Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

# Synthesis, crystal structure and Hirshfeld surface analysis of a copper(II) complex involving 3-methylbenzoate and 2,2′-bipyridine ligands

**Adnan Qadir***

Department of Chemistry, College of Science, Salahaddin University, Erbil 44001, Iraq. *Correspondence e-mail: adnan.qadir@su.edu.krd

Received 24 January 2023
Accepted 5 August 2023

Edited by G. Diaz de Delgado, Universidad de Los Andes Mérida, Venezuela

**Keywords:** crystal structure; coordination compound; Hirshfeld surface analysis; 3-methylbenzoate.

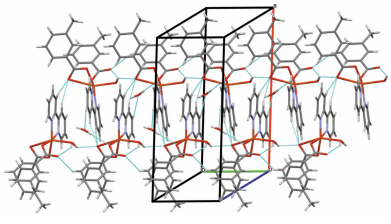
**CCDC reference:** 2117143

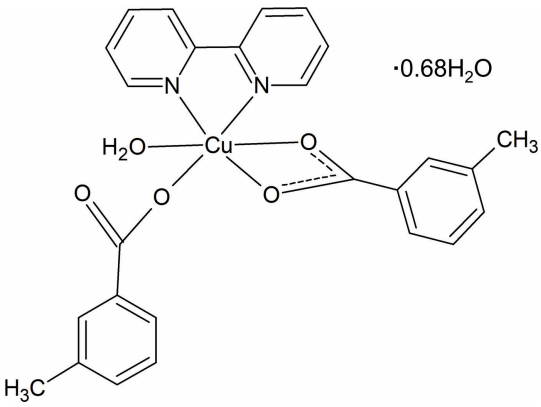
**Supporting information:** this article has supporting information at journals.iucr.org/e

3-Methylbenzoic acid (3-mbH) and 2,2′-bipyridine (bipy) reacted with a copper(II) salt forming a new mixed ligand complex, aqua(2,2′-bipyridine-$\kappa^2N,N'$)-bis(3-methylbenzoato)-$\kappa^2O,O';\kappa O$-copper(II) 0.68-hydrate, $[Cu(C_8H_7O_2)_2(C_{10}H_8N_2)(H_2O)]\cdot 0.68H_2O$ or $[Cu(3\text{-mb})_2(bipy)(H_2O)]\cdot 0.68H_2O$. The coordination environment of $Cu^{II}$ is a distorted octahedron. The metal atom is attached to two 3-mb moieties, which bind in monodentate and bidentate fashions. One of the 3-mb units is disordered. The coordination environment is completed by one bipy ligand and a water molecule. A second water molecule is outside the coordination sphere of the $Cu^{II}$ atom and its occupancy refined to 0.68. The structure consists of chains along the *b*-axis direction formed by complex units joined *via* hydrogen bonds between the coordinated water molecule and an O atom of a coordinated 3-mb unit. Hirshfeld surface analysis indicates that the most abundant contacts are H···H (56.8%), H···C/C···H (21.7%) and H···O/O···H (13.7%).

## 1. Chemical context

The coordination chemistry of mixed-ligand copper(II) complexes continues to be of interest. Copper is an important part of various metalloenzymes. It takes part in many metabolic processes such as iron metabolism, mitochondrial oxidative phosphorylation and catecholamine production (Chen *et al.*, 2020; De Freitas *et al.*, 2003). Mixed-ligand copper(II) carboxylates containing nitrogen donor ligands have been reported to display a variety of pharmacological and superoxide dismutase activities. For example, the bis(acetato)bis(imidazole)copper(II) complex exhibits antitumor activity (Tamura *et al.*, 1987) and copper(II) salicylate with imidazoles have dismutase activities (Abuhijleh, 2010). Incorporating nitrogen donor ligands in metal complexes has resulted in enhancement of the biological activity of these complexes (Patel *et al.*, 2012). It has been reported that the steric effect of a substituent on the phenyl group of carboxylate ligands in metal complexes affects the coordination number of the metal, the geometry of the complex and the coordination mode of the ligand (Saini *et al.*, 2015). In our previous contribution, the $Cu^{II}$ complex with 3-mb and *N*,*N*,*N*,*N*-tetramethylethylenediamine (tmeda), $[Cu(3\text{-mb})_2(tmeda)(H_2O)_2]$, was prepared and characterized by single-crystal X-ray diffraction. The complex was octahedral with 3-mb acting as monodentate (Kansız *et al.*, 2021). In view of the above information, a new $Cu^{II}$ carboxylate containing 2,2′-bipyridine was synthesized, characterized by X-ray crystallographic analysis and studied by Hirshfeld surface analysis.






## 2. Structural commentary

Complex **1** (Fig. 1) crystallizes in the monoclinic system in the $P2_1/c$ space group. The $Cu^{II}$ atom has a distorted octahedral environment with the central copper atom coordinated by $N_2O_4$ donor sets. The Cu—N bond lengths range from 2.0071 (18) to 2.0131 (18) Å and the N1—Cu1—N2 angle is 80.58 (7)° (Table 1). The Cu1—$O_{carboxylate}$ distances are 1.842 (17)–2.2988 (18) Å. The Cu—O and Cu—N values are very close to those reported for copper(II) complexes involving benzoate (BZA) as a ligand, for example [Cu(BZA)$_2$(bipy)($H_2O$)] [Cu—O = 1.9951 (12)–1.9633 (12) Å and Cu—N = 2.0064 (14)–2.0111 (13) Å; Devereux *et al.*, 2007]. This indicates that the presence of the methyl substituent has little or no effect on the Cu—O and Cu—N bond lengths. The 3-mb ligand defined by O3/O4/C9–C16 is disordered over two orientations related by an approximately 180° rotation.

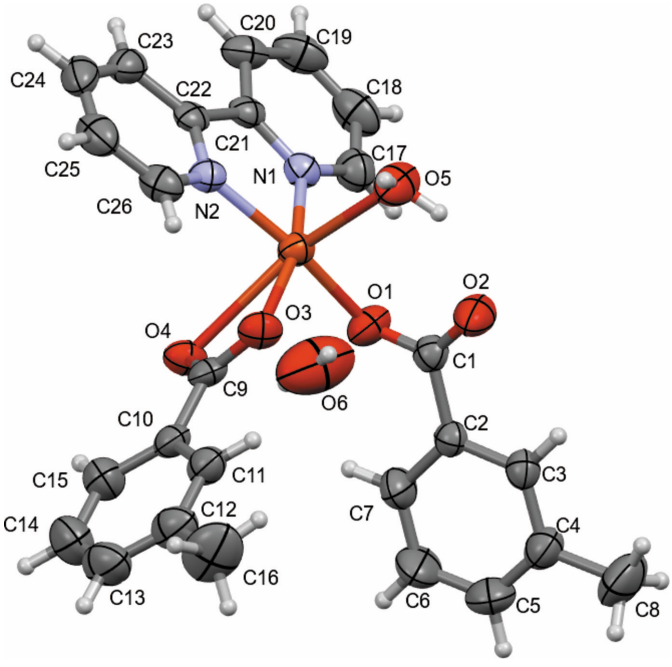



**Figure 1**
Molecular structure of complex **1** with ellipsoids drawn at the 50% probability level. Only the major component of disorder is shown.

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O5—H5$A$···O2 | 0.85 | 1.93 | 2.643 (3) | 140 |
| O5—H5$B$···O4$^{ai}$ | 0.85 | 2.09 | 2.694 (10) | 128 |
| C20—H20···O4$^{aii}$ | 0.93 | 2.40 | 3.324 (10) | 171 |
| C23—H23···O4$^{aii}$ | 0.93 | 2.51 | 3.405 (7) | 163 |
| C18—H18···O2$^{iii}$ | 0.93 | 2.51 | 3.371 (4) | 154 |
| C24—H24···O6$^{ii}$ | 0.93 | 2.36 | 3.200 (5) | 151 |
| C26—H26···O3$^{a}$ | 0.93 | 2.48 | 2.984 (13) | 115 |
| C17—H17···O1 | 0.93 | 2.59 | 3.093 (3) | 115 |
| C7—H7···O6 | 0.93 | 2.72 | 3.405 (6) | 131 |

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+1, -y+2, -z+1$.

## 3. Supramolecular features

In the crystal, hydrogen bonding between H atoms of the coordinated water molecule and the O atoms of the coordinated 3-mb (O5—H5$B$···O4) leads to the formation of a linear chain in the $b$-axis direction (Fig. 2 and Table 1). The chains interdigitate with other chains related by a screw-axis, connected *via* C—H···O interactions between O atoms of the 3-mb ligand and H atoms of the bipy ligand (Table 1), further consolidating the crystal. The occupancy of the solvent water (H6$A$—O6—H6$B$) refined to 0.68, which seems to be due to water escaping the crystal through the channels that run along the $b$-axis direction.

## 4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.42; Groom *et al.*, 2016) for compounds containing only Cu, O, N, C, and H resulted in 634 compounds containing bipy and 15 compounds containing 3-mb. In both lists, a dimeric compound containing bipy and 3-mb was identified (refcode PIGZAH; Li *et al.*, 2007). Other related compounds are AJEFEB (Wen, 2009), DUDYIN (He *et al.*, 2019), FERCOV (Wang *et al.*, 2005), GELXAX (Stephenson & Hardie, 2006), LEBOR (Tian *et al.*, 2011), QETNEJ (Chen *et al.*, 2006) and TOFZIZ (Gopalakrishnan *et al.*, 2014).

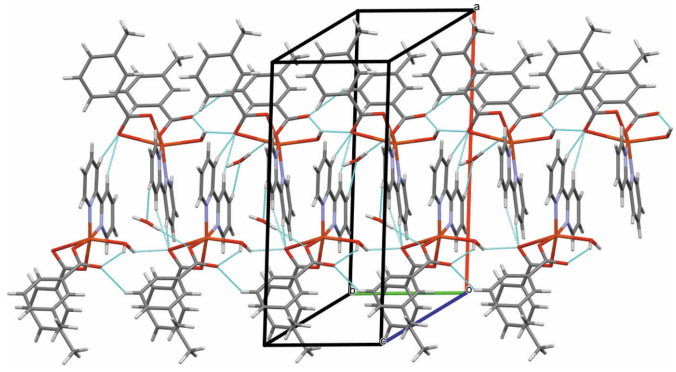


**Figure 2**
Partial view of the packing arrangement in compound **1** showing O—H···O interactions along the $b$-axis direction.

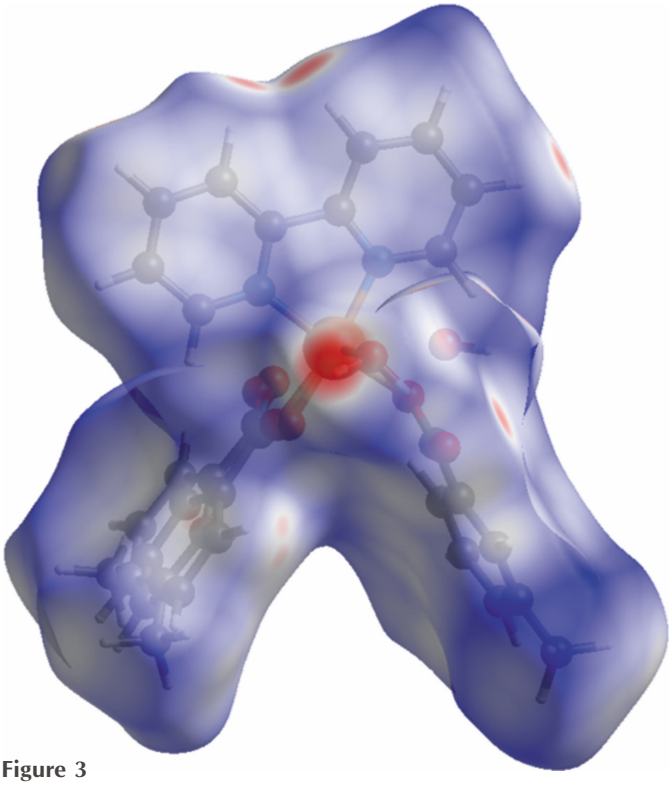


**Figure 3**
Hirshfeld surface map for the title complex.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[Cu(C_8HH_7O_2)_2(C_{10}H_8N_2)(H_2O)]\cdot 0.68H_2O$ |
| $M_r$ | 520.26 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 293 |
| $a, b, c$ (Å) | 16.754 (3), 7.0021 (12), 22.103 (4) |
| $\beta$ (°) | 106.522 (6) |
| $V$ (Å$^3$) | 2485.9 (8) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.92 |
| Crystal size (mm) | 0.20 × 0.15 × 0.12 |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 63716, 6171, 4874 |
| $R_{int}$ | 0.035 |
| $(\sin\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.670 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.042, 0.106, 1.09 |
| No. of reflections | 6171 |
| No. of parameters | 418 |
| No. of restraints | 347 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.30, −0.40 |

Computer programs: *APEX2* (Bruker, 2013), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *Mercury* (Macrae *et al.*, 2020).

## 5. Hirshfeld surface analysis

*CrystalExplorer* (Turner *et al.*, 2017) was used for Hirshfeld surface analysis and to generate the fingerprint plots. The purpose of using Hirshfeld surfaces, mapped onto $d_{norm}$, is to provide additional insight into intermolecular interactions. Close contacts shorter than van der Waals radii are shown as red spots on the surface. The closest contacts are responsible for directional supramolecular interactions. The blue areas in the surface map represent weak contacts that are longer than the sum of the van der Waals radii. The Hirshfeld surface mapped onto $d_{norm}$, is presented in Fig. 3. It displays several red spots due to O—H···O and C—H···O contacts. The intense spot near the coordinated water molecule in the complex is assigned to the O5—H5···O hydrogen bond, as confirmed by the X-ray analysis (Table 1). Fingerprint plots for the contacts are shown in Fig. 4. The contributions of the H···H (Fig. 4*b*), H···C/C···H (Fig. 4*c*) and H···O/O···H (Fig. 4*d*) contacts are 56.8, 21.7 and 13.7%, respectively.

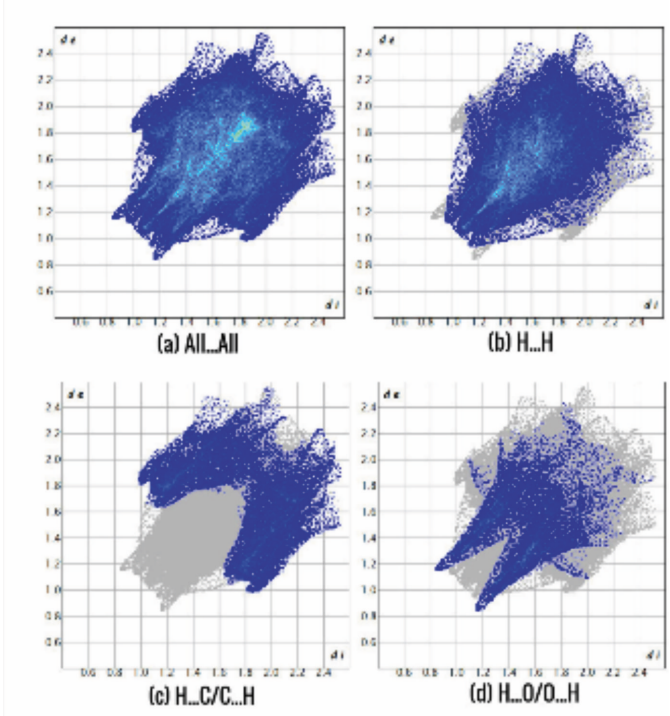



**Figure 4**
Fingerprint plot of the title compound showing all interactions and delineated into the most important intermolecular contacts.

## 6. Synthesis and crystallization

3-Methylbenzoic acid (4 mmol, 0.54 g) and sodium hydroxide (4 mmol, 0.16 g) in water (20 ml) were added to a solution of $Cu(NO_3)_2\cdot 3H_2O$ (2 mmol, 0.48 g) in water (20 ml) under stirring. A solution of 2,2′-bipyridine (2 mmol, 0.3 g) in EtOH (25 ml) was added and the color changed from greenish blue to blue. The precipitate was filtered off, washed with water and dried. Blue single crystals of the title complex suitable for X-ray diffraction studies were obtained after evaporation of an ethanol solution after several days.

## 7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. One of the 3-methylbenzoates (O3/O4/C9–C16) is disordered over two positions related by a 180° rotation. The occupancies of the two components refined to 0.664 (4):0.336 (4). The occupancy of the water molecule H6*A*–O6–H6*B* refined to 0.680 (10). The coordinates of the ordered water atom were refined with $U_{iso}$(H) = 1.5$U_{eq}$(O). All other H atoms were positioned geometrically and refined as riding with $U_{iso}$(H) = 1.2–1.5$U_{eq}$(parent atom).

## Acknowledgements

The author acknowledges the Scientific and Technological Research Application and Research Center, Sinop University, Turkey, for the use of the Bruker APEXII CCD diffractometer.

## Funding information

Funding for this research was provided by: Salahaddin University-Erbil.

## References

Abuhijleh, A. L. (2010). *J. Mol. Struct.* **980**, 201–207.
Bruker (2013). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, J., Jiang, Y., Shi, H., Peng, Y., Fan, X. & Li, C. (2020). *Eur. J. Physiol.* **472**, 1415–1429.
Chen, P.-K., Che, Y.-X. & Zheng, J. M. (2006). *Chin. J. Struct. Chem.* (Jiegou Huaxue) **25**, 1427-1430.
De Freitas, J., Wintz, H., Hyoun Kim, J., Poynton, H., Fox, T. & Vulpe, C. (2003). *BioMetals*, **16**, 185–197.
Devereux, M., O'Shea, D., O'Connor, M., Grehan, H., Connor, G., McCann, M., Rosair, G., Lyng, F., Kellett, A., Walsh, M., Egan, D. & Thati, B. (2007). *Polyhedron*, **26**, 4073–4084.
Gopalakrishnan, M., Senthilkumar, K., Rao, P. R., Siva, R. & Palanisami, N. (2014). *Inorg. Chem. Commun.* **46**, 54–59.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
He, X., Chen, F., Zhang, D., Li, Y., Yang, H.-L. & Zhang, X.-Q. (2019). *Z. Anorg. Allg. Chem.* **645**, 1341–1348.
Kansız, S., Qadir, M. Q., Dege, N. & Faizi, S. H. (2021). *J. Mol. Struct.* **1230**, 129916–129916.
Li, W., Li, C.-H., Yang, Y.-Q. & Kuang, Y.-F. (2007). *Wuji Huaxue Xuebao*, **23**, 1264.
Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
Patel, M. N., Dosi, P. A. & Bhatt, B. S. (2012). *J. Coord. Chem.* **65**, 3833–3844.
Saini, A., Sharma, R. P., Kumar, S., Venugopalan, P., Gubanov, A. I. & Smolentsev, A. I. (2015). *Polyhedron*, **100**, 155–163.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Stephenson, M. D. & Hardie, M. J. (2006). *Dalton Trans. pp.* 3407–3417.
Tamura, H., Imai, H., Kuwahara, J. & Sugiura, Y. (1987). *J. Am. Chem. Soc.* **109**, 6870–6871.
Tian, D., Zhou, Y., Guan, L. & Zhang, H. (2011). *J. Coord. Chem.* **64**, 565–573.
Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Spackman, P. R., Jayatilaka, D. & Spackman, M. A. (2017). *CrystalExplorer17*. The University of Western Australia.
Wang, P., Moorefield, C. N., Panzer, M. & Newkome, G. R. (2005). *Chem. Commun.* pp. 465–467.
Wen, G.-L. (2009). *Z. Krist. New Cryst. Struct.* **224**, 495–497.

# supporting information

*Acta Cryst.* (2023). E**79**, 804-807 [https://doi.org/10.1107/S2056989023006904]

# Synthesis, crystal structure and Hirshfeld surface analysis of a copper(II) complex involving 3-methylbenzoate and 2,2′-bipyridine ligands

**Adnan Qadir**

## Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *APEX2* (Bruker, 2013); data reduction: *APEX2* (Bruker, 2013); program(s) used to solve structure: *SHELXT2018/2* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2020).

**Aqua(2,2′-bipyridine$\kappa^2N,N'$)bis(3-methylbenzoato)-$\kappa^2O,O';\kappa O$-copper(II) 0.68-hydrate,**

*Crystal data*

$[Cu(C_8HH_7O_2)_2(C_{10}H_8N_2)(H_2O)]\cdot 0.68H_2O$
$M_r = 520.26$
Monoclinic, $P2_1/c$
$a = 16.754$ (3) Å
$b = 7.0021$ (12) Å
$c = 22.103$ (4) Å
$\beta = 106.522$ (6)°
$V = 2485.9$ (8) Å$^3$
$Z = 4$
$F(000) = 1079$
$D_x = 1.390$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9233 reflections
$\theta = 2.5$–26.6°
$\mu = 0.92$ mm$^{-1}$
$T = 293$ K
Block, blue
0.20 × 0.15 × 0.12 mm

*Data collection*

Bruker APEXII CCD diffractometer
$\varphi$ and $\omega$ scans
63716 measured reflections
6171 independent reflections
4874 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 28.5°$, $\theta_{min} = 2.5°$
$h = -22\rightarrow22$
$k = -9\rightarrow9$
$l = -29\rightarrow29$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.106$
$S = 1.09$
6171 reflections
418 parameters
347 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0389P)^2 + 1.6967P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å$^{-3}$
$\Delta\rho_{min} = -0.40$ e Å$^{-3}$

*Special details*

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

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Cu1 | 0.34763 (2) | 0.84495 (4) | 0.31767 (2) | 0.03879 (9) | |
| O1 | 0.32781 (10) | 0.7602 (3) | 0.39681 (8) | 0.0519 (4) | |
| O2 | 0.26638 (14) | 1.0161 (2) | 0.42229 (9) | 0.0664 (5) | |
| N1 | 0.47164 (11) | 0.8619 (2) | 0.35426 (8) | 0.0391 (4) | |
| N2 | 0.38047 (11) | 0.8817 (2) | 0.23762 (8) | 0.0377 (4) | |
| C1 | 0.27773 (13) | 0.8419 (3) | 0.42213 (10) | 0.0392 (4) | |
| C2 | 0.23017 (13) | 0.7151 (3) | 0.45422 (9) | 0.0372 (4) | |
| C3 | 0.18273 (14) | 0.7973 (3) | 0.48953 (10) | 0.0422 (5) | |
| H3 | 0.182368 | 0.929463 | 0.493519 | 0.051* | |
| C4 | 0.13590 (17) | 0.6878 (4) | 0.51900 (12) | 0.0563 (6) | |
| C5 | 0.1379 (2) | 0.4918 (5) | 0.51221 (15) | 0.0735 (9) | |
| H5 | 0.107167 | 0.415128 | 0.531672 | 0.088* | |
| C6 | 0.1844 (2) | 0.4077 (4) | 0.47736 (17) | 0.0801 (10) | |
| H6 | 0.184782 | 0.275525 | 0.473485 | 0.096* | |
| C7 | 0.23037 (18) | 0.5186 (4) | 0.44812 (13) | 0.0571 (6) | |
| H7 | 0.261503 | 0.461430 | 0.424335 | 0.069* | |
| C8 | 0.0844 (2) | 0.7820 (6) | 0.55660 (18) | 0.0969 (12) | |
| H8A | 0.113429 | 0.775074 | 0.600751 | 0.145* | |
| H8B | 0.031860 | 0.717351 | 0.548780 | 0.145* | |
| H8C | 0.074998 | 0.913325 | 0.544171 | 0.145* | |
| O3 | 0.2315 (6) | 0.7725 (11) | 0.2675 (5) | 0.0456 (16) | 0.664 (4) |
| O4 | 0.2993 (4) | 0.4976 (13) | 0.2761 (4) | 0.0443 (13) | 0.664 (4) |
| C9 | 0.2338 (3) | 0.5930 (10) | 0.2581 (4) | 0.0401 (12) | 0.664 (4) |
| C10 | 0.1531 (2) | 0.4981 (6) | 0.2230 (2) | 0.0427 (9) | 0.664 (4) |
| C11 | 0.0787 (3) | 0.5949 (7) | 0.21325 (19) | 0.0493 (9) | 0.664 (4) |
| H11 | 0.079230 | 0.717697 | 0.229388 | 0.059* | 0.664 (4) |
| C12 | 0.0028 (3) | 0.5143 (9) | 0.1799 (2) | 0.0644 (12) | 0.664 (4) |
| C13 | 0.0051 (3) | 0.3318 (9) | 0.1573 (3) | 0.0746 (14) | 0.664 (4) |
| H13 | −0.044531 | 0.273815 | 0.135003 | 0.090* | 0.664 (4) |
| C14 | 0.0781 (3) | 0.2330 (8) | 0.1666 (2) | 0.0792 (13) | 0.664 (4) |
| H14 | 0.077331 | 0.110027 | 0.150537 | 0.095* | 0.664 (4) |
| C15 | 0.1529 (3) | 0.3148 (7) | 0.1996 (2) | 0.0616 (11) | 0.664 (4) |
| H15 | 0.202420 | 0.247440 | 0.206067 | 0.074* | 0.664 (4) |
| C16 | −0.0769 (3) | 0.6241 (10) | 0.1687 (3) | 0.099 (2) | 0.664 (4) |
| H16A | −0.100922 | 0.642619 | 0.124164 | 0.148* | 0.664 (4) |
| H16B | −0.065780 | 0.745972 | 0.189242 | 0.148* | 0.664 (4) |
| H16C | −0.115080 | 0.553947 | 0.185422 | 0.148* | 0.664 (4) |
| O3′ | 0.2373 (12) | 0.789 (2) | 0.2796 (10) | 0.040 (2) | 0.336 (4) |
| O4′ | 0.2799 (8) | 0.498 (3) | 0.2621 (9) | 0.047 (3) | 0.336 (4) |

| | | | | | |
|---|---|---|---|---|---|
| C9′ | 0.2241 (6) | 0.618 (2) | 0.2594 (9) | 0.042 (2) | 0.336 (4) |
| C10′ | 0.1349 (5) | 0.5677 (11) | 0.2262 (4) | 0.0430 (16) | 0.336 (4) |
| C11′ | 0.1173 (5) | 0.3862 (12) | 0.2021 (4) | 0.0552 (16) | 0.336 (4) |
| H11′ | 0.160250 | 0.298071 | 0.207060 | 0.066* | 0.336 (4) |
| C12′ | 0.0359 (6) | 0.3330 (15) | 0.1703 (6) | 0.068 (2) | 0.336 (4) |
| C13′ | −0.0260 (6) | 0.4669 (14) | 0.1651 (5) | 0.067 (2) | 0.336 (4) |
| H13′ | −0.080912 | 0.432829 | 0.145436 | 0.081* | 0.336 (4) |
| C14′ | −0.0089 (5) | 0.6484 (14) | 0.1879 (4) | 0.0641 (19) | 0.336 (4) |
| H14′ | −0.051704 | 0.737327 | 0.182021 | 0.077* | 0.336 (4) |
| C15′ | 0.0720 (4) | 0.7003 (13) | 0.2197 (4) | 0.0503 (16) | 0.336 (4) |
| H15′ | 0.083741 | 0.822434 | 0.236369 | 0.060* | 0.336 (4) |
| C16′ | 0.0144 (7) | 0.1356 (13) | 0.1463 (5) | 0.090 (3) | 0.336 (4) |
| H16D | −0.002135 | 0.136810 | 0.101007 | 0.135* | 0.336 (4) |
| H16E | −0.030539 | 0.088314 | 0.160979 | 0.135* | 0.336 (4) |
| H16F | 0.062117 | 0.054395 | 0.161428 | 0.135* | 0.336 (4) |
| C17 | 0.51321 (16) | 0.8587 (4) | 0.41546 (12) | 0.0524 (6) | |
| H17 | 0.483401 | 0.844910 | 0.444839 | 0.063* | |
| C18 | 0.59886 (18) | 0.8753 (4) | 0.43692 (14) | 0.0647 (7) | |
| H18 | 0.626326 | 0.873196 | 0.479876 | 0.078* | |
| C19 | 0.64208 (17) | 0.8947 (4) | 0.39341 (15) | 0.0650 (8) | |
| H19 | 0.699777 | 0.905457 | 0.406664 | 0.078* | |
| C20 | 0.60063 (14) | 0.8983 (3) | 0.33014 (13) | 0.0507 (6) | |
| H20 | 0.629658 | 0.911990 | 0.300250 | 0.061* | |
| C21 | 0.51485 (13) | 0.8811 (3) | 0.31178 (11) | 0.0369 (4) | |
| C22 | 0.46312 (13) | 0.8851 (3) | 0.24534 (10) | 0.0370 (4) | |
| C23 | 0.49461 (16) | 0.8923 (3) | 0.19373 (12) | 0.0492 (6) | |
| H23 | 0.551776 | 0.893392 | 0.199385 | 0.059* | |
| C24 | 0.4399 (2) | 0.8979 (4) | 0.13391 (13) | 0.0593 (7) | |
| H24 | 0.459856 | 0.901430 | 0.098753 | 0.071* | |
| C25 | 0.35603 (19) | 0.8982 (4) | 0.12654 (12) | 0.0591 (7) | |
| H25 | 0.318396 | 0.904644 | 0.086519 | 0.071* | |
| C26 | 0.32842 (16) | 0.8888 (3) | 0.17930 (11) | 0.0501 (6) | |
| H26 | 0.271393 | 0.887348 | 0.174260 | 0.060* | |
| O5 | 0.33408 (13) | 1.1632 (2) | 0.33836 (11) | 0.0676 (5) | |
| H5A | 0.311059 | 1.174260 | 0.367935 | 0.101* | |
| H5B | 0.299885 | 1.215072 | 0.306576 | 0.101* | |
| O6 | 0.4289 (3) | 0.4219 (8) | 0.4465 (3) | 0.119 (2) | 0.680 (10) |
| H6A | 0.441 (6) | 0.309 (10) | 0.446 (4) | 0.178* | 0.680 (10) |
| H6B | 0.435 (6) | 0.490 (13) | 0.478 (4) | 0.178* | 0.680 (10) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.03652 (14) | 0.03638 (15) | 0.04663 (16) | 0.00129 (11) | 0.01693 (11) | 0.00307 (11) |
| O1 | 0.0532 (9) | 0.0548 (10) | 0.0559 (10) | 0.0099 (8) | 0.0286 (8) | 0.0131 (8) |
| O2 | 0.1003 (15) | 0.0395 (10) | 0.0768 (13) | 0.0003 (9) | 0.0534 (12) | 0.0043 (9) |
| N1 | 0.0404 (9) | 0.0344 (9) | 0.0418 (10) | −0.0003 (7) | 0.0107 (8) | −0.0015 (7) |
| N2 | 0.0392 (9) | 0.0334 (9) | 0.0409 (9) | −0.0016 (7) | 0.0118 (7) | 0.0026 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C1 | 0.0423 (11) | 0.0412 (12) | 0.0339 (10) | 0.0002 (9) | 0.0105 (8) | 0.0004 (9) |
| C2 | 0.0405 (11) | 0.0386 (11) | 0.0321 (10) | −0.0017 (9) | 0.0095 (8) | −0.0013 (8) |
| C3 | 0.0492 (12) | 0.0418 (12) | 0.0359 (11) | 0.0028 (10) | 0.0126 (9) | −0.0023 (9) |
| C4 | 0.0593 (15) | 0.0674 (18) | 0.0479 (14) | −0.0020 (13) | 0.0244 (12) | −0.0018 (12) |
| C5 | 0.088 (2) | 0.0661 (19) | 0.080 (2) | −0.0222 (16) | 0.0450 (17) | 0.0024 (16) |
| C6 | 0.120 (3) | 0.0390 (14) | 0.097 (2) | −0.0164 (16) | 0.056 (2) | −0.0061 (15) |
| C7 | 0.0755 (17) | 0.0394 (13) | 0.0652 (16) | −0.0015 (12) | 0.0343 (14) | −0.0083 (12) |
| C8 | 0.104 (3) | 0.112 (3) | 0.102 (3) | 0.003 (2) | 0.073 (2) | −0.006 (2) |
| O3 | 0.0315 (18) | 0.047 (2) | 0.055 (4) | 0.0020 (17) | 0.007 (2) | 0.005 (2) |
| O4 | 0.035 (3) | 0.0400 (18) | 0.057 (4) | 0.002 (2) | 0.011 (2) | 0.006 (2) |
| C9 | 0.038 (2) | 0.044 (2) | 0.044 (2) | −0.006 (2) | 0.0222 (19) | 0.007 (2) |
| C10 | 0.0408 (19) | 0.051 (2) | 0.0411 (17) | −0.0051 (17) | 0.0202 (15) | 0.0005 (18) |
| C11 | 0.0437 (19) | 0.063 (2) | 0.0424 (18) | −0.005 (2) | 0.0149 (15) | −0.0017 (19) |
| C12 | 0.049 (2) | 0.092 (3) | 0.049 (2) | −0.014 (2) | 0.0094 (19) | −0.002 (2) |
| C13 | 0.066 (3) | 0.096 (3) | 0.058 (3) | −0.029 (3) | 0.011 (2) | −0.010 (2) |
| C14 | 0.088 (3) | 0.077 (3) | 0.072 (3) | −0.023 (3) | 0.023 (2) | −0.022 (2) |
| C15 | 0.064 (2) | 0.059 (2) | 0.065 (2) | −0.010 (2) | 0.024 (2) | −0.0119 (19) |
| C16 | 0.041 (2) | 0.159 (6) | 0.085 (3) | 0.001 (3) | 0.000 (2) | −0.008 (4) |
| O3′ | 0.035 (4) | 0.046 (4) | 0.041 (5) | −0.001 (3) | 0.015 (3) | −0.006 (3) |
| O4′ | 0.032 (5) | 0.050 (4) | 0.054 (7) | 0.001 (4) | 0.005 (4) | 0.010 (4) |
| C9′ | 0.036 (3) | 0.048 (4) | 0.044 (3) | 0.000 (3) | 0.018 (3) | 0.005 (3) |
| C10′ | 0.038 (3) | 0.053 (4) | 0.043 (3) | −0.007 (3) | 0.020 (3) | 0.000 (3) |
| C11′ | 0.051 (3) | 0.065 (3) | 0.053 (3) | −0.009 (3) | 0.021 (3) | −0.003 (3) |
| C12′ | 0.058 (4) | 0.084 (4) | 0.060 (4) | −0.019 (4) | 0.016 (3) | −0.005 (3) |
| C13′ | 0.054 (4) | 0.089 (4) | 0.055 (4) | −0.024 (4) | 0.010 (3) | −0.002 (4) |
| C14′ | 0.046 (3) | 0.087 (4) | 0.058 (4) | −0.002 (4) | 0.012 (3) | 0.000 (4) |
| C15′ | 0.038 (3) | 0.066 (4) | 0.048 (3) | −0.002 (3) | 0.014 (2) | −0.003 (3) |
| C16′ | 0.088 (6) | 0.093 (7) | 0.084 (6) | −0.028 (5) | 0.017 (5) | −0.025 (5) |
| C17 | 0.0596 (15) | 0.0513 (14) | 0.0447 (13) | −0.0019 (12) | 0.0123 (11) | −0.0024 (11) |
| C18 | 0.0619 (16) | 0.0594 (17) | 0.0576 (16) | −0.0058 (13) | −0.0075 (13) | −0.0029 (13) |
| C19 | 0.0416 (13) | 0.0574 (16) | 0.085 (2) | −0.0084 (12) | 0.0003 (13) | 0.0048 (15) |
| C20 | 0.0394 (12) | 0.0397 (12) | 0.0741 (17) | −0.0039 (9) | 0.0179 (12) | 0.0059 (11) |
| C21 | 0.0387 (10) | 0.0227 (9) | 0.0512 (12) | −0.0009 (8) | 0.0160 (9) | 0.0010 (8) |
| C22 | 0.0446 (11) | 0.0198 (9) | 0.0494 (12) | −0.0021 (8) | 0.0177 (9) | 0.0015 (8) |
| C23 | 0.0557 (14) | 0.0368 (12) | 0.0641 (16) | −0.0040 (10) | 0.0312 (12) | −0.0008 (11) |
| C24 | 0.094 (2) | 0.0431 (13) | 0.0502 (15) | −0.0102 (13) | 0.0362 (15) | −0.0023 (11) |
| C25 | 0.0802 (19) | 0.0492 (14) | 0.0423 (13) | −0.0130 (13) | 0.0084 (13) | 0.0026 (11) |
| C26 | 0.0501 (13) | 0.0444 (13) | 0.0507 (14) | −0.0057 (10) | 0.0061 (11) | 0.0054 (10) |
| O5 | 0.0899 (14) | 0.0395 (9) | 0.0894 (14) | 0.0115 (9) | 0.0516 (12) | 0.0108 (9) |
| O6 | 0.103 (3) | 0.113 (4) | 0.157 (5) | 0.023 (3) | 0.064 (3) | 0.043 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—O3′ | 1.842 (17) | C16—H16A | 0.9600 |
| Cu1—O1 | 1.9628 (16) | C16—H16B | 0.9600 |
| Cu1—N1 | 2.0072 (18) | C16—H16C | 0.9600 |
| Cu1—O3 | 2.011 (8) | O3′—C9′ | 1.275 (8) |
| Cu1—N2 | 2.0131 (18) | O4′—C9′ | 1.248 (8) |

| | | | |
|---|---|---|---|
| Cu1—O5 | 2.2988 (18) | C9′—C10′ | 1.509 (7) |
| O1—C1 | 1.269 (3) | C10′—C11′ | 1.377 (8) |
| O2—C1 | 1.235 (3) | C10′—C15′ | 1.381 (8) |
| N1—C17 | 1.334 (3) | C11′—C12′ | 1.396 (9) |
| N1—C21 | 1.346 (3) | C11′—H11′ | 0.9300 |
| N2—C26 | 1.336 (3) | C12′—C13′ | 1.378 (9) |
| N2—C22 | 1.346 (3) | C12′—C16′ | 1.488 (10) |
| C1—C2 | 1.499 (3) | C13′—C14′ | 1.367 (10) |
| C2—C7 | 1.382 (3) | C13′—H13′ | 0.9300 |
| C2—C3 | 1.387 (3) | C14′—C15′ | 1.387 (8) |
| C3—C4 | 1.385 (3) | C14′—H14′ | 0.9300 |
| C3—H3 | 0.9300 | C15′—H15′ | 0.9300 |
| C4—C5 | 1.382 (4) | C16′—H16D | 0.9600 |
| C4—C8 | 1.510 (4) | C16′—H16E | 0.9600 |
| C5—C6 | 1.373 (4) | C16′—H16F | 0.9600 |
| C5—H5 | 0.9300 | C17—C18 | 1.382 (4) |
| C6—C7 | 1.377 (4) | C17—H17 | 0.9300 |
| C6—H6 | 0.9300 | C18—C19 | 1.365 (4) |
| C7—H7 | 0.9300 | C18—H18 | 0.9300 |
| C8—H8A | 0.9600 | C19—C20 | 1.373 (4) |
| C8—H8B | 0.9600 | C19—H19 | 0.9300 |
| C8—H8C | 0.9600 | C20—C21 | 1.383 (3) |
| O3—C9 | 1.277 (5) | C20—H20 | 0.9300 |
| O4—C9 | 1.250 (5) | C21—C22 | 1.478 (3) |
| C9—C10 | 1.508 (5) | C22—C23 | 1.387 (3) |
| C10—C11 | 1.380 (5) | C23—C24 | 1.379 (4) |
| C10—C15 | 1.384 (5) | C23—H23 | 0.9300 |
| C11—C12 | 1.395 (6) | C24—C25 | 1.367 (4) |
| C11—H11 | 0.9300 | C24—H24 | 0.9300 |
| C12—C13 | 1.377 (7) | C25—C26 | 1.373 (4) |
| C12—C16 | 1.499 (7) | C25—H25 | 0.9300 |
| C13—C14 | 1.369 (7) | C26—H26 | 0.9300 |
| C13—H13 | 0.9300 | O5—H5A | 0.8517 |
| C14—C15 | 1.383 (6) | O5—H5B | 0.8515 |
| C14—H14 | 0.9300 | O6—H6A | 0.82 (7) |
| C15—H15 | 0.9300 | O6—H6B | 0.82 (7) |

| | | | |
|---|---|---|---|
| O3′—Cu1—O1 | 86.6 (7) | C10—C15—H15 | 120.4 |
| O3′—Cu1—N1 | 170.4 (5) | C12—C16—H16A | 109.5 |
| O1—Cu1—N1 | 94.41 (7) | C12—C16—H16B | 109.5 |
| O1—Cu1—O3 | 91.9 (4) | H16A—C16—H16B | 109.5 |
| N1—Cu1—O3 | 164.9 (3) | C12—C16—H16C | 109.5 |
| O3′—Cu1—N2 | 96.6 (7) | H16A—C16—H16C | 109.5 |
| O1—Cu1—N2 | 168.42 (7) | H16B—C16—H16C | 109.5 |
| N1—Cu1—N2 | 80.58 (7) | C9′—O3′—Cu1 | 114.1 (12) |
| O3—Cu1—N2 | 90.7 (3) | O4′—C9′—O3′ | 124.5 (10) |
| O3′—Cu1—O5 | 98.8 (5) | O4′—C9′—C10′ | 119.3 (9) |
| O1—Cu1—O5 | 93.69 (7) | O3′—C9′—C10′ | 116.1 (9) |

| | | | |
|---|---|---|---|
| N1—Cu1—O5 | 90.69 (7) | C11′—C10′—C15′ | 120.5 (7) |
| O3—Cu1—O5 | 102.7 (2) | C11′—C10′—C9′ | 118.6 (7) |
| N2—Cu1—O5 | 96.79 (7) | C15′—C10′—C9′ | 120.9 (7) |
| C1—O1—Cu1 | 123.87 (15) | C10′—C11′—C12′ | 120.8 (8) |
| C17—N1—C21 | 118.7 (2) | C10′—C11′—H11′ | 119.6 |
| C17—N1—Cu1 | 126.13 (17) | C12′—C11′—H11′ | 119.6 |
| C21—N1—Cu1 | 115.18 (14) | C13′—C12′—C11′ | 117.7 (8) |
| C26—N2—C22 | 119.2 (2) | C13′—C12′—C16′ | 120.1 (8) |
| C26—N2—Cu1 | 125.89 (16) | C11′—C12′—C16′ | 122.0 (9) |
| C22—N2—Cu1 | 114.78 (14) | C14′—C13′—C12′ | 121.9 (8) |
| O2—C1—O1 | 124.6 (2) | C14′—C13′—H13′ | 119.1 |
| O2—C1—C2 | 118.7 (2) | C12′—C13′—H13′ | 119.1 |
| O1—C1—C2 | 116.66 (19) | C13′—C14′—C15′ | 120.1 (8) |
| C7—C2—C3 | 119.0 (2) | C13′—C14′—H14′ | 119.9 |
| C7—C2—C1 | 121.8 (2) | C15′—C14′—H14′ | 119.9 |
| C3—C2—C1 | 119.2 (2) | C10′—C15′—C14′ | 118.9 (8) |
| C4—C3—C2 | 121.8 (2) | C10′—C15′—H15′ | 120.5 |
| C4—C3—H3 | 119.1 | C14′—C15′—H15′ | 120.5 |
| C2—C3—H3 | 119.1 | C12′—C16′—H16D | 109.5 |
| C5—C4—C3 | 117.6 (2) | C12′—C16′—H16E | 109.5 |
| C5—C4—C8 | 121.9 (3) | H16D—C16′—H16E | 109.5 |
| C3—C4—C8 | 120.4 (3) | C12′—C16′—H16F | 109.5 |
| C6—C5—C4 | 121.5 (3) | H16D—C16′—H16F | 109.5 |
| C6—C5—H5 | 119.3 | H16E—C16′—H16F | 109.5 |
| C4—C5—H5 | 119.3 | N1—C17—C18 | 122.6 (3) |
| C5—C6—C7 | 120.2 (3) | N1—C17—H17 | 118.7 |
| C5—C6—H6 | 119.9 | C18—C17—H17 | 118.7 |
| C7—C6—H6 | 119.9 | C19—C18—C17 | 118.3 (3) |
| C6—C7—C2 | 119.9 (2) | C19—C18—H18 | 120.9 |
| C6—C7—H7 | 120.1 | C17—C18—H18 | 120.9 |
| C2—C7—H7 | 120.1 | C18—C19—C20 | 120.2 (2) |
| C4—C8—H8A | 109.5 | C18—C19—H19 | 119.9 |
| C4—C8—H8B | 109.5 | C20—C19—H19 | 119.9 |
| H8A—C8—H8B | 109.5 | C19—C20—C21 | 118.7 (2) |
| C4—C8—H8C | 109.5 | C19—C20—H20 | 120.7 |
| H8A—C8—H8C | 109.5 | C21—C20—H20 | 120.7 |
| H8B—C8—H8C | 109.5 | N1—C21—C20 | 121.6 (2) |
| C9—O3—Cu1 | 105.6 (6) | N1—C21—C22 | 114.54 (18) |
| O4—C9—O3 | 122.6 (5) | C20—C21—C22 | 123.8 (2) |
| O4—C9—C10 | 120.4 (5) | N2—C22—C23 | 121.0 (2) |
| O3—C9—C10 | 117.0 (5) | N2—C22—C21 | 114.65 (18) |
| C11—C10—C15 | 119.4 (4) | C23—C22—C21 | 124.4 (2) |
| C11—C10—C9 | 120.1 (4) | C24—C23—C22 | 119.0 (2) |
| C15—C10—C9 | 120.5 (4) | C24—C23—H23 | 120.5 |
| C10—C11—C12 | 122.1 (5) | C22—C23—H23 | 120.5 |
| C10—C11—H11 | 119.0 | C25—C24—C23 | 119.7 (2) |
| C12—C11—H11 | 119.0 | C25—C24—H24 | 120.2 |
| C13—C12—C11 | 116.9 (5) | C23—C24—H24 | 120.2 |

| | | | |
|---|---|---|---|
| C13—C12—C16 | 122.1 (5) | C24—C25—C26 | 118.8 (2) |
| C11—C12—C16 | 121.0 (5) | C24—C25—H25 | 120.6 |
| C14—C13—C12 | 122.0 (5) | C26—C25—H25 | 120.6 |
| C14—C13—H13 | 119.0 | N2—C26—C25 | 122.4 (2) |
| C12—C13—H13 | 119.0 | N2—C26—H26 | 118.8 |
| C13—C14—C15 | 120.5 (5) | C25—C26—H26 | 118.8 |
| C13—C14—H14 | 119.8 | Cu1—O5—H5A | 109.4 |
| C15—C14—H14 | 119.8 | Cu1—O5—H5B | 109.3 |
| C14—C15—C10 | 119.2 (5) | H5A—O5—H5B | 104.4 |
| C14—C15—H15 | 120.4 | H6A—O6—H6B | 126 (9) |
| | | | |
| Cu1—O1—C1—O2 | −36.8 (3) | O4′—C9′—C10′—C15′ | −176.9 (19) |
| Cu1—O1—C1—C2 | 143.68 (16) | O3′—C9′—C10′—C15′ | −1 (2) |
| O2—C1—C2—C7 | 170.4 (2) | C15′—C10′—C11′—C12′ | 0.4 (13) |
| O1—C1—C2—C7 | −10.0 (3) | C9′—C10′—C11′—C12′ | −179.2 (10) |
| O2—C1—C2—C3 | −7.7 (3) | C10′—C11′—C12′—C13′ | −1.1 (17) |
| O1—C1—C2—C3 | 171.8 (2) | C10′—C11′—C12′—C16′ | −177.2 (10) |
| C7—C2—C3—C4 | 0.3 (4) | C11′—C12′—C13′—C14′ | 2.3 (19) |
| C1—C2—C3—C4 | 178.4 (2) | C16′—C12′—C13′—C14′ | 178.5 (11) |
| C2—C3—C4—C5 | 0.1 (4) | C12′—C13′—C14′—C15′ | −2.7 (17) |
| C2—C3—C4—C8 | −179.4 (3) | C11′—C10′—C15′—C14′ | −0.7 (13) |
| C3—C4—C5—C6 | −0.2 (5) | C9′—C10′—C15′—C14′ | 178.9 (9) |
| C8—C4—C5—C6 | 179.3 (3) | C13′—C14′—C15′—C10′ | 1.9 (14) |
| C4—C5—C6—C7 | 0.0 (6) | C21—N1—C17—C18 | 0.3 (3) |
| C5—C6—C7—C2 | 0.4 (5) | Cu1—N1—C17—C18 | −178.59 (19) |
| C3—C2—C7—C6 | −0.5 (4) | N1—C17—C18—C19 | −0.3 (4) |
| C1—C2—C7—C6 | −178.6 (3) | C17—C18—C19—C20 | 0.3 (4) |
| Cu1—O3—C9—O4 | −2.8 (14) | C18—C19—C20—C21 | −0.3 (4) |
| Cu1—O3—C9—C10 | 177.9 (6) | C17—N1—C21—C20 | −0.3 (3) |
| O4—C9—C10—C11 | 168.3 (9) | Cu1—N1—C21—C20 | 178.71 (16) |
| O3—C9—C10—C11 | −12.4 (11) | C17—N1—C21—C22 | −179.34 (19) |
| O4—C9—C10—C15 | −12.5 (11) | Cu1—N1—C21—C22 | −0.3 (2) |
| O3—C9—C10—C15 | 166.7 (9) | C19—C20—C21—N1 | 0.3 (3) |
| C15—C10—C11—C12 | −0.5 (7) | C19—C20—C21—C22 | 179.3 (2) |
| C9—C10—C11—C12 | 178.6 (5) | C26—N2—C22—C23 | −1.2 (3) |
| C10—C11—C12—C13 | 0.4 (8) | Cu1—N2—C22—C23 | 174.20 (16) |
| C10—C11—C12—C16 | −178.6 (5) | C26—N2—C22—C21 | 178.66 (18) |
| C11—C12—C13—C14 | −0.2 (9) | Cu1—N2—C22—C21 | −5.9 (2) |
| C16—C12—C13—C14 | 178.7 (6) | N1—C21—C22—N2 | 4.1 (2) |
| C12—C13—C14—C15 | 0.2 (10) | C20—C21—C22—N2 | −174.88 (19) |
| C13—C14—C15—C10 | −0.2 (8) | N1—C21—C22—C23 | −175.98 (19) |
| C11—C10—C15—C14 | 0.4 (7) | C20—C21—C22—C23 | 5.0 (3) |
| C9—C10—C15—C14 | −178.7 (5) | N2—C22—C23—C24 | 0.6 (3) |
| O1—Cu1—O3′—C9′ | −89.7 (18) | C21—C22—C23—C24 | −179.2 (2) |
| N2—Cu1—O3′—C9′ | 79.1 (18) | C22—C23—C24—C25 | 0.7 (4) |
| O5—Cu1—O3′—C9′ | 177.1 (17) | C23—C24—C25—C26 | −1.4 (4) |
| Cu1—O3′—C9′—O4′ | −3 (3) | C22—N2—C26—C25 | 0.5 (3) |
| Cu1—O3′—C9′—C10′ | −178.4 (11) | Cu1—N2—C26—C25 | −174.38 (19) |

| | | | |
|---|---|---|---|
| O4′—C9′—C10′—C11′ | 3 (2) | C24—C25—C26—N2 | 0.8 (4) |
| O3′—C9′—C10′—C11′ | 178.4 (17) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O5—H5*A*···O2 | 0.85 | 1.93 | 2.643 (3) | 140 |
| O5—H5*B*···O4$^{ai}$ | 0.85 | 2.09 | 2.694 (10) | 128 |
| C20—H20···O4$^{aii}$ | 0.93 | 2.40 | 3.324 (10) | 171 |
| C23—H23···O4$^{aii}$ | 0.93 | 2.51 | 3.405 (7) | 163 |
| C18—H18···O2$^{iii}$ | 0.93 | 2.51 | 3.371 (4) | 154 |
| C24—H24···O6$^{ii}$ | 0.93 | 2.36 | 3.200 (5) | 151 |
| C26—H26···O3$^{a}$ | 0.93 | 2.48 | 2.984 (13) | 115 |
| C17—H17···O1 | 0.93 | 2.59 | 3.093 (3) | 115 |
| C7—H7···O6 | 0.93 | 2.72 | 3.405 (6) | 131 |

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*+1, *y*+1/2, −*z*+1/2; (iii) −*x*+1, −*y*+2, −*z*+1.