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# Diaquabis(4-bromobenzoato-$\kappa O$)bis-(*N*,*N*-diethylnicotinamide-$\kappa N^1$)copper(II)

**Hacali Necefoğlu,[a] Füreya Elif Özbek,[a] Vijdan Öztürk,[a] Vedat Adıgüzel[a] and Tuncer Hökelek[b]***

[a]Department of Chemistry, Kafkas University, 36100 Kars, Turkey, and [b]Department of Physics, Hacettepe University, 06800 Beytepe, Ankara, Turkey
Correspondence e-mail: merzifon@hacettepe.edu.tr

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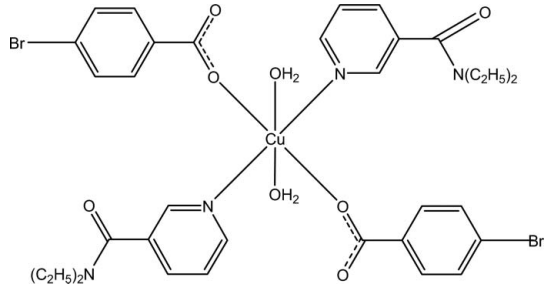
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.035; $wR$ factor = 0.079; data-to-parameter ratio = 15.1.

The title $Cu^{II}$ complex, $[Cu(C_7H_4BrO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$, contains two 4-bromobenzoate (PBB), two diethylnicotinamide (DENA) monodentate ligands and two water molecules. The four O atoms in the equatorial plane around the $Cu^{II}$ ion form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by two N atoms of the DENA ligands in the axial positions. Intramolecular O—H···O hydrogen bonds link the water molecules to the carboxylate groups. The dihedral angles between the carboxylate groups and the adjacent benzene rings are 3.1 (3) and 3.74 (17)°, while the pyridine rings and the benzene rings are oriented at dihedral angles of 6.81 (10) and 3.38 (12)°. In the crystal, intermolecular O—H···O hydrogen bonds link the molecules into double chains along the $b$ axis. C—H···O interactions are also observed. $\pi$–$\pi$ contacts between pyridine rings [centroid–centroid distance = 3.485 (2) Å] may further stabilize the crystal structure.

## Related literature

For literature on niacin, see: Krishnamachari (1974). For information on the nicotinic acid derivative *N*,*N*-diethylnicotinamide, see: Bigoli *et al.* (1972). For related structures, see: Hökelek *et al.* (1996, 2009*a*,*b*); Hökelek & Necefoğlu (1998, 2007); Necefoğlu *et al.* (2011). For bond-length data, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$[Cu(C_7H_4BrO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$
$M_r$ = 856.05
Monoclinic, $P2_1$
$a$ = 8.3621 (2) Å
$b$ = 12.2183 (3) Å
$c$ = 17.6504 (4) Å
$\beta$ = 101.478 (3)°
$V$ = 1767.29 (8) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 2.94 mm$^{-1}$
$T$ = 100 K
0.41 × 0.18 × 0.12 mm

### Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.536, $T_{max}$ = 0.703
17073 measured reflections
7011 independent reflections
6116 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.036

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.079
$S$ = 1.03
7011 reflections
463 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.08 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.59 e Å$^{-3}$
Absolute structure: Flack (1983), 2353 Friedel pairs
Flack parameter: 0.412 (7)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O7—H71···O2 | 0.83 (2) | 1.93 (3) | 2.692 (4) | 154 (5) |
| O7—H72···O4$^{i}$ | 0.83 (4) | 2.04 (4) | 2.834 (4) | 163 (3) |
| O8—H81···O4 | 0.84 (2) | 1.88 (2) | 2.702 (4) | 170 (4) |
| O8—H82···O6$^{ii}$ | 0.82 (4) | 2.05 (4) | 2.848 (4) | 168 (5) |
| C11—H11···O5$^{iii}$ | 0.93 | 2.41 | 3.106 (5) | 133 |
| C16—H16···O4$^{iii}$ | 0.93 | 2.46 | 3.359 (5) | 162 |
| C26—H26···O6$^{iv}$ | 0.93 | 2.37 | 3.261 (4) | 160 |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

The authors are indebted to Anadolu University and the Medicinal Plants and Medicine Research Centre of Anadolu University, Eskişehir, Turkey, for the use of the X-ray

diffractometer. This work was supported financially by the Scientific and Technological Research Council of Turkey (grant No. 106 T472).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2303).

## References


Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.

Bigoli, F., Braibanti, A., Pellinghelli, M. A. & Tiripicchio, A. (1972). *Acta Cryst.* B**28**, 962–966.

Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Hökelek, T., Dal, H., Tercan, B., Özbek, F. E. & Necefoğlu, H. (2009*a*). *Acta Cryst.* E**65**, m466–m467.

Hökelek, T., Dal, H., Tercan, B., Özbek, F. E. & Necefoğlu, H. (2009*b*). *Acta Cryst.* E**65**, m607–m608.

Hökelek, T., Gündüz, H. & Necefoğlu, H. (1996). *Acta Cryst.* C**52**, 2470–2473.

Hökelek, T. & Necefoğlu, H. (1998). *Acta Cryst.* C**54**, 1242–1244.

Hökelek, T. & Necefoğlu, H. (2007). *Acta Cryst.* E**63**, m821–m823.

Krishnamachari, K. A. V. R. (1974). *Am. J. Clin. Nutr.* **27**, 108–111.

Necefoğlu, H., Maracı, A., Özbek, F. E., Tercan, B. & Hökelek, T. (2011). *Acta Cryst.* E**67**, m619–m620.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

# supporting information

*Acta Cryst.* (2011). E**67**, m1317–m1318 [doi:10.1107/S1600536811034787]

## Diaquabis(4-bromobenzoato-$\kappa O$)bis(*N*,*N*-diethylnicotinamide-$\kappa N^1$)copper(II)

**Hacali Necefoğlu, Füreya Elif Özbek, Vijdan Öztürk, Vedat Adıgüzel and Tuncer Hökelek**

### S1. Comment

As a part of our ongoing investigations of transition metal complexes of nicotinamide (NA), one form of niacin (Krishnamachari, 1974), and/or the nicotinic acid derivative *N*,*N*-diethylnicotinamide (DENA), an important respiratory stimulant (Bigoli *et al.*, 1972), the title compound was synthesized and its crystal structure is reported on herein.

The title complex, (Fig. 1), is a mononuclear $Cu^{II}$complex, consisting of two *N*,*N*-diethylnicotinamide (DENA), two 4-bromobenzoate (PBB) ligands and two coordinated water molecules, all ligands coordinating in a monodentate manner. The crystal structures of similar omplexes of $Cu^{II}$, $Co^{II}$, $Ni^{II}$, $Mn^{II}$ and $Zn^{II}$ ions, $[Cu(C_7H_5O_2)_2(C_{10}H_{14}N_2O)_2]$ (Hökelek *et al.*, 1996), $[Co(C_6H_6N_2O)_2(C_7H_4NO_4)_2(H_2O)_2]$ (Hökelek & Necefoğlu, 1998), $[Co(C_9H_9O_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$ (Necefoğlu *et al.*, 2011), $[Ni(C_7H_4ClO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$ (Hökelek *et al.*, 2009*a*), $[Mn(C_9H_{10}NO_2)_2(H_2O)_4].2H_2O$ (Hökelek & Necefoğlu, 2007) and $[Zn(C_7H_4BrO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$ (Hökelek *et al.*, 2009*b*) have also been reported. In the copper(II) complex mentioned above the two benzoate ions coordinate to the $Cu^{II}$ atom as bidentate ligands, while in the other structures all the ligands coordinate in a monodentate manner.

In the title complex (Fig. 1), the four O atoms (O1, O3, O7 and O8) in the equatorial plane around the $Cu^{II}$ ion form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by the two N atoms of the DENA ligands (N1 and N3) in the axial positions. The intramolecular O—H···O hydrogen bonds link the water molecules to the carboxylate groups (Table 1). The near equalities of the C1—O1 [1.289 (4) Å], C1—O2 [1.200 (5) Å] and C8—O3 [1.277 (4) Å], C8—O4 [1.229 (4) Å] bonds in the carboxylate groups indicate delocalized bonding arrangements, rather than localized single and double bonds. The Cu—O bond lengths are 1.985 (2) and 1.979 (2) Å (for benzoate oxygens) and 2.377 (3) and 2.543 (3) Å (for water oxygens), and the Cu—N bond lengths are 1.996 (3) and 1.998 (3) Å, close to standard values (Allen *et al.*, 1987). The Cu atom is displaced out of the least-squares planes of the carboxylate groups (O1/C1/O2) and (O3/C8/O4) by -0.7206 (4) and 0.6797 (4) Å, respectively. The dihedral angles between the planar carboxylate groups and the adjacent benzene rings A (C2—C7) and B (C9—C14) are 3.06 (28) and 3.74 (17) °, respectively. The benzene A (C2—C7) and B (C9—C14) rings and the pyridine C (N1/C15—C19) and D (N3/C25—C29) rings are oriented at dihedral angles of A/B = 3.38 (12), A/C = 67.74 (11), A/D = 61.26 (11), B/C = 67.57 (11), B/D = 61.24 (11) and C/D = 6.81 (10) °.

In the crystal, intermolecular O—H···O hydrogen bonds link the molecules into double chains along the b-axis (Table 1 and Fig. 2). There also exist C—H···O interactions. The $\pi$–$\pi$ contact between the pyridine rings, Cg3—Cg4$^{i}$, [symmetry code: (i) 1 + x, y, z, where Cg3 and Cg4 are centroids of the rings C (N1/C15—C19) and D (N3/C25—C29), respectively], may further stabilize the structure, with centroid-centroid distance of 3.485 (2) Å.

### S2. Experimental

The title compound was prepared by the reaction of $CuSO_4.5H_2O$ (1.23 g, 5 mmol) in $H_2O$ (20 ml) and DENA (1.78 g, 10 mmol) in $H_2O$ (20 ml) with sodium 4-bromobenzoate (2.23 g, 10 mmol) in $H_2O$ (50 ml) at room temperature. The

mixture was filtered and set aside to crystallize at ambient temperature for two weeks, giving blue single crystals.

### S3. Refinement

The compound crystallized as an inversion twin: refined BASF parameter = 0.412 (7), for 2353 Friedel pairs (50.5% coverage). Atoms H71, H72, H81 and H82 (for water molecules) were located in a difference Fourier map and were freely refined. The C-bound H-atoms were positioned geometrically with C—H = 0.93, 0.97 and 0.96 Å, for aromatic, methylene and methyl H-atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}$(H) = k × $U_{eq}$(C), where k = 1.5 for methyl H-atoms and k = 1.2 for all other H-atoms.

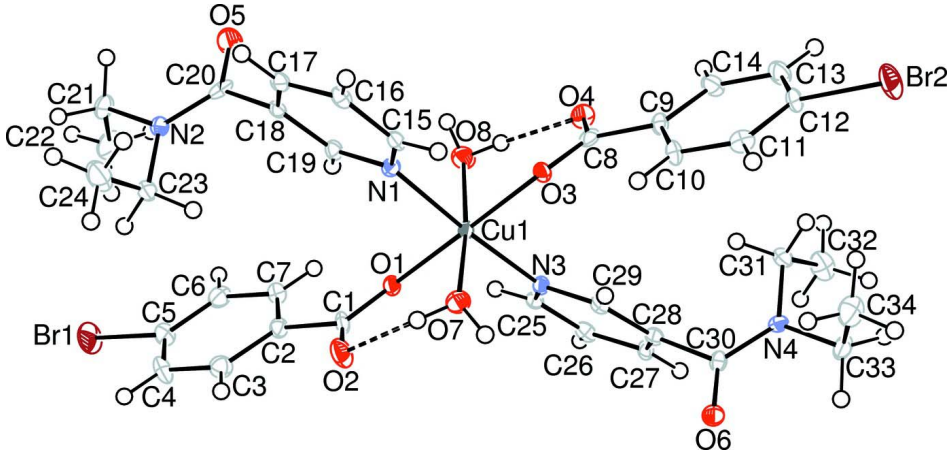



**Figure 1**

The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The intramolecular O—H···O hydrogen bonds are shown as dashed lines [see Table 1 for details].

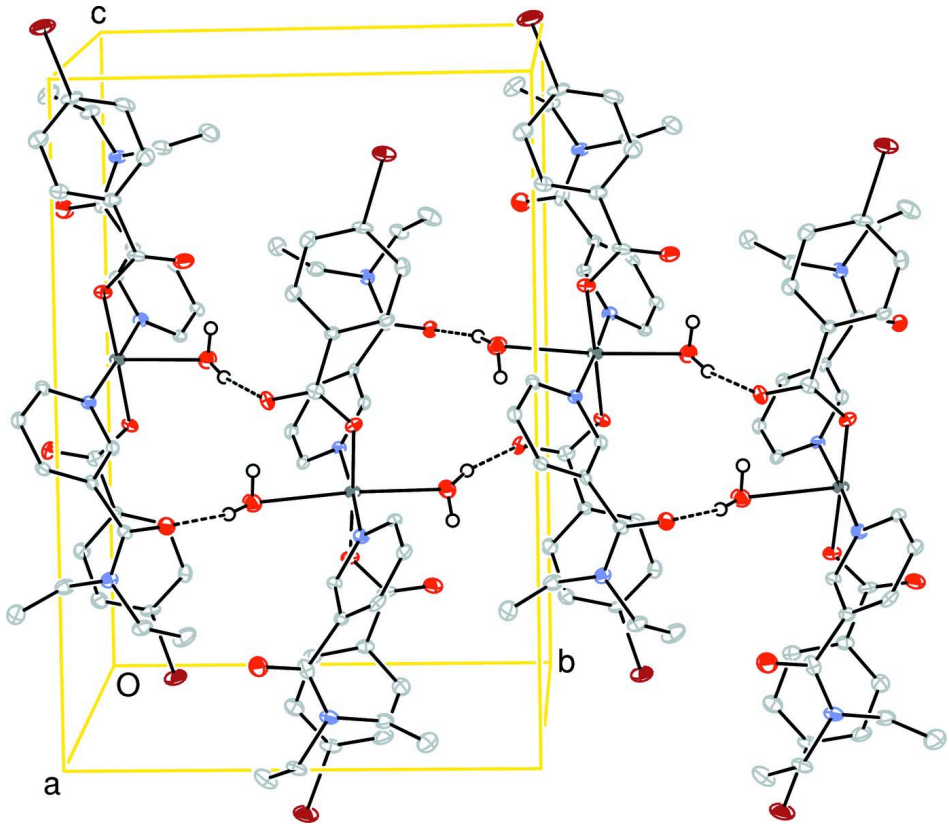



**Figure 2**

A view along the a-axis of the crystal packing of the title compound. Only the intermolecular O—H···O hydrogen bonds are shown as dashed lines [see Table 1 for details; H-atoms not involved in hydrogen bonding have been omitted for clarity].

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*Crystal data*

$[Cu(C_7H_4BrO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$
$M_r = 856.05$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 8.3621\ (2)$ Å
$b = 12.2183\ (3)$ Å
$c = 17.6504\ (4)$ Å
$\beta = 101.478\ (3)°$
$V = 1767.29\ (8)$ Å$^3$
$Z = 2$
$F(000) = 870$
$D_x = 1.609$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6540 reflections
$\theta = 2.4–27.7°$
$\mu = 2.94$ mm$^{-1}$
$T = 100$ K
Block, blue
0.41 × 0.18 × 0.12 mm

*Data collection*

Bruker Kappa APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.536$, $T_{max} = 0.703$
17073 measured reflections
7011 independent reflections
6116 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.036
$\theta_{max}$ = 28.4°, $\theta_{min}$ = 2.0°
$h$ = −11→11
$k$ = −13→16
$l$ = −23→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.079
$S$ = 1.03
7011 reflections
463 parameters
5 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.040P)^2 + 0.1414P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.08 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.59 e Å$^{-3}$
Absolute structure: Flack (1983), 2353 Friedel pairs
Absolute structure parameter: 0.412 (7)

*Special details*

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

**Refinement**. Refinement 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 $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.09645 (6) | 0.00081 (4) | 1.08082 (2) | 0.03240 (12) |
| Br2 | −0.29887 (6) | 0.21016 (3) | 0.08947 (2) | 0.03089 (12) |
| Cu1 | −0.08109 (5) | 0.12231 (3) | 0.58764 (2) | 0.01174 (10) |
| O1 | 0.0327 (3) | 0.1074 (2) | 0.69709 (12) | 0.0142 (5) |
| O2 | 0.0556 (4) | 0.2787 (2) | 0.74212 (14) | 0.0256 (7) |
| O3 | −0.1953 (3) | 0.1336 (2) | 0.47839 (12) | 0.0134 (5) |
| O4 | −0.2014 (3) | −0.0418 (2) | 0.44161 (14) | 0.0182 (6) |
| O5 | −0.5601 (4) | −0.0408 (2) | 0.76338 (15) | 0.0286 (7) |
| O6 | 0.3897 (3) | 0.2655 (2) | 0.40749 (14) | 0.0174 (6) |
| O7 | −0.0443 (3) | 0.3152 (2) | 0.58962 (15) | 0.0198 (6) |
| H71 | −0.026 (5) | 0.325 (4) | 0.6372 (12) | 0.045 (15)* |
| H72 | 0.018 (4) | 0.355 (3) | 0.571 (2) | 0.030 (13)* |
| O8 | −0.1305 (4) | −0.0824 (2) | 0.59515 (15) | 0.0217 (6) |
| H81 | −0.153 (4) | −0.078 (3) | 0.5467 (11) | 0.012 (9)* |
| H82 | −0.204 (4) | −0.125 (3) | 0.601 (3) | 0.042 (15)* |
| N1 | −0.2899 (3) | 0.1512 (2) | 0.62260 (15) | 0.0126 (6) |
| N2 | −0.4635 (3) | 0.0913 (2) | 0.84909 (15) | 0.0157 (7) |
| N3 | 0.1205 (3) | 0.0828 (2) | 0.54918 (15) | 0.0118 (6) |
| N4 | 0.2885 (3) | 0.1367 (2) | 0.31866 (15) | 0.0139 (6) |
| C1 | 0.0513 (4) | 0.1813 (3) | 0.75019 (18) | 0.0151 (8) |

| | | | | |
|---|---|---|---|---|
| C2 | 0.0678 (4) | 0.1339 (3) | 0.83163 (18) | 0.0147 (7) |
| C3 | 0.0873 (4) | 0.2070 (4) | 0.89380 (19) | 0.0196 (8) |
| H3 | 0.0935 | 0.2818 | 0.8854 | 0.023* |
| C4 | 0.0972 (5) | 0.1667 (3) | 0.9687 (2) | 0.0232 (9) |
| H4 | 0.1122 | 0.2141 | 1.0107 | 0.028* |
| C5 | 0.0848 (5) | 0.0566 (3) | 0.97913 (19) | 0.0191 (8) |
| C6 | 0.0646 (4) | −0.0172 (3) | 0.91911 (19) | 0.0199 (8) |
| H6 | 0.0569 | −0.0918 | 0.9281 | 0.024* |
| C7 | 0.0559 (4) | 0.0232 (3) | 0.84411 (19) | 0.0177 (8) |
| H7 | 0.0421 | −0.0250 | 0.8025 | 0.021* |
| C8 | −0.2081 (4) | 0.0570 (3) | 0.42829 (19) | 0.0142 (8) |
| C9 | −0.2320 (4) | 0.0953 (3) | 0.34487 (18) | 0.0128 (7) |
| C10 | −0.2276 (4) | 0.2049 (3) | 0.32745 (18) | 0.0149 (7) |
| H10 | −0.2114 | 0.2559 | 0.3673 | 0.018* |
| C11 | −0.2466 (4) | 0.2406 (3) | 0.2520 (2) | 0.0160 (8) |
| H11 | −0.2445 | 0.3148 | 0.2405 | 0.019* |
| C12 | −0.2690 (5) | 0.1626 (3) | 0.19390 (19) | 0.0183 (8) |
| C13 | −0.2709 (5) | 0.0525 (3) | 0.2096 (2) | 0.0204 (9) |
| H13 | −0.2847 | 0.0014 | 0.1697 | 0.024* |
| C14 | −0.2517 (4) | 0.0190 (3) | 0.28592 (19) | 0.0179 (8) |
| H14 | −0.2522 | −0.0552 | 0.2975 | 0.021* |
| C15 | −0.3960 (4) | 0.2245 (3) | 0.58675 (17) | 0.0124 (7) |
| H15 | −0.3736 | 0.2599 | 0.5434 | 0.015* |
| C16 | −0.5378 (5) | 0.2501 (3) | 0.61129 (19) | 0.0151 (8) |
| H16 | −0.6095 | 0.3020 | 0.5850 | 0.018* |
| C17 | −0.5719 (4) | 0.1976 (3) | 0.67556 (18) | 0.0153 (7) |
| H17 | −0.6658 | 0.2146 | 0.6938 | 0.018* |
| C18 | −0.4640 (4) | 0.1192 (3) | 0.71239 (17) | 0.0131 (7) |
| C19 | −0.3252 (4) | 0.0974 (3) | 0.68331 (17) | 0.0130 (7) |
| H19 | −0.2539 | 0.0434 | 0.7068 | 0.016* |
| C20 | −0.4993 (4) | 0.0495 (3) | 0.7767 (2) | 0.0160 (8) |
| C21 | −0.5022 (5) | 0.0272 (3) | 0.9134 (2) | 0.0197 (9) |
| H21A | −0.5973 | −0.0177 | 0.8944 | 0.024* |
| H21B | −0.5295 | 0.0769 | 0.9518 | 0.024* |
| C22 | −0.3628 (5) | −0.0458 (4) | 0.9514 (2) | 0.0278 (10) |
| H22A | −0.3900 | −0.0801 | 0.9961 | 0.042* |
| H22B | −0.2659 | −0.0025 | 0.9667 | 0.042* |
| H22C | −0.3440 | −0.1009 | 0.9154 | 0.042* |
| C23 | −0.3767 (5) | 0.1954 (3) | 0.86888 (19) | 0.0196 (8) |
| H23A | −0.3204 | 0.2151 | 0.8278 | 0.024* |
| H23B | −0.2952 | 0.1857 | 0.9159 | 0.024* |
| C24 | −0.4906 (6) | 0.2879 (4) | 0.8806 (2) | 0.0303 (10) |
| H24A | −0.4283 | 0.3534 | 0.8946 | 0.045* |
| H24B | −0.5470 | 0.2687 | 0.9210 | 0.045* |
| H24C | −0.5684 | 0.3001 | 0.8335 | 0.045* |
| C25 | 0.2162 (4) | 0.0000 (3) | 0.58143 (17) | 0.0128 (7) |
| H25 | 0.1921 | −0.0352 | 0.6245 | 0.015* |
| C26 | 0.3494 (4) | −0.0343 (3) | 0.55230 (18) | 0.0152 (8) |

| | | | | |
|---|---|---|---|---|
| H26 | 0.4136 | −0.0921 | 0.5753 | 0.018* |
| C27 | 0.3865 (4) | 0.0181 (3) | 0.48863 (18) | 0.0134 (7) |
| H27 | 0.4752 | −0.0041 | 0.4679 | 0.016* |
| C28 | 0.2882 (4) | 0.1048 (3) | 0.45606 (18) | 0.0124 (7) |
| C29 | 0.1590 (4) | 0.1348 (3) | 0.48858 (17) | 0.0124 (7) |
| H29 | 0.0952 | 0.1939 | 0.4676 | 0.015* |
| C30 | 0.3275 (4) | 0.1746 (3) | 0.3915 (2) | 0.0129 (8) |
| C31 | 0.1984 (5) | 0.0353 (3) | 0.2969 (2) | 0.0186 (8) |
| H31A | 0.1083 | 0.0501 | 0.2542 | 0.022* |
| H31B | 0.1530 | 0.0098 | 0.3402 | 0.022* |
| C32 | 0.3040 (5) | −0.0541 (3) | 0.2733 (2) | 0.0265 (9) |
| H32A | 0.2398 | −0.1190 | 0.2602 | 0.040* |
| H32B | 0.3930 | −0.0695 | 0.3154 | 0.040* |
| H32C | 0.3462 | −0.0304 | 0.2293 | 0.040* |
| C33 | 0.3236 (4) | 0.2055 (4) | 0.25605 (19) | 0.0191 (8) |
| H33A | 0.3514 | 0.1591 | 0.2160 | 0.023* |
| H33B | 0.4174 | 0.2512 | 0.2759 | 0.023* |
| C34 | 0.1815 (5) | 0.2775 (4) | 0.2212 (2) | 0.0269 (9) |
| H34A | 0.2118 | 0.3232 | 0.1821 | 0.040* |
| H34B | 0.1518 | 0.3224 | 0.2608 | 0.040* |
| H34C | 0.0903 | 0.2325 | 0.1984 | 0.040* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0422 (3) | 0.0408 (3) | 0.01315 (17) | 0.0001 (2) | 0.00294 (16) | 0.00690 (18) |
| Br2 | 0.0464 (3) | 0.0329 (2) | 0.01177 (17) | −0.0012 (2) | 0.00189 (16) | 0.00394 (17) |
| Cu1 | 0.01055 (19) | 0.0157 (2) | 0.00941 (18) | 0.0017 (2) | 0.00319 (15) | 0.00015 (17) |
| O1 | 0.0124 (11) | 0.0200 (15) | 0.0102 (11) | 0.0010 (11) | 0.0022 (9) | −0.0007 (9) |
| O2 | 0.0405 (18) | 0.0236 (16) | 0.0123 (13) | −0.0064 (14) | 0.0046 (12) | 0.0003 (11) |
| O3 | 0.0130 (12) | 0.0162 (13) | 0.0112 (11) | 0.0004 (11) | 0.0026 (9) | −0.0036 (10) |
| O4 | 0.0232 (15) | 0.0117 (13) | 0.0201 (13) | −0.0012 (11) | 0.0054 (11) | 0.0032 (10) |
| O5 | 0.0404 (19) | 0.0231 (16) | 0.0244 (15) | −0.0148 (14) | 0.0112 (13) | −0.0034 (12) |
| O6 | 0.0201 (15) | 0.0150 (14) | 0.0178 (13) | −0.0043 (12) | 0.0053 (11) | −0.0018 (10) |
| O7 | 0.0217 (15) | 0.0183 (15) | 0.0198 (14) | −0.0056 (13) | 0.0051 (12) | 0.0006 (12) |
| O8 | 0.0232 (15) | 0.0228 (15) | 0.0182 (14) | −0.0045 (14) | 0.0018 (12) | 0.0013 (12) |
| N1 | 0.0114 (14) | 0.0144 (16) | 0.0122 (13) | −0.0002 (12) | 0.0028 (11) | 0.0004 (11) |
| N2 | 0.0158 (15) | 0.0213 (18) | 0.0106 (14) | −0.0042 (14) | 0.0036 (12) | 0.0008 (12) |
| N3 | 0.0136 (14) | 0.0119 (14) | 0.0105 (13) | −0.0009 (13) | 0.0037 (11) | −0.0001 (11) |
| N4 | 0.0119 (14) | 0.0156 (16) | 0.0141 (14) | −0.0043 (14) | 0.0024 (11) | 0.0006 (12) |
| C1 | 0.0138 (19) | 0.024 (2) | 0.0070 (15) | 0.0050 (16) | 0.0019 (13) | −0.0017 (14) |
| C2 | 0.0122 (16) | 0.021 (2) | 0.0112 (15) | 0.0020 (17) | 0.0016 (13) | 0.0008 (15) |
| C3 | 0.019 (2) | 0.020 (2) | 0.0192 (17) | −0.0008 (19) | 0.0028 (15) | 0.0008 (17) |
| C4 | 0.030 (2) | 0.028 (2) | 0.0111 (17) | 0.0016 (19) | 0.0016 (16) | −0.0051 (15) |
| C5 | 0.0164 (19) | 0.031 (2) | 0.0080 (16) | 0.0027 (18) | −0.0032 (14) | 0.0059 (15) |
| C6 | 0.0165 (19) | 0.024 (2) | 0.0194 (18) | −0.0006 (18) | 0.0040 (15) | 0.0042 (16) |
| C7 | 0.0184 (19) | 0.022 (2) | 0.0132 (16) | −0.0016 (17) | 0.0035 (14) | −0.0014 (14) |
| C8 | 0.0073 (17) | 0.020 (2) | 0.0163 (17) | 0.0011 (16) | 0.0038 (14) | 0.0015 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9 | 0.0141 (17) | 0.014 (2) | 0.0112 (16) | 0.0033 (15) | 0.0043 (13) | −0.0003 (13) |
| C10 | 0.0196 (18) | 0.0157 (18) | 0.0101 (15) | 0.0033 (17) | 0.0046 (13) | −0.0020 (15) |
| C11 | 0.0136 (18) | 0.0130 (19) | 0.0213 (19) | 0.0040 (15) | 0.0028 (15) | 0.0017 (14) |
| C12 | 0.020 (2) | 0.027 (2) | 0.0069 (15) | −0.0013 (17) | 0.0008 (14) | 0.0031 (14) |
| C13 | 0.027 (2) | 0.018 (2) | 0.0164 (18) | −0.0051 (18) | 0.0032 (16) | −0.0047 (15) |
| C14 | 0.021 (2) | 0.016 (2) | 0.0153 (16) | −0.0035 (16) | 0.0000 (15) | −0.0016 (14) |
| C15 | 0.0152 (18) | 0.0125 (19) | 0.0087 (15) | −0.0014 (15) | 0.0007 (13) | −0.0011 (13) |
| C16 | 0.0189 (19) | 0.0131 (18) | 0.0127 (16) | −0.0014 (16) | 0.0014 (14) | −0.0032 (13) |
| C17 | 0.0127 (17) | 0.0168 (19) | 0.0168 (16) | −0.0004 (16) | 0.0040 (14) | −0.0091 (15) |
| C18 | 0.0157 (16) | 0.0136 (17) | 0.0098 (15) | −0.0061 (18) | 0.0022 (12) | −0.0027 (15) |
| C19 | 0.0160 (17) | 0.0132 (19) | 0.0096 (15) | −0.0006 (14) | 0.0021 (13) | 0.0012 (12) |
| C20 | 0.0085 (17) | 0.0154 (19) | 0.026 (2) | 0.0001 (16) | 0.0071 (15) | 0.0049 (16) |
| C21 | 0.022 (2) | 0.025 (2) | 0.0144 (17) | −0.0032 (17) | 0.0085 (15) | 0.0047 (15) |
| C22 | 0.028 (2) | 0.031 (2) | 0.026 (2) | 0.0022 (19) | 0.0084 (18) | 0.0126 (17) |
| C23 | 0.021 (2) | 0.025 (2) | 0.0132 (16) | −0.0096 (18) | 0.0050 (15) | −0.0036 (16) |
| C24 | 0.042 (3) | 0.027 (2) | 0.022 (2) | −0.007 (2) | 0.0066 (19) | −0.0067 (17) |
| C25 | 0.0144 (18) | 0.0114 (17) | 0.0125 (15) | −0.0026 (16) | 0.0028 (13) | −0.0029 (14) |
| C26 | 0.0187 (19) | 0.0116 (18) | 0.0137 (16) | 0.0009 (15) | −0.0010 (14) | −0.0005 (13) |
| C27 | 0.0172 (18) | 0.0125 (19) | 0.0117 (15) | −0.0009 (16) | 0.0055 (13) | −0.0025 (13) |
| C28 | 0.0163 (17) | 0.0079 (19) | 0.0134 (16) | −0.0025 (15) | 0.0039 (13) | −0.0035 (13) |
| C29 | 0.0144 (16) | 0.0095 (17) | 0.0125 (15) | 0.0004 (16) | 0.0009 (13) | −0.0004 (14) |
| C30 | 0.0129 (18) | 0.0138 (18) | 0.0134 (16) | 0.0028 (15) | 0.0057 (14) | −0.0012 (14) |
| C31 | 0.0188 (19) | 0.024 (2) | 0.0116 (16) | −0.0060 (17) | −0.0005 (14) | 0.0002 (14) |
| C32 | 0.037 (3) | 0.020 (2) | 0.0215 (19) | 0.0020 (19) | 0.0039 (18) | 0.0010 (16) |
| C33 | 0.0181 (19) | 0.024 (2) | 0.0168 (16) | −0.0004 (18) | 0.0085 (15) | 0.0043 (17) |
| C34 | 0.023 (2) | 0.035 (2) | 0.022 (2) | 0.008 (2) | 0.0038 (17) | 0.0130 (17) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—C5 | 1.904 (3) | C15—C16 | 1.377 (5) |
| Br2—C12 | 1.901 (3) | C15—H15 | 0.9300 |
| Cu1—O1 | 1.985 (2) | C16—H16 | 0.9300 |
| Cu1—O3 | 1.979 (2) | C17—C16 | 1.382 (5) |
| Cu1—O7 | 2.377 (3) | C17—C18 | 1.386 (5) |
| Cu1—O8 | 2.543 (3) | C17—H17 | 0.9300 |
| Cu1—N1 | 1.996 (3) | C18—C19 | 1.385 (4) |
| Cu1—N3 | 1.998 (3) | C18—C20 | 1.495 (5) |
| O1—C1 | 1.289 (4) | C19—H19 | 0.9300 |
| O2—C1 | 1.200 (5) | C20—N2 | 1.354 (4) |
| O3—C8 | 1.277 (4) | C21—N2 | 1.467 (4) |
| O4—C8 | 1.229 (4) | C21—C22 | 1.515 (5) |
| O5—C20 | 1.217 (5) | C21—H21A | 0.9700 |
| O6—C30 | 1.235 (4) | C21—H21B | 0.9700 |
| O7—H71 | 0.831 (19) | C22—H22A | 0.9600 |
| O7—H72 | 0.823 (19) | C22—H22B | 0.9600 |
| O8—H81 | 0.841 (18) | C22—H22C | 0.9600 |
| O8—H82 | 0.826 (19) | C23—N2 | 1.472 (5) |
| N1—C19 | 1.339 (4) | C23—C24 | 1.518 (6) |

| | | | |
|---|---|---|---|
| N3—C29 | 1.337 (4) | C23—H23A | 0.9700 |
| N4—C30 | 1.343 (4) | C23—H23B | 0.9700 |
| N4—C31 | 1.462 (5) | C24—H24A | 0.9600 |
| N4—C33 | 1.464 (4) | C24—H24B | 0.9600 |
| C2—C1 | 1.531 (4) | C24—H24C | 0.9600 |
| C2—C7 | 1.377 (5) | C25—N3 | 1.344 (5) |
| C3—C2 | 1.399 (5) | C25—C26 | 1.382 (5) |
| C3—C4 | 1.397 (5) | C25—H25 | 0.9300 |
| C3—H3 | 0.9300 | C26—H26 | 0.9300 |
| C4—H4 | 0.9300 | C27—C26 | 1.381 (5) |
| C5—C4 | 1.364 (6) | C27—H27 | 0.9300 |
| C5—C6 | 1.376 (5) | C28—C27 | 1.393 (5) |
| C6—C7 | 1.401 (5) | C28—C29 | 1.371 (4) |
| C6—H6 | 0.9300 | C29—H29 | 0.9300 |
| C7—H7 | 0.9300 | C30—C28 | 1.511 (5) |
| C8—C9 | 1.520 (4) | C31—C32 | 1.514 (5) |
| C10—C9 | 1.376 (5) | C31—H31A | 0.9700 |
| C10—H10 | 0.9300 | C31—H31B | 0.9700 |
| C11—C10 | 1.381 (5) | C32—H32A | 0.9600 |
| C11—C12 | 1.385 (5) | C32—H32B | 0.9600 |
| C11—H11 | 0.9300 | C32—H32C | 0.9600 |
| C13—C12 | 1.374 (6) | C33—C34 | 1.507 (5) |
| C13—H13 | 0.9300 | C33—H33A | 0.9700 |
| C14—C9 | 1.382 (4) | C33—H33B | 0.9700 |
| C14—C13 | 1.387 (5) | C34—H34A | 0.9600 |
| C14—H14 | 0.9300 | C34—H34B | 0.9600 |
| C15—N1 | 1.329 (4) | C34—H34C | 0.9600 |

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|---|---|---|---|
| O1—Cu1—O7 | 92.38 (10) | C16—C17—H17 | 120.5 |
| O1—Cu1—N1 | 89.72 (10) | C18—C17—H17 | 120.5 |
| O1—Cu1—N3 | 91.99 (10) | C17—C18—C20 | 122.8 (3) |
| O3—Cu1—O1 | 178.70 (11) | C19—C18—C17 | 118.3 (3) |
| O3—Cu1—O7 | 88.92 (10) | C19—C18—C20 | 118.6 (3) |
| O3—Cu1—N1 | 90.39 (10) | N1—C19—C18 | 122.4 (3) |
| O3—Cu1—N3 | 87.81 (10) | N1—C19—H19 | 118.8 |
| N1—Cu1—O7 | 86.50 (10) | C18—C19—H19 | 118.8 |
| N1—Cu1—N3 | 175.65 (12) | O5—C20—N2 | 122.0 (3) |
| N3—Cu1—O7 | 97.43 (11) | O5—C20—C18 | 120.6 (3) |
| C1—O1—Cu1 | 127.5 (2) | N2—C20—C18 | 117.5 (3) |
| C8—O3—Cu1 | 125.5 (2) | N2—C21—C22 | 112.8 (3) |
| Cu1—O7—H71 | 99 (3) | N2—C21—H21A | 109.0 |
| Cu1—O7—H72 | 132 (3) | N2—C21—H21B | 109.0 |
| H71—O7—H72 | 108 (5) | C22—C21—H21A | 109.0 |
| H81—O8—H82 | 99 (4) | C22—C21—H21B | 109.0 |
| C15—N1—Cu1 | 120.9 (2) | H21A—C21—H21B | 107.8 |
| C15—N1—C19 | 118.6 (3) | C21—C22—H22A | 109.5 |
| C19—N1—Cu1 | 120.4 (2) | C21—C22—H22B | 109.5 |
| C20—N2—C21 | 119.2 (3) | C21—C22—H22C | 109.5 |

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|---|---|---|---|
| C20—N2—C23 | 123.8 (3) | H22A—C22—H22B | 109.5 |
| C21—N2—C23 | 116.9 (3) | H22A—C22—H22C | 109.5 |
| C25—N3—Cu1 | 120.6 (2) | H22B—C22—H22C | 109.5 |
| C29—N3—Cu1 | 120.7 (2) | N2—C23—C24 | 112.5 (3) |
| C29—N3—C25 | 118.6 (3) | N2—C23—H23A | 109.1 |
| C30—N4—C31 | 123.9 (3) | N2—C23—H23B | 109.1 |
| C30—N4—C33 | 118.5 (3) | C24—C23—H23A | 109.1 |
| C31—N4—C33 | 117.3 (3) | C24—C23—H23B | 109.1 |
| O1—C1—C2 | 113.1 (3) | H23A—C23—H23B | 107.8 |
| O2—C1—O1 | 127.7 (3) | C23—C24—H24A | 109.5 |
| O2—C1—C2 | 119.2 (3) | C23—C24—H24B | 109.5 |
| C3—C2—C1 | 118.0 (3) | C23—C24—H24C | 109.5 |
| C7—C2—C1 | 121.8 (3) | H24A—C24—H24B | 109.5 |
| C7—C2—C3 | 120.2 (3) | H24A—C24—H24C | 109.5 |
| C2—C3—H3 | 120.2 | H24B—C24—H24C | 109.5 |
| C4—C3—C2 | 119.5 (4) | N3—C25—C26 | 121.8 (3) |
| C4—C3—H3 | 120.2 | N3—C25—H25 | 119.1 |
| C3—C4—H4 | 120.5 | C26—C25—H25 | 119.1 |
| C5—C4—C3 | 118.9 (4) | C25—C26—H26 | 120.3 |
| C5—C4—H4 | 120.5 | C27—C26—C25 | 119.4 (3) |
| C4—C5—Br1 | 119.3 (3) | C27—C26—H26 | 120.3 |
| C4—C5—C6 | 122.9 (3) | C26—C27—C28 | 118.6 (3) |
| C6—C5—Br1 | 117.8 (3) | C26—C27—H27 | 120.7 |
| C5—C6—C7 | 118.1 (4) | C28—C27—H27 | 120.7 |
| C5—C6—H6 | 120.9 | C27—C28—C30 | 122.8 (3) |
| C7—C6—H6 | 120.9 | C29—C28—C27 | 118.7 (3) |
| C2—C7—C6 | 120.4 (3) | C29—C28—C30 | 118.2 (3) |
| C2—C7—H7 | 119.8 | N3—C29—C28 | 122.9 (3) |
| C6—C7—H7 | 119.8 | N3—C29—H29 | 118.6 |
| O3—C8—C9 | 114.9 (3) | C28—C29—H29 | 118.6 |
| O4—C8—O3 | 126.4 (3) | O6—C30—N4 | 122.7 (3) |
| O4—C8—C9 | 118.7 (3) | O6—C30—C28 | 118.7 (3) |
| C10—C9—C8 | 120.8 (3) | N4—C30—C28 | 118.7 (3) |
| C10—C9—C14 | 119.5 (3) | N4—C31—C32 | 112.7 (3) |
| C14—C9—C8 | 119.6 (3) | N4—C31—H31A | 109.1 |
| C9—C10—C11 | 121.3 (3) | N4—C31—H31B | 109.1 |
| C9—C10—H10 | 119.3 | C32—C31—H31A | 109.1 |
| C11—C10—H10 | 119.3 | C32—C31—H31B | 109.1 |
| C10—C11—C12 | 118.0 (3) | H31A—C31—H31B | 107.8 |
| C10—C11—H11 | 121.0 | C31—C32—H32A | 109.5 |
| C12—C11—H11 | 121.0 | C31—C32—H32B | 109.5 |
| C11—C12—Br2 | 118.6 (3) | C31—C32—H32C | 109.5 |
| C13—C12—Br2 | 119.3 (3) | H32A—C32—H32B | 109.5 |
| C13—C12—C11 | 122.0 (3) | H32A—C32—H32C | 109.5 |
| C12—C13—C14 | 118.7 (3) | H32B—C32—H32C | 109.5 |
| C12—C13—H13 | 120.6 | N4—C33—C34 | 112.5 (3) |
| C14—C13—H13 | 120.6 | N4—C33—H33A | 109.1 |
| C9—C14—C13 | 120.4 (3) | N4—C33—H33B | 109.1 |

| | | | |
|---|---|---|---|
| C9—C14—H14 | 119.8 | C34—C33—H33A | 109.1 |
| C13—C14—H14 | 119.8 | C34—C33—H33B | 109.1 |
| N1—C15—C16 | 122.6 (3) | H33A—C33—H33B | 107.8 |
| N1—C15—H15 | 118.7 | C33—C34—H34A | 109.5 |
| C16—C15—H15 | 118.7 | C33—C34—H34B | 109.5 |
| C15—C16—C17 | 118.9 (3) | C33—C34—H34C | 109.5 |
| C15—C16—H16 | 120.5 | H34A—C34—H34B | 109.5 |
| C17—C16—H16 | 120.5 | H34A—C34—H34C | 109.5 |
| C16—C17—C18 | 119.0 (3) | H34B—C34—H34C | 109.5 |
| | | | |
| O7—Cu1—O1—C1 | 23.4 (3) | C5—C6—C7—C2 | 0.1 (5) |
| N1—Cu1—O1—C1 | −63.1 (3) | O3—C8—C9—C10 | 4.5 (5) |
| N3—Cu1—O1—C1 | 120.9 (3) | O3—C8—C9—C14 | −178.2 (3) |
| O7—Cu1—O3—C8 | 155.5 (3) | O4—C8—C9—C10 | −174.9 (4) |
| N1—Cu1—O3—C8 | −118.0 (3) | O4—C8—C9—C14 | 2.4 (5) |
| N3—Cu1—O3—C8 | 58.1 (3) | C11—C10—C9—C8 | 179.0 (3) |
| O1—Cu1—N1—C15 | 141.7 (3) | C11—C10—C9—C14 | 1.7 (6) |
| O1—Cu1—N1—C19 | −37.7 (2) | C12—C11—C10—C9 | −0.6 (5) |
| O3—Cu1—N1—C15 | −39.6 (3) | C10—C11—C12—Br2 | 179.1 (3) |
| O3—Cu1—N1—C19 | 141.0 (3) | C10—C11—C12—C13 | −0.7 (6) |
| O7—Cu1—N1—C15 | 49.3 (2) | C14—C13—C12—Br2 | −178.9 (3) |
| O7—Cu1—N1—C19 | −130.1 (3) | C14—C13—C12—C11 | 0.8 (6) |
| O1—Cu1—N3—C25 | 43.0 (3) | C13—C14—C9—C8 | −178.9 (3) |
| O1—Cu1—N3—C29 | −140.1 (2) | C13—C14—C9—C10 | −1.5 (5) |
| O3—Cu1—N3—C25 | −135.7 (3) | C9—C14—C13—C12 | 0.3 (6) |
| O3—Cu1—N3—C29 | 41.2 (3) | C16—C15—N1—C19 | 2.4 (5) |
| O7—Cu1—N3—C25 | 135.7 (2) | C16—C15—N1—Cu1 | −177.0 (3) |
| O7—Cu1—N3—C29 | −47.5 (3) | N1—C15—C16—C17 | −0.2 (5) |
| Cu1—O1—C1—O2 | −27.2 (6) | C18—C17—C16—C15 | −1.3 (5) |
| Cu1—O1—C1—C2 | 152.3 (2) | C16—C17—C18—C19 | 0.5 (5) |
| Cu1—O3—C8—O4 | 25.0 (5) | C16—C17—C18—C20 | −173.0 (3) |
| Cu1—O3—C8—C9 | −154.4 (2) | C17—C18—C19—N1 | 1.9 (5) |
| Cu1—N1—C19—C18 | 176.1 (2) | C20—C18—C19—N1 | 175.6 (3) |
| C15—N1—C19—C18 | −3.3 (5) | C17—C18—C20—O5 | 94.2 (5) |
| Cu1—N3—C29—C28 | −174.5 (3) | C17—C18—C20—N2 | −84.9 (4) |
| C25—N3—C29—C28 | 2.5 (5) | C19—C18—C20—O5 | −79.3 (4) |
| C31—N4—C30—O6 | −172.8 (3) | C19—C18—C20—N2 | 101.7 (4) |
| C31—N4—C30—C28 | 4.9 (5) | O5—C20—N2—C21 | −1.4 (5) |
| C33—N4—C30—O6 | 1.0 (5) | O5—C20—N2—C23 | 174.3 (3) |
| C33—N4—C30—C28 | 178.7 (3) | C18—C20—N2—C21 | 177.6 (3) |
| C30—N4—C31—C32 | −109.2 (4) | C18—C20—N2—C23 | −6.7 (5) |
| C33—N4—C31—C32 | 76.9 (4) | C22—C21—N2—C20 | 90.9 (4) |
| C30—N4—C33—C34 | −92.0 (4) | C22—C21—N2—C23 | −85.0 (4) |
| C31—N4—C33—C34 | 82.2 (4) | C24—C23—N2—C20 | 102.7 (4) |
| C3—C2—C1—O1 | −179.5 (3) | C24—C23—N2—C21 | −81.5 (4) |
| C3—C2—C1—O2 | 0.0 (5) | C26—C25—N3—Cu1 | 175.1 (2) |
| C7—C2—C1—O1 | −2.7 (5) | C26—C25—N3—C29 | −1.8 (5) |
| C7—C2—C1—O2 | 176.8 (4) | N3—C25—C26—C27 | 0.4 (5) |

| | | | |
|---|---|---|---|
| C1—C2—C7—C6 | −177.2 (3) | C28—C27—C26—C25 | 0.5 (5) |
| C3—C2—C7—C6 | −0.5 (5) | C29—C28—C27—C26 | 0.1 (5) |
| C4—C3—C2—C1 | 177.9 (3) | C30—C28—C27—C26 | 173.8 (3) |
| C4—C3—C2—C7 | 1.0 (5) | C27—C28—C29—N3 | −1.6 (5) |
| C2—C3—C4—C5 | −1.2 (6) | C30—C28—C29—N3 | −175.6 (3) |
| Br1—C5—C4—C3 | −179.5 (3) | O6—C30—C28—C27 | −101.2 (4) |
| C6—C5—C4—C3 | 0.8 (7) | O6—C30—C28—C29 | 72.5 (4) |
| Br1—C5—C6—C7 | −180.0 (3) | N4—C30—C28—C27 | 81.0 (4) |
| C4—C5—C6—C7 | −0.3 (6) | N4—C30—C28—C29 | −105.3 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O7—H71···O2 | 0.83 (2) | 1.93 (3) | 2.692 (4) | 154 (5) |
| O7—H72···O4$^{i}$ | 0.83 (4) | 2.04 (4) | 2.834 (4) | 163 (3) |
| O8—H81···O4 | 0.84 (2) | 1.88 (2) | 2.702 (4) | 170 (4) |
| O8—H82···O6$^{ii}$ | 0.82 (4) | 2.05 (4) | 2.848 (4) | 168 (5) |
| C11—H11···O5$^{iii}$ | 0.93 | 2.41 | 3.106 (5) | 133 |
| C16—H16···O4$^{iii}$ | 0.93 | 2.46 | 3.359 (5) | 162 |
| C26—H26···O6$^{iv}$ | 0.93 | 2.37 | 3.261 (4) | 160 |

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