С18—Н18	120.1
C3-C4-H4 125.3 C18-C19-C20 120.0 (3) N3-C4-H4 125.3 C18-C19-H19 120.0 C6-C5-N1 109.3 (3) C20-C19-H19 120.0 C6-C5-H5 125.4 C19-C20-H20 119.5 C5-C6-N2 106.3 (3) C21-C20-H20 119.5 C5-C6-N2 106.3 (3) C21-C20-H20 119.5 C5-C6-H6 126.8 C20-C21-C16 120.2 (3) N1-C7-N2 109.4 (3) C16-C21-C22 123.0 (2) N1-C7-N2 109.4 (3) O3-C22-O4 122.0 (2) N2-C7-C8 123.7 (3) O3-C22-C21 168.3 (3) C7-C8-H8A 109.5 C7-N1-C5 106.2 (2) H8A-C8-H8B 109.5 C7-N1-C41 128.57 (19) C7-C8-H8C 109.5 C7-N2-C6 108.8 (3) H8B-C8-H8C 109.5 C7-N2-C6 108.8 (3) O1-C9-O2 122.4 (2) C1-N3-C4 106.5 (2) O2-C9-C10 153.3 (2) C1-N3-C4 106.5 (2) O2-C9-C10 153.3 (2)<	C3—C4—N3	109.5 (3)	С17—С18—Н18	120.1
N3-C4-H4 125.3 $C18-C19-H19$ 120.0 C6-C5-N1 109.3 (3) C20-C19-H19 120.0 C6-C5-H5 125.4 C19-C20-C21 120.9 (3) N1-C5-H5 125.4 C19-C20-H20 119.5 C5-C6-N2 106.3 (3) C21-C20-H20 119.5 C5-C6-H6 126.8 C20-C21-C16 120.2 (3) N1-C7-N2 109.4 (3) C16-C21-C22 116.8 (3) N1-C7-C8 126.9 (3) 0.3-C22-O4 122.0 (2) N2-C7-C8 123.7 (3) 0.3-C22-C21 121.2 (3) C7-C8-H8A 109.5 C7-N1-C5 106.2 (2) H8A-C8-H8B 109.5 C7-N1-C4I 125.7 (19) C7-C8-H8B 109.5 C7-N2-C6 108.8 (3) H8A-C8-H8C 109.5 C7-N2-C6 108.8 (3) H8B-C8-H8C 109.5 C7-N2-C6 108.8 (3) H8B-C8-H8C 109.5 C7-N2-H2 125.6 O1-C9-O2 122.4 (2) C1-N3-C41 125.6 O1-C9-C10 122.4 (2) C1-N3-C41 126.1 (2) C15-C10-C9 122.6 (2)	C3—C4—H4	125.3	C18—C19—C20	120.0 (3)
C6—C5—N1 109.3 (3) C20—C19—H19 120.0 C6—C5—H5 125.4 C19—C20—C21 120.9 (3) N1—C5—H5 125.4 C19—C20—H20 119.5 C5—C6—N2 106.3 (3) C21—C20—H20 119.5 C5—C6—H6 126.8 C20—C21—C16 120.2 (3) N2—C6—H6 126.8 C20—C21—C22 116.8 (3) N1—C7—N2 109.4 (3) C16—C21—C22 123.0 (2) N1—C7—C8 125.7 (3) O3—C22—C4 122.0 (2) N2—C7—C8 123.7 (3) O3—C22—C21 121.2 (3) C7—C8—H8A 109.5 C7—N1—C5 106.2 (2) H8A—C8—H8B 109.5 C7—N1—Cul 128.57 (19) C7—C8—H8C 109.5 C7—N2—H2 125.6 O1—C9—C2 122.4 (2) C6—N2—H2 125.6 O1—C9—C10 122.4 (2) C6—N2—H2 125.6 O1—C9—C10 15.3 (2) C1—N3—Cul 128.17 (19) C11—C10—C15 119.5 (3) C4—N3—Cul 125.6 C12—C10—C1 122.4 (2) C6—N2—H2 125.6 C11—C10—C15 119.5 (3)	N3—C4—H4	125.3	С18—С19—Н19	120.0
C6-C5-H5 125.4 $C19-C20-C21$ 120.9 (3) $N1-C5-H5$ 125.4 $C19-C20-H20$ 119.5 $C5-C6-N2$ 106.3 (3) $C21-C20-H20$ 119.5 $C5-C6-H6$ 126.8 $C20-C21-C16$ 120.2 (3) $N2-C6-H6$ 126.8 $C20-C21-C22$ 116.8 (3) $N1-C7-N2$ 109.4 (3) $C16-C21-C22$ 123.0 (2) $N1-C7-C8$ 126.9 (3) $O3-C22-C41$ 122.0 (2) $N2-C6-H8$ 120.7 (3) $O3-C22-C21$ 116.8 (3) $N1-C7-C8$ 123.7 (3) $O3-C22-C21$ 116.8 (2) $C7-C8-H8A$ 109.5 $C7-N1-C5$ 106.2 (2) $N8-C8-H8B$ 109.5 $C7-N1-C41$ 128.57 (19) $C7-C8-H8C$ 109.5 $C7-N2-C6$ 108.8 (3) $NB-C8-H8C$ 109.5 $C7-N2-C6$ 108.8 (3) $NB-C8-H8C$ 109.5 $C7-N2-H2$ 125.6 $O1-C9-O2$ 122.4 (2) $C1-N3-C4$ 106.5 (2) $O1-C9-C10$ 123.3 (2) $C1-N4-C3$ 108.9 (2) $C11-C10-C9$ 117.9 (3) $C1-N4-C3$ 108.9 (2)	C6—C5—N1	109.3 (3)	С20—С19—Н19	120.0
N1-C5-H5 125.4 C19-C20-H20 119.5 C5-C6-N2 106.3 (3) C21-C20-H20 119.5 C5-C6-H6 126.8 C20-C21-C16 120.2 (3) N1-C7-N2 109.4 (3) C16-C21-C22 123.0 (2) N1-C7-N2 109.4 (3) C16-C21-C22 123.0 (2) N1-C7-R2 109.4 (3) C3-C22-C4 122.0 (2) N2-C7-C8 123.7 (3) 03-C22-C21 121.2 (3) C7-C8-H8A 109.5 C7-N1-C5 106.2 (2) H8A-C8-H8B 109.5 C7-N1-Cul 125.17 (19) C7-C8-H8C 109.5 C7-N2-C6 108.8 (3) H8A-C8-H8C 109.5 C7-N2-C6 108.8 (3) H8A-C8-H8C 109.5 C7-N2-C6 108.8 (3) H8B-C8-H8C 109.5 C7-N2-H2 125.6 O1-C9-O1 122.4 (2) C1-N3-Cul 128.17 (19) C11-C10-C15 119.5 (3) C4-N3-Cul 125.1 (2) C11-C10-C15 119.5 (3) C4-N3-Cul 125.6 C12-C11-H11 <td< td=""><td>С6—С5—Н5</td><td>125.4</td><td>C19—C20—C21</td><td>120.9 (3)</td></td<>	С6—С5—Н5	125.4	C19—C20—C21	120.9 (3)
C5C6N2106.3 (3)C21C20H20119.5C5C6H6126.8C20C21C16120.2 (3)N2C6H6126.8C20C21C22116.8 (3)N1C7N2109.4 (3)C16C21C22123.0 (2)N1C7C8126.9 (3)03C22C21121.2 (3)C7C8H8A109.5O4C22C21116.8 (2)C7C8H8B109.5C7N1C5106.2 (2)H8AC8H8B109.5C7N1C1128.57 (19)C7C8H8C109.5C7N2C6108.8 (3)H8BC8H8C109.5C7N2C6108.8 (3)H8B-C8H8C109.5C7N2C6108.8 (3)10-C9C10122.4 (2)C1N3C4106.5 (2)02C9C10115.3 (2)C1N3C4106.5 (2)02-C9C10115.3 (2)C1N4C3108.9 (2)C15C10C9122.6 (2)C1-N4H4A125.6C12C11C10121.2 (3)C3N4H4A125.6C12C11C10121.2 (3)C3N4H4A125.6C12C11C10121.2 (3)C3N4H4A125.6C12C11C10121.2 (3)C3N4H4A125.6C12C11C10121.2 (3)C3N4H4A125.6C12C11C10121.2 (3)C3N4H4A125.6C12C11C10121.2 (3)C3N4H4A125.6C12C11H11119.4HW11-O1WHW12112 (3)C13C12H12120.2C2O4Cu1106.61 (16)C10C13H13119.9N3Cu1	N1—C5—H5	125.4	С19—С20—Н20	119.5
C5-C6-H6126.8C20-C21-C16120.2 (3)N2-C6-H6126.8C20-C21-C22116.8 (3)N1-C7-N2109.4 (3)C16-C21-C22123.0 (2)N1-C7-C8126.9 (3)O3-C22-O4122.0 (2)N2-C7-C8123.7 (3)O3-C22-C21121.2 (3)C7-C8-H8A109.5O4-C22-C21116.8 (2)C7-C8-H8B109.5C7-N1-C5106.2 (2)H8A-C8-H8B109.5C7-N1-Cu1128.57 (19)C7-C8-H8C109.5C7-N2-C6108.8 (3)H8B-C8-H8C109.5C7-N2-C6108.8 (3)1H8B-C8-H8C109.5C7-N2-C4125.601-C9-O2122.4 (2)C6-N2-H2125.601-C9-O2122.4 (2)C1-N3-C4106.5 (2)02-C9-C10115.3 (2)C1-N3-Cu1128.17 (19)C11-C10-C15119.5 (3)C4-N3-Cu1125.1 (2)C11-C10-C917.9 (3)C1-N4-C3108.9 (2)C12-C11-C10121.2 (3)C3-N4-H4A125.6C12-C11-H11119.4HW11-O1W-HW12112 (3)C13-C12-C11119.6 (3)HW21-O2W-HW22109 (3)C13-C12-C11119.6 (3)HW21-O2W-HW22109 (3)C13-C12-C11119.6 (3)HW21-O2W-HW22109 (3)C13-C12-C11119.6 (3)HW21-O2W-HW22109 (3)C13-C12-C11119.6 (3)HW21-O2W-HW22109 (3)C13-C12-C11119.9N3-Cu1-N191.99 (9)C13-C12-C11119.6 (3)HW21-O2W-HW22109 (3)C13-C12-C11	C5—C6—N2	106.3 (3)	С21—С20—Н20	119.5
N2C6H6 126.8 C20C21C22 116.8 (3) N1C7N2 109.4 (3) C16C21C22 123.0 (2) N1C7C8 126.9 (3) O3C22O4 122.0 (2) N2C7C8 123.7 (3) O3C22C21 121.2 (3) C7C8H8A 109.5 O4C22C21 116.8 (2) C7C8H8B 109.5 C7N1C5 106.2 (2) H8AC8H8B 109.5 C7N1Cu1 128.57 (19) C7C8H8C 109.5 C7N1Cu1 125.17 (19) H8AC8H8C 109.5 C7N2C6 108.8 (3) H8BC8H8C 109.5 C7N2C6 108.8 (3) H8BC8H8C 109.5 C7N2H2 125.6 O1C9-O2 122.4 (2) C6N2H2 125.6 O1C9-C10 115.3 (2) C1N3Cu1 128.17 (19) C11C10-C15 119.5 (3) C4N3Cu1 128.17 (19) C15C10-C9 117.9 (3) C1N4C3 108.9 (2) C15C10-C9 122.6 (2) C1N4C3 108.9 (2) C15C10-C9 122.6 (2) C1N4H4A 12	С5—С6—Н6	126.8	C20—C21—C16	120.2 (3)
N1C7N2 109.4 (3) C16C21C22 123.0 (2) N1C7C8 126.9 (3) O3C22O4 122.0 (2) N2C7C8 123.7 (3) O3C22C21 121.2 (3) C7C8H8A 109.5 O4C22C21 116.8 (2) C7C8H8B 109.5 C7N1C5 106.2 (2) H8AC8H8B 109.5 C7N1Cu1 128.57 (19) C7C8H8C 109.5 C7N2C6 108.8 (3) H8AC8H8C 109.5 C7N2C6 108.8 (3) H8BC8H8C 109.5 C7N2H2 125.6 O1C9-O2 122.4 (2) C6-N2H2 125.6 O1-C9-O2 122.4 (2) C1N3Cu1 128.17 (19) C11C10-C15 119.5 (3) C4N3Cu1 125.1 (2) C11C10-C5 117.9 (3) C1N4C3 108.9 (2) C15C10-C9 122.6 (2) C1N4H4A 125.6 C12C11C10 121.2 (3) C3N4H4A 125.6 C12C11C10 121.2 (3) C3N4H4A 125.6 C12C11H11 119.4 HW11O1WHW12 112 (3)<	N2—C6—H6	126.8	C20—C21—C22	116.8 (3)
N1C7C8 126.9 (3) O3C22O4 122.0 (2) N2C7C8 123.7 (3) O3C22C21 121.2 (3) C7C8H8A 109.5 O4C22C21 116.8 (2) C7C8H8B 109.5 C7N1C5 106.2 (2) H8AC8H8B 109.5 C7N1Cul 128.57 (19) C7C8H8C 109.5 C5N1Cul 125.17 (19) H8AC8H8C 109.5 C7N2C6 108.8 (3) H8BC8H8C 109.5 C7N2C6 108.8 (3) H8B-C902 122.4 (2) C6N2H2 125.6 O1-C9-O2 122.4 (2) C1N3Cul 128.17 (19) C11C10C15 119.5 (3) C4N3Cul 125.1 (2) C11C10-C9 117.9 (3) C1N4C3 108.9 (2) C15C10-C9 122.6 (2) C1N4H4A 125.6 C12C11C10 121.2 (3) C3N4H4A 125.6 C12C11C10 121.2 (3) C3N4H4A 125.6 C12C11H11 119.4 HW11O1WHW12 112	N1—C7—N2	109.4 (3)	C16—C21—C22	123.0 (2)
N2C7C8123.7 (3)O3C22C21121.2 (3)C7C8H8A109.5O4C22C21116.8 (2)C7C8H8B109.5C7N1C5106.2 (2)H8AC8H8B109.5C7N1Cul128.57 (19)C7C8H8C109.5C5N1Cul125.17 (19)H8AC8H8C109.5C7N2C6108.8 (3)H8BC8H8C109.5C7N2H2125.6O1C9O2122.4 (2)C6-N2H2125.6O1-C9O10122.4 (2)C1N3C4106.5 (2)O2C9C10115.3 (2)C1N4C3108.9 (2)C11C10C15119.5 (3)C4N3Cul125.6C12C11C10121.2 (3)C3N4H4A125.6C12C11C10121.2 (3)C3N4H4A125.6C12C11H11119.4H911O1WHW12112 (3)C13C12C11119.6 (3)HW21O2WHW22109 (3)C13C12H12120.2C2O4Cul^i104.84 (16)C11C12H12120.2C2O4Cul^i104.84 (16)C11C12H13119.9N3Cu1N190.72 (9)C14C13H13119.9N3Cu1O4 ⁱⁱ 89.39 (8)C13C14C15121.4 (3)N3Cu1O4 ⁱⁱ 90.88 (9)C13C14H14119.3N1Cu1Q4 ⁱⁱ 168.31 (8)	N1—C7—C8	126.9 (3)	O3—C22—O4	122.0 (2)
$C7-C8-H8A$ 109.5 $O4-C22-C21$ 116.8 (2) $C7-C8-H8B$ 109.5 $C7-N1-C5$ 106.2 (2) $H8A-C8-H8B$ 109.5 $C7-N1-Cu1$ 128.57 (19) $C7-C8-H8C$ 109.5 $C5-N1-Cu1$ 125.17 (19) $H8A-C8-H8C$ 109.5 $C7-N2-C6$ 108.8 (3) $H8B-C8-H8C$ 109.5 $C7-N2-H2$ 125.6 $O1-C9-O2$ 122.4 (2) $C6-N2-H2$ 125.6 $O1-C9-C10$ 122.4 (2) $C1-N3-C4$ 106.5 (2) $O2-C9-C10$ 115.3 (2) $C1-N3-Cu1$ 128.17 (19) $C11-C10-C15$ 119.5 (3) $C4-N3-Cu1$ 125.1 (2) $C11-C10-C9$ 117.9 (3) $C1-N4-H4A$ 125.6 $C12-C11-C10$ 121.2 (3) $C3-N4-H4A$ 125.6 $C12-C11-H11$ 119.4 $C9-O2-Cu1$ 106.61 (16) $C10-C11-H11$ 119.4 $W11-O1W-HW12$ 112 (3) $C13-C12-C11$ 119.6 (3) $HW21-O2W-HW22$ 109 (3) $C13-C12-H12$ 120.2 $O2-Cu1-N3$ 165.28 (8) $C12-C13-H13$ 119.9 $N3-Cu1-N1$ 91.99 (9) $C12-C13-H13$ 119.9 $O2-Cu1-O4^{ii}$ 89.39 (8) $C13-C14-C15$ 121.4 (3) $N3-Cu1-O4^{ii}$ 90.88 (9) $C13-C14-H14$ 119.3 $N1-Cn1-O4^{ii}$ 168.31 (8)	N2—C7—C8	123.7 (3)	O3—C22—C21	121.2 (3)
C7C8H8B109.5C7N1C5106.2 (2)H8AC8H8B109.5C7N1Cu1128.57 (19)C7C8H8C109.5C5N1Cu1125.17 (19)H8AC8H8C109.5C7N2C6108.8 (3)H8BC8H8C109.5C7N2H2125.6O1C9O2122.4 (2)C6N2H2125.6O1C9C10122.4 (2)C1N3C4106.5 (2)O2C9C10115.3 (2)C1N3Cu1128.17 (19)C11C10C15119.5 (3)C4N3Cu1125.1 (2)C11C10-C9117.9 (3)C1N4C3108.9 (2)C15C10-C9122.6 (2)C1N4H4A125.6C12C11C10121.2 (3)C3N4H4A125.6C12C11H11119.4HW11O1WHW12112 (3)C13C12C11119.6 (3)HW21O2WHW22109 (3)C13C12C14120.2C22O4Cu1^i104.84 (16)C11C12H12120.2O2Cu1N191.99 (9)C12C13C14120.1 (3)O2Cu1N191.99 (9)C12C13H13119.9N3Cu1N190.72 (9)C14C13H13119.9O2Cu1O4 ⁱⁱ 89.39 (8)C13C14C15121.4 (3)N3Cu1O4 ⁱⁱ 90.88 (9)C13C14H14119.3N1Cn1O4 ⁱⁱ 168.31 (8)	С7—С8—Н8А	109.5	O4—C22—C21	116.8 (2)
H8A—C8—H8B109.5C7—N1—Cu1128.57 (19)C7—C8—H8C109.5C5—N1—Cu1125.17 (19)H8A—C8—H8C109.5C7—N2—C6108.8 (3)H8B—C8—H8C109.5C7—N2—H2125.6O1—C9—O2122.4 (2)C6—N2—H2125.6O1—C9—C10122.4 (2)C1—N3—C4106.5 (2)O2—C9—C10115.3 (2)C1—N3—Cu1128.17 (19)C11—C10—C15119.5 (3)C4—N3—Cu1125.1 (2)C11—C10—C9117.9 (3)C1—N4—C3108.9 (2)C15—C10—C9122.6 (2)C1—N4—H4A125.6C12—C11—H11119.4C9—O2—Cu1106.61 (16)C10—C11—H11119.4HW11—O1W—HW12112 (3)C13—C12—C11119.6 (3)HW21—O2W—HW22109 (3)C13—C12—H12120.2C2—O4—Cu1 ⁱ 104.84 (16)C11—C12—H12120.1 (3)O2—Cu1—N191.99 (9)C12—C13—H13119.9N3—Cu1—N190.72 (9)C14—C13—H13119.9N3—Cu1—O4 ⁱⁱ 89.39 (8)C13—C14—C15121.4 (3)N3—Cu1—O4 ⁱⁱ 90.88 (9)C13—C14—H14119.3N1—Cu1—O4 ⁱⁱ 168.31 (8)	С7—С8—Н8В	109.5	C7—N1—C5	106.2 (2)
C7—C8—H8C109.5C5—N1—Cu1125.17 (19)H8A—C8—H8C109.5C7—N2—C6108.8 (3)H8B—C8—H8C109.5C7—N2—H2125.6O1—C9—O2122.4 (2)C6—N2—H2125.6O1—C9—C10122.4 (2)C1—N3—C4106.5 (2)O2—C9—C10115.3 (2)C1—N3—Cu1128.17 (19)C11—C10—C15119.5 (3)C4—N3—Cu1125.1 (2)C11—C10—C9117.9 (3)C1—N4—C3108.9 (2)C15—C10—C9122.6 (2)C1—N4—H4A125.6C12—C11—H11119.4C9—O2—Cu1106.61 (16)C10—C11—H11119.4HW11—O1W—HW12112 (3)C13—C12—C11119.6 (3)HW21—O2W—HW22109 (3)C13—C12—H12120.2C22—O4—Cu1 ⁱ 104.84 (16)C11—C12—H12120.1 (3)O2—Cu1—N191.99 (9)C12—C13—H13119.9N3—Cu1—N190.72 (9)C14—C13—H13119.9O2—Cu1—O4 ⁱⁱ 89.39 (8)C13—C14—C15121.4 (3)N3—Cu1—O4 ⁱⁱ 90.88 (9)C13—C14—H14119.3N1—Cu1—O4 ⁱⁱ 168.31 (8)	H8A—C8—H8B	109.5	C7—N1—Cu1	128.57 (19)
H8A—C8—H8C109.5C7—N2—C6108.8 (3)H8B—C8—H8C109.5C7—N2—H2125.6O1—C9—O2122.4 (2)C6—N2—H2125.6O1—C9—C10122.4 (2)C1—N3—C4106.5 (2)O2—C9—C10115.3 (2)C1—N3—Cu1128.17 (19)C11—C10—C15119.5 (3)C4—N3—Cu1125.1 (2)C11—C10—C9117.9 (3)C1—N4—C3108.9 (2)C15—C10—C9122.6 (2)C1—N4—H4A125.6C12—C11—C10121.2 (3)C3—N4—H4A125.6C12—C11—H11119.4HW11—O1W—HW12112 (3)C13—C12—C11119.6 (3)HW21—O2W—HW22109 (3)C13—C12—H12120.2C22—O4—Cu1 ⁱ 104.84 (16)C11—C12—H12120.1 (3)O2—Cu1—N191.99 (9)C12—C13—H13119.9N3—Cu1—N190.72 (9)C14—C13—H13119.9O2—Cu1—Q4 ⁱⁱ 89.39 (8)C13—C14—C15121.4 (3)N3—Cu1—Q4 ⁱⁱ 90.88 (9)C13—C14—H14119.3N1—Cu1—Q4 ⁱⁱ 168.31 (8)	С7—С8—Н8С	109.5	C5—N1—Cu1	125.17 (19)
H8B—C8—H8C109.5C7—N2—H2125.6O1—C9—O2122.4 (2)C6—N2—H2125.6O1—C9—C10122.4 (2)C1—N3—C4106.5 (2)O2—C9—C10115.3 (2)C1—N3—Cu1128.17 (19)C11—C10—C15119.5 (3)C4—N3—Cu1125.1 (2)C11—C10—C9117.9 (3)C1—N4—C3108.9 (2)C15—C10—C9122.6 (2)C1—N4—H4A125.6C12—C11—C10121.2 (3)C3—N4—H4A125.6C12—C11—H11119.4C9—O2—Cu1106.61 (16)C10—C11—H11119.4HW11—O1W—HW12112 (3)C13—C12—C11119.6 (3)HW21—O2W—HW22109 (3)C13—C12—H12120.2C22—O4—Cu1 ⁱ 104.84 (16)C11—C12—H12120.1 (3)O2—Cu1—N191.99 (9)C12—C13—C14120.1 (3)O2—Cu1—N190.72 (9)C14—C13—H13119.9O2—Cu1—O4 ⁱⁱ 89.39 (8)C13—C14—C15121.4 (3)N3—Cu1—O4 ⁱⁱⁱ 90.88 (9)C13—C14—H14119.3N1—Cu1—O4 ⁱⁱⁱ 168.31 (8)	H8A—C8—H8C	109.5	C7—N2—C6	108.8 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H8B—C8—H8C	109.5	C7—N2—H2	125.6
$01-C9-C10$ 122.4 (2) $C1-N3-C4$ 106.5 (2) $02-C9-C10$ 115.3 (2) $C1-N3-Cu1$ 128.17 (19) $C11-C10-C15$ 119.5 (3) $C4-N3-Cu1$ 125.1 (2) $C11-C10-C9$ 117.9 (3) $C1-N4-C3$ 108.9 (2) $C15-C10-C9$ 122.6 (2) $C1-N4-H4A$ 125.6 $C12-C11-C10$ 121.2 (3) $C3-N4-H4A$ 125.6 $C12-C11-H11$ 119.4 $C9-O2-Cu1$ 106.61 (16) $C10-C11-H11$ 119.4 $HW11-O1W-HW12$ 112 (3) $C13-C12-C11$ 119.6 (3) $HW21-O2W-HW22$ 109 (3) $C13-C12-H12$ 120.2 $C22-O4-Cu1^i$ 104.84 (16) $C11-C12-H12$ 120.2 $O2-Cu1-N3$ 165.28 (8) $C12-C13-C14$ 120.1 (3) $O2-Cu1-N1$ 91.99 (9) $C12-C13-H13$ 119.9 $N3-Cu1-N1$ 90.72 (9) $C14-C13-H13$ 119.9 $O2-Cu1-O4^{ii}$ 89.39 (8) $C13-C14-C15$ 121.4 (3) $N3-Cu1-O4^{ii}$ 90.88 (9) $C13-C14-H14$ 119.3 $N1-Cu1-O4^{ii}$ 168.31 (8)	01—C9—O2	122.4 (2)	C6—N2—H2	125.6
$02-C9-C10$ 115.3 (2) $C1-N3-Cu1$ 128.17 (19) $C11-C10-C15$ 119.5 (3) $C4-N3-Cu1$ 125.1 (2) $C11-C10-C9$ 117.9 (3) $C1-N4-C3$ 108.9 (2) $C15-C10-C9$ 122.6 (2) $C1-N4-H4A$ 125.6 $C12-C11-C10$ 121.2 (3) $C3-N4-H4A$ 125.6 $C12-C11-H11$ 119.4 $C9-O2-Cu1$ 106.61 (16) $C10-C11-H11$ 119.4 $C9-O2-Cu1$ 106.61 (16) $C13-C12-C11$ 119.6 (3) $HW21-O2W-HW22$ 109 (3) $C13-C12-H12$ 120.2 $C22-O4-Cu1^{i}$ 104.84 (16) $C12-C13-C14$ 120.1 (3) $O2-Cu1-N3$ 165.28 (8) $C12-C13-H13$ 119.9 $N3-Cu1-N1$ 91.99 (9) $C12-C13-H13$ 119.9 $O2-Cu1-O4^{ii}$ 89.39 (8) $C13-C14-C15$ 121.4 (3) $N3-Cu1-O4^{ii}$ 90.88 (9) $C13-C14-H14$ 119.3 $N1-Cu1-O4^{ii}$ 168.31 (8)	O1—C9—C10	122.4 (2)	C1—N3—C4	106.5 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2—C9—C10	115.3 (2)	C1—N3—Cu1	128.17 (19)
C11—C10—C9117.9 (3)C1—N4—C3108.9 (2)C15—C10—C9122.6 (2)C1—N4—H4A125.6C12—C11—C10121.2 (3)C3—N4—H4A125.6C12—C11—H11119.4C9—O2—Cu1106.61 (16)C10—C11—H11119.4HW11—O1W—HW12112 (3)C13—C12—C11119.6 (3)HW21—O2W—HW22109 (3)C13—C12—H12120.2C22—O4—Cu1 ⁱ 104.84 (16)C11—C12—H12120.2O2—Cu1—N3165.28 (8)C12—C13—C14120.1 (3)O2—Cu1—N191.99 (9)C14—C13—H13119.9N3—Cu1—N190.72 (9)C13—C14—C15121.4 (3)N3—Cu1—O4 ⁱⁱ 90.88 (9)C13—C14—H14119.3N1—Cu1—O4 ⁱⁱ 168.31 (8)	C11—C10—C15	119.5 (3)	C4—N3—Cu1	125.1 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C11—C10—C9	117.9 (3)	C1—N4—C3	108.9 (2)
C12—C11—C10121.2 (3)C3—N4—H4A125.6C12—C11—H11119.4C9—O2—Cu1106.61 (16)C10—C11—H11119.4HW11—O1W—HW12112 (3)C13—C12—C11119.6 (3)HW21—O2W—HW22109 (3)C13—C12—H12120.2C22—O4—Cu1 ⁱ 104.84 (16)C11—C12—H12120.2O2—Cu1—N3165.28 (8)C12—C13—C14120.1 (3)O2—Cu1—N191.99 (9)C14—C13—H13119.9N3—Cu1—N190.72 (9)C13—C14—C15121.4 (3)N3—Cu1—O4 ⁱⁱ 90.88 (9)C13—C14—H14119.3N1—Cu1—O4 ⁱⁱ 168.31 (8)	C15—C10—C9	122.6 (2)	C1—N4—H4A	125.6
C12—C11—H11119.4C9—O2—Cu1106.61 (16)C10—C11—H11119.4HW11—O1W—HW12112 (3)C13—C12—C11119.6 (3)HW21—O2W—HW22109 (3)C13—C12—H12120.2C22—O4—Cu1 ⁱ 104.84 (16)C11—C12—H12120.2O2—Cu1—N3165.28 (8)C12—C13—C14120.1 (3)O2—Cu1—N191.99 (9)C12—C13—H13119.9N3—Cu1—N190.72 (9)C14—C13—H13119.9O2—Cu1—O4 ⁱⁱ 89.39 (8)C13—C14—C15121.4 (3)N3—Cu1—O4 ⁱⁱ 90.88 (9)C13—C14—H14119.3N1—Cu1—O4 ⁱⁱ 168.31 (8)	C12-C11-C10	121.2 (3)	C3—N4—H4A	125.6
C10—C11—H11119.4HW11—O1W—HW12112 (3)C13—C12—C11119.6 (3)HW21—O2W—HW22109 (3)C13—C12—H12120.2 $C22$ —O4—Cu1 ⁱ 104.84 (16)C11—C12—H12120.2O2—Cu1—N3165.28 (8)C12—C13—C14120.1 (3)O2—Cu1—N191.99 (9)C12—C13—H13119.9N3—Cu1—N190.72 (9)C14—C13—H13119.9O2—Cu1—O4 ⁱⁱ 89.39 (8)C13—C14—C15121.4 (3)N3—Cu1—O4 ⁱⁱ 90.88 (9)C13—C14—H14119.3N1—Cu1—O4 ⁱⁱ 168.31 (8)	C12—C11—H11	119.4	C9—O2—Cu1	106.61 (16)
C13—C12—C11119.6 (3)HW21—O2W—HW22109 (3)C13—C12—H12120.2C22—O4—Cu1 ⁱ 104.84 (16)C11—C12—H12120.2O2—Cu1—N3165.28 (8)C12—C13—C14120.1 (3)O2—Cu1—N191.99 (9)C12—C13—H13119.9N3—Cu1—N190.72 (9)C14—C13—H13119.9O2—Cu1—O4 ⁱⁱ 89.39 (8)C13—C14—C15121.4 (3)N3—Cu1—O4 ⁱⁱ 90.88 (9)C13—C14—H14119.3N1—Cu1—O4 ⁱⁱ 168.31 (8)	C10-C11-H11	119.4	HW11—O1W—HW12	112 (3)
C13C12H12120.2C22O4Cu1i104.84 (16)C11C12H12120.2O2Cu1N3165.28 (8)C12C13C14120.1 (3)O2Cu1N191.99 (9)C12C13H13119.9N3Cu1N190.72 (9)C14C13H13119.9O2Cu1O4 ⁱⁱ 89.39 (8)C13C14C15121.4 (3)N3Cu1O4 ⁱⁱ 90.88 (9)C13C14H14119.3N1Cu1O4 ⁱⁱ 168.31 (8)	C13—C12—C11	119.6 (3)	HW21—O2W—HW22	109 (3)
C11—C12—H12120.2O2—Cu1—N3165.28 (8)C12—C13—C14120.1 (3)O2—Cu1—N191.99 (9)C12—C13—H13119.9N3—Cu1—N190.72 (9)C14—C13—H13119.9O2—Cu1—O4 ⁱⁱ 89.39 (8)C13—C14—C15121.4 (3)N3—Cu1—O4 ⁱⁱ 90.88 (9)C13—C14—H14119.3N1—Cu1—O4 ⁱⁱ 168.31 (8)	C13—C12—H12	120.2	C22—O4—Cu1 ⁱ	104.84 (16)
C12—C13—C14120.1 (3)O2—Cu1—N191.99 (9)C12—C13—H13119.9N3—Cu1—N190.72 (9)C14—C13—H13119.9O2—Cu1—O4 ⁱⁱ 89.39 (8)C13—C14—C15121.4 (3)N3—Cu1—O4 ⁱⁱ 90.88 (9)C13—C14—H14119.3N1—Cu1—O4 ⁱⁱ 168.31 (8)	C11—C12—H12	120.2	O2—Cu1—N3	165.28 (8)
C12—C13—H13 119.9 N3—Cu1—N1 90.72 (9) C14—C13—H13 119.9 O2—Cu1—O4 ⁱⁱ 89.39 (8) C13—C14—C15 121.4 (3) N3—Cu1—O4 ⁱⁱ 90.88 (9) C13—C14—H14 119.3 N1—Cu1—O4 ⁱⁱ 168.31 (8)	C12—C13—C14	120.1 (3)	O2—Cu1—N1	91.99 (9)
C14—C13—H13119.9 $O2$ —Cu1— $O4^{ii}$ 89.39 (8)C13—C14—C15121.4 (3)N3—Cu1— $O4^{ii}$ 90.88 (9)C13—C14—H14119.3N1—Cu1— $O4^{ii}$ 168.31 (8)	C12—C13—H13	119.9	N3—Cu1—N1	90.72 (9)
C13—C14—C15 121.4 (3) N3—Cu1—O4 ⁱⁱ 90.88 (9) C13—C14—H14 119.3 N1—Cu1—O4 ⁱⁱ 168.31 (8)	С14—С13—Н13	119.9	O2—Cu1—O4 ⁱⁱ	89.39 (8)
C13—C14—H14 119.3 N1—Cu1—O4 ⁱⁱ 168.31 (8)	C13—C14—C15	121.4 (3)	N3—Cu1—O4 ⁱⁱ	90.88 (9)
	C13—C14—H14	119.3	N1—Cu1—O4 ⁱⁱ	168.31 (8)

Symmetry codes: (i) -x+1/2, y+1/2, -z+3/2; (ii) -x+1/2, y-1/2, -z+3/2.

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	D—H··· A		
O1W—HW12···O2W ⁱⁱⁱ	0.840 (17)	1.94 (2)	2.757 (4)	163 (3)		
O1W—HW11···O2W ^{iv}	0.837 (17)	2.02 (2)	2.846 (4)	169 (3)		
O2W—HW21…O1	0.842 (17)	1.922 (18)	2.761 (3)	174 (4)		
O2W—HW22…O3	0.859 (18)	1.884 (18)	2.738 (3)	173 (4)		
N2—H2…O4 ^v	0.86	1.98	2.814 (3)	164		
N4—H4A…O1W	0.86	1.90	2.738 (4)	163		
Symmetry codes: (iii) $-x-1/2$, $y-1/2$, $-z+3/2$; (iv) $x-1/2$, $-y+1/2$, $z+1/2$; (v) $-x+1$, $-y+1$, $-z+2$.						

sup-7







Fig. 2