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# Tetra-$\mu$-acetato-$\kappa^8O:O'$-bis{[2-(2-furyl)-1-(2-furylmethyl)-1*H*-benzimidazole-$\kappa N^3$]copper(II)}

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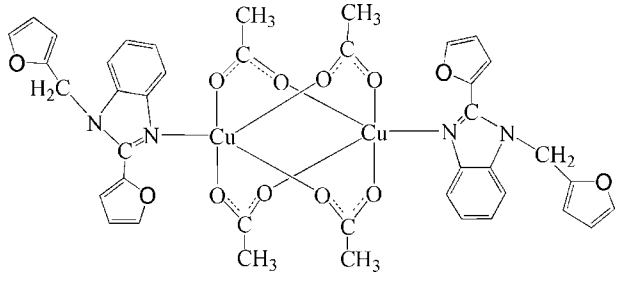
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.009 Å; disorder in main residue; $R$ factor = 0.057; $wR$ factor = 0.152; data-to-parameter ratio = 11.2.

The title complex, $[Cu_2(CH_3COO)_4(C_{16}H_{12}N_2O_2)_2]$, forms a dimer of the paddle-wheel type located on a crystallographic inversion centre. The two $Cu^{II}$ atoms [Cu···Cu = 2.7254 (11) Å] are bridged by four acetate anions. The geometry of the polyhedron around the metal centre can be described as tetragonal-pyramidal derived from the calculation of the value $\tau$ = 0.0018. The apical positions of the tetragonal-pyramidal copper coordination polyhedra are occupied by the N atoms of 2-(2-furyl)-1-(2-furylmethyl)-1*H*-benzimidazole ligands. In the crystal structure, molecules are linked into a chain by intermolecular C—H···O hydrogen bonds parallel to [010]. Two furan rings are disordered over two positions in ratios of 0.55:0.45 and 0.69:0.31.

## Related literature

For general background, see: Solomon *et al.* (1992). For the chemical, physical and structural properties of tripodal copper complexes, see: Malachowski *et al.* (1995); Mclachlan *et al.* (1995). For Cu—Cu distances in dimeric copper(II) carboxylate complexes, see: Liu *et al.* (2007). For the $\tau$ parameter, see: Addison *et al.* (1984).



## Experimental

### Crystal data

$[Cu_2(C_2H_3O_2)_4(C_{16}H_{12}N_2O_2)_2]$
$M_r$ = 891.81
Triclinic, $P\overline{1}$
$a$ = 9.6617 (15) Å
$b$ = 11.2779 (19) Å
$c$ = 19.233 (2) Å
$\alpha$ = 75.817 (1)°
$\beta$ = 80.031 (2)°
$\gamma$ = 76.168 (1)°
$V$ = 1958.3 (5) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.16 mm$^{-1}$
$T$ = 298 K
0.48 × 0.23 × 0.12 mm

### Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.607, $T_{max}$ = 0.874
10261 measured reflections
6802 independent reflections
4761 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.023

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.152
$S$ = 1.02
6802 reflections
606 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.62 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cu1—O4$^{i}$ | 1.961 (3) | Cu1—O6$^{i}$ | 1.989 (3) |
| Cu1—O3 | 1.966 (3) | Cu1—N1 | 2.233 (4) |
| Cu1—O5 | 1.977 (3) | | |
| O4$^{i}$—Cu1—O3 | 165.00 (14) | O5—Cu1—O6$^{i}$ | 165.11 (15) |

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

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C12—H12$B$···O3$^{ii}$ | 0.97 | 2.55 | 3.426 (7) | 151 |
| C31—H31···O6$^{iii}$ | 0.93 | 2.54 | 3.44 (3) | 166 |
| C36—H36···O4$^{i}$ | 0.93 | 2.50 | 3.371 (19) | 157 |

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2119).

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# supporting information

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## Tetra-$\mu$-acetato-$\kappa^8O:O'$-bis{[2-(2-furyl)-1-(2-furylmethyl)-1*H*-benzimidazole-$\kappa N^3$]copper(II)}

**Qiang Wang, Cai-Feng Bi, Da-Qi Wang, Yu-Hua Fan and Ji-Tian Liu**

### S1. Comment

Investigations of the coordination chemistry of copper(II) continue to be stimulated by interest in developing models for copper proteins and in understanding the factors which give rise to the seemingly infinite variety of distortions from regular stereochemistry observed in $Cu^{II}$ complexes (Solomon *et al.*, 1992). Due to the unique coordination polyhedra and their ease of preparation, tripodal copper complexes have attracted much attention in addition to their special chemical, physical and structure properties (Malachowski *et al.*, 1995; Mclachlan *et al.*, 1995). We report here the synthesis and crystal structure of the title compound, a new binuclear copper(II) complex.

The molecular structure of the title complex is shown in Fig.1. The $Cu^{II}$ atom is five-coordinated, with a coordination geometry that is best described as distorted square pyramidal. The Cu1—Cu1A distance is 2.7254 (11) Å, very similar to the values found in other dimeric copper(II) carboxylate complexes (Liu *et al.*, 2007). The basal plane for a tetragonal-pyramidal geometry is defined by the atoms O3, O4, O5 and O6, their mean deviation from this plane is 0.0031 Å, and the Cu atom just out of this plane by 0.4762 Å. The axial position of the pyramid is occupied by atom N1. For this point of view, a geometry parameter $\tau$, which is defined $\tau = (\beta - \alpha)/60$, applicable to 5-coordinate structures within the structural continuum between trigonal bipyramidal and tetragonal or rectangular pyramidal. For a perfect tetragonal symmetry $\tau$ is zero, and for a perfect trigonal-bipyramidal geometry $\tau$ becomes 1.0 (Addison *et al.* 1984). In the title compound, the largest angles within the four atoms O3, O4, O5, O6, are $\beta$ = 165.11 (15)° for O5–Cu1–O6, and $\alpha$ = 165.00 (14)° for O3–Cu1–O4. Thus, $\tau$ is (165.11–165.00)/60 = 0.0018, indicating a 98% rectangular pyramidal geometry. The 2-(furan-2-yl)-1-((furan-2-yl)methyl) -1*H*-benzo[*d*]imidazole molecules are coordinated to $Cu^{II}$ through their midazole N atom and occupy the axial position. Four acetate ligands act as bridges to connect the two $Cu^{II}$ centers into a dinuclear complex across a crystallographic centre of inversion. In the ligand, the dihedral angle between furyl rings and phenyl ring are 24.50 (3)°, 55.22 (2)° and 30.84 (2) °. Selected bond distances and angles are presented in Table 1.

As seen in Fig. 2, the molecules are linked into a one-dimensional chain by intermolecular C—H···O hydrogen bonds. (Table 2).

### S2. Experimental

furfuraldehyde (10 mmol, 960 mg) was added dropwise to a absolute ethanol (20 ml) of *o*-phenylenediamine (5 mmol, 547 mg). The mixture was heated under reflux with stirring for 2 h. An absolute ethanol solution (10 ml) of cupric acetate monohydrate (5 mmol, 850 mg) was then added dropwise, and the mixture was stirred at room temperature for another 20 h. The solution was filtered off, the filterate was kept at room temperature for about several weeks, after which the green crystals were obtained.

### S3. Refinement

All H-atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.96 Å, with $U_{iso}$(H) =1.2$U_{eq}$(C).

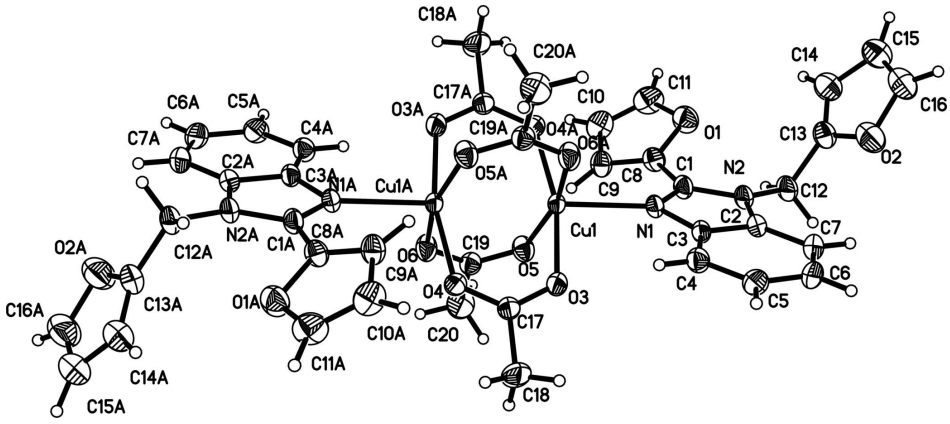


**Figure 1**

The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

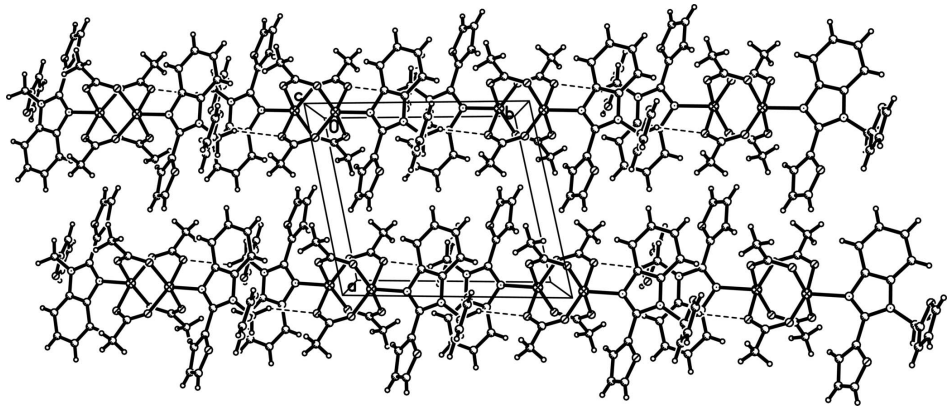

**Figure 2**

The crystal packing of the title complex, viewed approximately along the *b* axis.

**Tetra-$\mu$-acetato-$\kappa^8O$:$O'$-bis{[2-(2-furyl)-1-(2-furylmethyl)- 1*H*-benzimidazole-$\kappa N^3$]copper(II)}

*Crystal data*

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$M_r$ = 891.81
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 9.6617 (15) Å
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$c$ = 19.233 (2) Å
$\alpha$ = 75.817 (1)°
$\beta$ = 80.031 (2)°
$\gamma$ = 76.168 (1)°
$V$ = 1958.3 (5) Å$^3$
$Z$ = 2
$F$(000) = 916
$D_x$ = 1.512 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2908 reflections
$\theta$ = 2.4–24.7°
$\mu$ = 1.16 mm$^{-1}$
$T$ = 298 K
Block, green
0.48 × 0.23 × 0.12 mm

*Data collection*

Siemens SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.607, $T_{max}$ = 0.874
10261 measured reflections
6802 independent reflections
4761 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.023
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 1.9°
$h$ = −11→11
$k$ = −13→13
$l$ = −17→22

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.152
$S$ = 1.02
6802 reflections
606 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0617P)^2 + 4.0885P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.59 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.62 e Å$^{-3}$

*Special details*

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

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness of fit $S$ are based on $F^2$, conventional $R$-factors $R$ are based on $F$, with $F$ set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating $R$-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. $R$-factors based on $F^2$ are statistically about twice as large as those based on $F$, and $R$- factors based on ALL data will be even larger.

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Cu1 | 0.99281 (6) | 0.89727 (5) | 0.47651 (3) | 0.03232 (18) | |
| Cu2 | 0.53213 (7) | 0.60430 (6) | 0.01052 (3) | 0.0440 (2) | |
| N1 | 0.9845 (4) | 0.7264 (4) | 0.4396 (2) | 0.0365 (9) | |
| N2 | 0.9293 (5) | 0.5746 (4) | 0.3999 (2) | 0.0436 (10) | |
| N3 | 0.5831 (5) | 0.7740 (4) | 0.0330 (3) | 0.0551 (12) | |
| N4 | 0.6085 (6) | 0.9327 (5) | 0.0755 (3) | 0.0654 (14) | |
| O1 | 0.6522 (4) | 0.7372 (4) | 0.3768 (2) | 0.0650 (11) | |
| O2 | 0.9699 (6) | 0.4443 (5) | 0.2714 (3) | 0.0931 (16) | |
| O3 | 1.1457 (4) | 0.8153 (3) | 0.53831 (19) | 0.0480 (9) | |
| O4 | 1.1553 (4) | 0.9823 (3) | 0.57688 (19) | 0.0471 (9) | |
| O5 | 0.8573 (4) | 0.8762 (3) | 0.56612 (19) | 0.0487 (9) | |
| O6 | 0.8639 (4) | 1.0444 (3) | 0.60436 (19) | 0.0507 (9) | |
| O7 | 0.3864 (18) | 0.8787 (16) | 0.1965 (9) | 0.072 (5) | 0.55 (3) |
| O8 | 0.7106 (13) | 1.0211 (14) | 0.2262 (8) | 0.083 (4) | 0.69 (3) |
| O7′ | 0.3368 (18) | 0.7504 (16) | 0.1357 (12) | 0.076 (6) | 0.45 (3) |
| O8′ | 0.752 (3) | 1.082 (3) | 0.1872 (18) | 0.076 (9) | 0.31 (3) |

| | | | | |
|---|---|---|---|---|
| O9 | 0.7334 (4) | 0.5180 (4) | −0.0055 (2) | 0.0673 (12) |
| O10 | 0.6774 (5) | 0.3442 (4) | −0.0174 (2) | 0.0682 (12) |
| O11 | 0.5353 (5) | 0.6649 (4) | −0.0946 (2) | 0.0626 (11) |
| O12 | 0.4755 (5) | 0.4963 (4) | −0.1098 (2) | 0.0628 (11) |
| C1 | 0.8807 (6) | 0.6855 (5) | 0.4222 (3) | 0.0423 (12) |
| C2 | 1.0751 (6) | 0.5432 (5) | 0.4036 (3) | 0.0430 (12) |
| C3 | 1.1091 (5) | 0.6365 (4) | 0.4280 (3) | 0.0369 (11) |
| C4 | 1.2510 (5) | 0.6321 (5) | 0.4367 (3) | 0.0462 (13) |
| H4 | 1.2761 | 0.6946 | 0.4527 | 0.055* |
| C5 | 1.3516 (6) | 0.5306 (5) | 0.4203 (3) | 0.0541 (14) |
| H5 | 1.4471 | 0.5242 | 0.4256 | 0.065* |
| C6 | 1.3142 (7) | 0.4375 (5) | 0.3961 (3) | 0.0574 (16) |
| H6 | 1.3859 | 0.3708 | 0.3855 | 0.069* |
| C7 | 1.1777 (6) | 0.4401 (5) | 0.3875 (3) | 0.0522 (14) |
| H7 | 1.1534 | 0.3770 | 0.3717 | 0.063* |
| C8 | 0.7319 (6) | 0.7505 (5) | 0.4262 (3) | 0.0463 (13) |
| C9 | 0.6530 (6) | 0.8268 (5) | 0.4672 (3) | 0.0509 (14) |
| H9 | 0.6820 | 0.8506 | 0.5045 | 0.061* |
| C10 | 0.5158 (6) | 0.8650 (6) | 0.4429 (4) | 0.0658 (17) |
| H10 | 0.4369 | 0.9183 | 0.4616 | 0.079* |
| C11 | 0.5204 (7) | 0.8118 (7) | 0.3896 (4) | 0.0720 (19) |
| H11 | 0.4441 | 0.8231 | 0.3634 | 0.086* |
| C12 | 0.8467 (6) | 0.4934 (5) | 0.3834 (3) | 0.0528 (14) |
| H12A | 0.7483 | 0.5143 | 0.4054 | 0.063* |
| H12B | 0.8857 | 0.4075 | 0.4056 | 0.063* |
| C13 | 0.8457 (7) | 0.5017 (6) | 0.3052 (3) | 0.0614 (16) |
| C14 | 0.7492 (8) | 0.5439 (7) | 0.2608 (4) | 0.077 (2) |
| H14 | 0.6554 | 0.5856 | 0.2717 | 0.093* |
| C15 | 0.8107 (10) | 0.5159 (8) | 0.1935 (4) | 0.087 (2) |
| H15 | 0.7661 | 0.5360 | 0.1518 | 0.104* |
| C16 | 0.9412 (10) | 0.4566 (8) | 0.2008 (4) | 0.097 (3) |
| H16 | 1.0066 | 0.4264 | 0.1645 | 0.117* |
| C17 | 1.1925 (5) | 0.8705 (5) | 0.5751 (3) | 0.0408 (12) |
| C18 | 1.3045 (7) | 0.7915 (6) | 0.6228 (4) | 0.0682 (18) |
| H18A | 1.3664 | 0.8424 | 0.6288 | 0.102* |
| H18B | 1.3603 | 0.7248 | 0.6007 | 0.102* |
| H18C | 1.2579 | 0.7572 | 0.6691 | 0.102* |
| C19 | 0.8264 (5) | 0.9439 (5) | 0.6114 (3) | 0.0424 (12) |
| C20 | 0.7392 (7) | 0.8957 (6) | 0.6811 (3) | 0.0714 (19) |
| H20A | 0.7889 | 0.8145 | 0.7035 | 0.107* |
| H20B | 0.6473 | 0.8898 | 0.6712 | 0.107* |
| H20C | 0.7259 | 0.9520 | 0.7131 | 0.107* |
| C21 | 0.5397 (7) | 0.8363 (6) | 0.0854 (4) | 0.0631 (17) |
| C22 | 0.7013 (7) | 0.9309 (6) | 0.0141 (4) | 0.0654 (17) |
| C23 | 0.8006 (8) | 1.0051 (6) | −0.0221 (4) | 0.076 (2) |
| H23 | 0.8120 | 1.0710 | −0.0041 | 0.091* |
| C24 | 0.8779 (8) | 0.9787 (7) | −0.0827 (5) | 0.082 (2) |
| H24 | 0.9444 | 1.0271 | −0.1067 | 0.098* |

| | | | | | |
|---|---|---|---|---|---|
| C25 | 0.8630 (8) | 0.8812 (7) | −0.1118 (4) | 0.079 (2) | |
| H25 | 0.9182 | 0.8668 | −0.1547 | 0.094* | |
| C26 | 0.7671 (7) | 0.8059 (6) | −0.0773 (4) | 0.0671 (18) | |
| H26 | 0.7563 | 0.7406 | −0.0961 | 0.081* | |
| C27 | 0.6876 (7) | 0.8316 (5) | −0.0134 (4) | 0.0596 (16) | |
| C28 | 0.4355 (8) | 0.8056 (6) | 0.1463 (4) | 0.0667 (17) | |
| C29 | 0.371 (2) | 0.705 (2) | 0.1747 (15) | 0.078 (5) | 0.55 (3) |
| H29 | 0.3907 | 0.6345 | 0.1548 | 0.093* | 0.55 (3) |
| C30 | 0.275 (3) | 0.719 (3) | 0.2356 (16) | 0.073 (6) | 0.55 (3) |
| H30 | 0.2177 | 0.6646 | 0.2630 | 0.088* | 0.55 (3) |
| C31 | 0.285 (3) | 0.832 (3) | 0.2461 (15) | 0.072 (6) | 0.55 (3) |
| H31 | 0.2300 | 0.8709 | 0.2820 | 0.086* | 0.55 (3) |
| C29′ | 0.421 (3) | 0.819 (3) | 0.2146 (16) | 0.069 (6) | 0.45 (3) |
| H29′ | 0.4782 | 0.8546 | 0.2346 | 0.083* | 0.45 (3) |
| C30′ | 0.306 (4) | 0.772 (3) | 0.2482 (18) | 0.073 (8) | 0.45 (3) |
| H30′ | 0.2689 | 0.7660 | 0.2966 | 0.088* | 0.45 (3) |
| C31′ | 0.255 (3) | 0.735 (2) | 0.198 (2) | 0.077 (7) | 0.45 (3) |
| H31′ | 0.1723 | 0.7018 | 0.2069 | 0.093* | 0.45 (3) |
| C32 | 0.5972 (8) | 1.0210 (6) | 0.1213 (4) | 0.0725 (19) | |
| H32A | 0.5005 | 1.0383 | 0.1460 | 0.087* | 0.69 (3) |
| H32B | 0.6202 | 1.0989 | 0.0926 | 0.087* | 0.69 (3) |
| H32C | 0.5067 | 1.0239 | 0.1526 | 0.087* | 0.31 (3) |
| H32D | 0.5950 | 1.1036 | 0.0908 | 0.087* | 0.31 (3) |
| C33 | 0.703 (11) | 0.960 (6) | 0.175 (5) | 0.069 (9) | 0.69 (3) |
| C34 | 0.808 (5) | 0.854 (3) | 0.1808 (18) | 0.070 (6) | 0.69 (3) |
| H34 | 0.8277 | 0.7962 | 0.1513 | 0.085* | 0.69 (3) |
| C35 | 0.879 (3) | 0.848 (2) | 0.2387 (14) | 0.072 (5) | 0.69 (3) |
| H35 | 0.9523 | 0.7839 | 0.2571 | 0.086* | 0.69 (3) |
| C36 | 0.821 (2) | 0.956 (2) | 0.2633 (13) | 0.071 (5) | 0.69 (3) |
| H36 | 0.8522 | 0.9797 | 0.2999 | 0.086* | 0.69 (3) |
| C33′ | 0.72 (2) | 0.992 (14) | 0.166 (12) | 0.07 (2) | 0.31 (3) |
| C34′ | 0.783 (10) | 0.881 (7) | 0.200 (4) | 0.073 (13) | 0.31 (3) |
| H34′ | 0.7785 | 0.8034 | 0.1935 | 0.088* | 0.31 (3) |
| C35′ | 0.861 (5) | 0.903 (5) | 0.246 (3) | 0.067 (13) | 0.31 (3) |
| H35′ | 0.9158 | 0.8440 | 0.2786 | 0.081* | 0.31 (3) |
| C36′ | 0.842 (3) | 1.028 (4) | 0.235 (2) | 0.074 (10) | 0.31 (3) |
| H36′ | 0.8867 | 1.0695 | 0.2583 | 0.089* | 0.31 (3) |
| C37 | 0.7653 (7) | 0.4081 (6) | −0.0139 (4) | 0.0640 (17) | |
| C38 | 0.9219 (7) | 0.3457 (7) | −0.0194 (5) | 0.099 (3) | |
| H38A | 0.9787 | 0.4047 | −0.0191 | 0.149* | |
| H38B | 0.9488 | 0.3159 | −0.0635 | 0.149* | |
| H38C | 0.9380 | 0.2766 | 0.0210 | 0.149* | |
| C39 | 0.5055 (7) | 0.6021 (6) | −0.1320 (3) | 0.0583 (15) | |
| C40 | 0.5108 (9) | 0.6544 (8) | −0.2121 (3) | 0.093 (3) | |
| H40A | 0.5917 | 0.6069 | −0.2369 | 0.140* | |
| H40B | 0.5199 | 0.7401 | −0.2223 | 0.140* | |
| H40C | 0.4240 | 0.6497 | −0.2283 | 0.140* | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0369 (3) | 0.0277 (3) | 0.0352 (3) | −0.0056 (2) | −0.0076 (2) | −0.0107 (2) |
| Cu2 | 0.0564 (4) | 0.0363 (4) | 0.0446 (4) | −0.0141 (3) | −0.0139 (3) | −0.0089 (3) |
| N1 | 0.038 (2) | 0.037 (2) | 0.039 (2) | −0.0074 (18) | −0.0056 (18) | −0.0167 (18) |
| N2 | 0.055 (3) | 0.039 (2) | 0.045 (2) | −0.014 (2) | −0.009 (2) | −0.017 (2) |
| N3 | 0.071 (3) | 0.042 (3) | 0.064 (3) | −0.016 (2) | −0.025 (3) | −0.016 (2) |
| N4 | 0.086 (4) | 0.050 (3) | 0.073 (4) | −0.013 (3) | −0.035 (3) | −0.021 (3) |
| O1 | 0.063 (3) | 0.071 (3) | 0.070 (3) | −0.015 (2) | −0.020 (2) | −0.022 (2) |
| O2 | 0.107 (4) | 0.104 (4) | 0.070 (3) | −0.001 (3) | −0.024 (3) | −0.034 (3) |
| O3 | 0.054 (2) | 0.039 (2) | 0.054 (2) | 0.0039 (17) | −0.0209 (18) | −0.0181 (17) |
| O4 | 0.057 (2) | 0.037 (2) | 0.052 (2) | −0.0056 (17) | −0.0248 (18) | −0.0101 (17) |
| O5 | 0.054 (2) | 0.051 (2) | 0.047 (2) | −0.0209 (18) | 0.0022 (18) | −0.0164 (18) |
| O6 | 0.058 (2) | 0.047 (2) | 0.047 (2) | −0.0133 (18) | 0.0108 (18) | −0.0192 (18) |
| O7 | 0.091 (9) | 0.061 (9) | 0.073 (9) | −0.011 (7) | −0.019 (6) | −0.029 (7) |
| O8 | 0.106 (7) | 0.072 (7) | 0.079 (8) | −0.013 (6) | −0.026 (6) | −0.028 (6) |
| O7′ | 0.094 (10) | 0.061 (9) | 0.076 (12) | −0.003 (7) | −0.023 (8) | −0.023 (8) |
| O8′ | 0.094 (14) | 0.068 (15) | 0.078 (17) | −0.016 (11) | −0.026 (12) | −0.026 (14) |
| O9 | 0.065 (3) | 0.052 (3) | 0.083 (3) | −0.014 (2) | −0.011 (2) | −0.007 (2) |
| O10 | 0.065 (3) | 0.057 (3) | 0.085 (3) | −0.006 (2) | −0.014 (2) | −0.023 (2) |
| O11 | 0.084 (3) | 0.057 (3) | 0.056 (2) | −0.032 (2) | −0.022 (2) | −0.003 (2) |
| O12 | 0.087 (3) | 0.066 (3) | 0.045 (2) | −0.030 (2) | −0.020 (2) | −0.007 (2) |
| C1 | 0.050 (3) | 0.039 (3) | 0.045 (3) | −0.015 (2) | −0.007 (2) | −0.016 (2) |
| C2 | 0.053 (3) | 0.039 (3) | 0.038 (3) | −0.005 (2) | −0.008 (2) | −0.015 (2) |
| C3 | 0.040 (3) | 0.036 (3) | 0.037 (3) | −0.005 (2) | −0.004 (2) | −0.014 (2) |
| C4 | 0.045 (3) | 0.047 (3) | 0.048 (3) | −0.003 (2) | −0.007 (2) | −0.017 (3) |
| C5 | 0.047 (3) | 0.056 (4) | 0.055 (3) | 0.004 (3) | −0.010 (3) | −0.016 (3) |
| C6 | 0.063 (4) | 0.046 (3) | 0.056 (4) | 0.011 (3) | −0.005 (3) | −0.020 (3) |
| C7 | 0.062 (4) | 0.043 (3) | 0.052 (3) | 0.000 (3) | −0.008 (3) | −0.020 (3) |
| C8 | 0.046 (3) | 0.050 (3) | 0.053 (3) | −0.020 (3) | −0.015 (3) | −0.015 (3) |
| C9 | 0.047 (3) | 0.051 (3) | 0.062 (4) | −0.015 (3) | −0.006 (3) | −0.021 (3) |
| C10 | 0.044 (3) | 0.066 (4) | 0.084 (5) | −0.007 (3) | −0.002 (3) | −0.018 (4) |
| C11 | 0.049 (4) | 0.081 (5) | 0.087 (5) | −0.011 (3) | −0.023 (4) | −0.013 (4) |
| C12 | 0.068 (4) | 0.049 (3) | 0.054 (3) | −0.022 (3) | −0.014 (3) | −0.020 (3) |
| C13 | 0.077 (4) | 0.058 (4) | 0.060 (4) | −0.019 (3) | −0.017 (4) | −0.023 (3) |
| C14 | 0.088 (5) | 0.079 (5) | 0.073 (5) | −0.015 (4) | −0.026 (4) | −0.022 (4) |
| C15 | 0.106 (6) | 0.091 (6) | 0.073 (5) | −0.018 (5) | −0.031 (5) | −0.023 (4) |
| C16 | 0.119 (7) | 0.106 (7) | 0.068 (5) | −0.002 (6) | −0.018 (5) | −0.037 (5) |
| C17 | 0.040 (3) | 0.040 (3) | 0.043 (3) | −0.005 (2) | −0.009 (2) | −0.010 (2) |
| C18 | 0.067 (4) | 0.056 (4) | 0.082 (5) | 0.006 (3) | −0.041 (4) | −0.011 (3) |
| C19 | 0.043 (3) | 0.040 (3) | 0.043 (3) | −0.008 (2) | −0.002 (2) | −0.009 (2) |
| C20 | 0.081 (5) | 0.070 (4) | 0.054 (4) | −0.020 (4) | 0.021 (3) | −0.012 (3) |
| C21 | 0.080 (4) | 0.050 (4) | 0.071 (4) | −0.013 (3) | −0.032 (4) | −0.018 (3) |
| C22 | 0.081 (5) | 0.050 (4) | 0.076 (5) | −0.020 (3) | −0.036 (4) | −0.008 (3) |
| C23 | 0.090 (5) | 0.060 (4) | 0.088 (5) | −0.027 (4) | −0.034 (4) | −0.008 (4) |
| C24 | 0.089 (5) | 0.066 (5) | 0.093 (6) | −0.035 (4) | −0.026 (5) | 0.006 (4) |
| C25 | 0.085 (5) | 0.070 (5) | 0.082 (5) | −0.028 (4) | −0.024 (4) | 0.003 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C26 | 0.079 (5) | 0.056 (4) | 0.073 (5) | −0.024 (3) | −0.025 (4) | −0.005 (3) |
| C27 | 0.073 (4) | 0.046 (3) | 0.070 (4) | −0.020 (3) | −0.031 (4) | −0.009 (3) |
| C28 | 0.085 (5) | 0.054 (4) | 0.068 (5) | −0.003 (4) | −0.026 (4) | −0.024 (4) |
| C29 | 0.098 (14) | 0.058 (10) | 0.076 (14) | −0.004 (9) | −0.016 (11) | −0.021 (10) |
| C30 | 0.095 (15) | 0.061 (15) | 0.068 (16) | −0.007 (10) | −0.018 (12) | −0.023 (12) |
| C31 | 0.090 (14) | 0.059 (15) | 0.072 (11) | −0.005 (13) | −0.020 (9) | −0.025 (13) |
| C29′ | 0.085 (16) | 0.060 (15) | 0.071 (14) | −0.012 (13) | −0.026 (11) | −0.021 (12) |
| C30′ | 0.091 (19) | 0.06 (2) | 0.072 (14) | −0.009 (18) | −0.018 (12) | −0.020 (19) |
| C31′ | 0.088 (17) | 0.064 (12) | 0.08 (2) | −0.007 (11) | −0.026 (16) | −0.015 (14) |
| C32 | 0.093 (5) | 0.059 (4) | 0.079 (5) | −0.014 (4) | −0.032 (4) | −0.027 (4) |
| C33 | 0.088 (19) | 0.06 (3) | 0.07 (2) | −0.019 (19) | −0.028 (14) | −0.03 (2) |
| C34 | 0.090 (16) | 0.063 (14) | 0.070 (16) | −0.016 (11) | −0.026 (12) | −0.026 (8) |
| C35 | 0.084 (10) | 0.066 (14) | 0.071 (9) | −0.014 (11) | −0.022 (7) | −0.018 (11) |
| C36 | 0.090 (12) | 0.065 (16) | 0.071 (12) | −0.017 (10) | −0.027 (10) | −0.022 (10) |
| C33′ | 0.09 (4) | 0.06 (6) | 0.07 (5) | −0.02 (4) | −0.03 (3) | −0.03 (5) |
| C34′ | 0.09 (4) | 0.06 (4) | 0.07 (4) | −0.02 (3) | −0.03 (3) | −0.02 (2) |
| C35′ | 0.08 (3) | 0.06 (4) | 0.07 (3) | −0.01 (3) | −0.02 (2) | −0.02 (3) |
| C36′ | 0.09 (2) | 0.07 (2) | 0.07 (2) | −0.016 (17) | −0.027 (16) | −0.024 (17) |
| C37 | 0.065 (4) | 0.055 (4) | 0.069 (4) | −0.012 (3) | −0.007 (3) | −0.008 (3) |
| C38 | 0.062 (5) | 0.082 (6) | 0.141 (8) | 0.003 (4) | −0.014 (5) | −0.018 (5) |
| C39 | 0.071 (4) | 0.058 (4) | 0.052 (4) | −0.025 (3) | −0.016 (3) | −0.004 (3) |
| C40 | 0.136 (7) | 0.102 (6) | 0.047 (4) | −0.054 (5) | −0.020 (4) | 0.008 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—O4$^{i}$ | 1.961 (3) | C12—H12B | 0.9700 |
| Cu1—O3 | 1.966 (3) | C13—C14 | 1.300 (9) |
| Cu1—O5 | 1.977 (3) | C14—C15 | 1.403 (10) |
| Cu1—O6$^{i}$ | 1.989 (3) | C14—H14 | 0.9300 |
| Cu1—N1 | 2.233 (4) | C15—C16 | 1.292 (10) |
| Cu1—Cu1$^{i}$ | 2.7254 (11) | C15—H15 | 0.9300 |
| Cu2—O10$^{ii}$ | 1.959 (4) | C16—H16 | 0.9300 |
| Cu2—O9 | 1.964 (4) | C17—C18 | 1.512 (7) |
| Cu2—O11 | 1.966 (4) | C18—H18A | 0.9600 |
| Cu2—O12$^{ii}$ | 1.967 (4) | C18—H18B | 0.9600 |
| Cu2—N3 | 2.241 (4) | C18—H18C | 0.9600 |
| Cu2—Cu2$^{ii}$ | 2.7085 (12) | C19—C20 | 1.508 (7) |
| N1—C1 | 1.320 (6) | C20—H20A | 0.9600 |
| N1—C3 | 1.401 (6) | C20—H20B | 0.9600 |
| N2—C1 | 1.371 (6) | C20—H20C | 0.9600 |
| N2—C2 | 1.377 (7) | C21—C28 | 1.437 (10) |
| N2—C12 | 1.469 (6) | C22—C27 | 1.392 (8) |
| N3—C21 | 1.321 (8) | C22—C23 | 1.404 (9) |
| N3—C27 | 1.398 (8) | C23—C24 | 1.330 (10) |
| N4—C22 | 1.355 (8) | C23—H23 | 0.9300 |
| N4—C21 | 1.364 (8) | C24—C25 | 1.395 (10) |
| N4—C32 | 1.457 (7) | C24—H24 | 0.9300 |
| O1—C11 | 1.368 (7) | C25—C26 | 1.381 (9) |

| | | | |
|---|---|---|---|
| O1—C8 | 1.378 (6) | C25—H25 | 0.9300 |
| O2—C13 | 1.359 (8) | C26—C27 | 1.387 (9) |
| O2—C16 | 1.399 (8) | C26—H26 | 0.9300 |
| O3—C17 | 1.247 (6) | C28—C29′ | 1.34 (3) |
| O4—C17 | 1.233 (6) | C28—C29 | 1.37 (2) |
| O4—Cu1$^{i}$ | 1.961 (3) | C29—C30 | 1.38 (3) |
| O5—C19 | 1.248 (6) | C29—H29 | 0.9300 |
| O6—C19 | 1.240 (6) | C30—C31 | 1.36 (4) |
| O6—Cu1$^{i}$ | 1.989 (3) | C30—H30 | 0.9300 |
| O7—C31 | 1.35 (3) | C31—H31 | 0.9300 |
| O7—C28 | 1.371 (15) | C29′—C30′ | 1.34 (5) |
| O8—C36 | 1.35 (2) | C29′—H29′ | 0.9300 |
| O8—C33 | 1.35 (9) | C30′—C31′ | 1.34 (5) |
| O7′—C31′ | 1.32 (3) | C30′—H30′ | 0.9300 |
| O7′—C28 | 1.323 (15) | C31′—H31′ | 0.9300 |
| O8′—C33′ | 1.32 (15) | C32—C33′ | 1.5 (2) |
| O8′—C36′ | 1.32 (3) | C32—C33 | 1.50 (10) |
| O9—C37 | 1.247 (7) | C32—H32A | 0.9700 |
| O10—C37 | 1.257 (7) | C32—H32B | 0.9700 |
| O10—Cu2$^{ii}$ | 1.959 (4) | C32—H32C | 0.9700 |
| O11—C39 | 1.234 (7) | C32—H32D | 0.9700 |
| O12—C39 | 1.251 (7) | C33—C34 | 1.37 (10) |
| O12—Cu2$^{ii}$ | 1.967 (4) | C34—C35 | 1.39 (5) |
| C1—C8 | 1.447 (7) | C34—H34 | 0.9300 |
| C2—C3 | 1.377 (7) | C35—C36 | 1.37 (2) |
| C2—C7 | 1.396 (7) | C35—H35 | 0.9300 |
| C3—C4 | 1.397 (7) | C36—H36 | 0.9300 |
| C4—C5 | 1.375 (7) | C33′—C34′ | 1.3 (2) |
| C4—H4 | 0.9300 | C34′—C35′ | 1.35 (10) |
| C5—C6 | 1.388 (8) | C34′—H34′ | 0.9300 |
| C5—H5 | 0.9300 | C35′—C36′ | 1.34 (5) |
| C6—C7 | 1.350 (8) | C35′—H35′ | 0.9300 |
| C6—H6 | 0.9300 | C36′—H36′ | 0.9300 |
| C7—H7 | 0.9300 | C37—C38 | 1.506 (9) |
| C8—C9 | 1.323 (7) | C38—H38A | 0.9600 |
| C9—C10 | 1.416 (8) | C38—H38B | 0.9600 |
| C9—H9 | 0.9300 | C38—H38C | 0.9600 |
| C10—C11 | 1.298 (9) | C39—C40 | 1.505 (8) |
| C10—H10 | 0.9300 | C40—H40A | 0.9600 |
| C11—H11 | 0.9300 | C40—H40B | 0.9600 |
| C12—C13 | 1.486 (8) | C40—H40C | 0.9600 |
| C12—H12A | 0.9700 | | |

| | | | |
|---|---|---|---|
| O4$^{i}$—Cu1—O3 | 165.00 (14) | C19—C20—H20A | 109.5 |
| O4$^{i}$—Cu1—O5 | 91.84 (16) | C19—C20—H20B | 109.5 |
| O3—Cu1—O5 | 86.28 (16) | H20A—C20—H20B | 109.5 |
| O4$^{i}$—Cu1—O6$^{i}$ | 87.21 (16) | C19—C20—H20C | 109.5 |
| O3—Cu1—O6$^{i}$ | 90.80 (16) | H20A—C20—H20C | 109.5 |

| | | | |
|---|---|---|---|
| O5—Cu1—O6$^{i}$ | 165.11 (15) | H20B—C20—H20C | 109.5 |
| O4$^{i}$—Cu1—N1 | 99.23 (14) | N3—C21—N4 | 111.6 (6) |
| O3—Cu1—N1 | 95.76 (14) | N3—C21—C28 | 124.7 (6) |
| O5—Cu1—N1 | 98.95 (14) | N4—C21—C28 | 123.7 (6) |
| O6$^{i}$—Cu1—N1 | 95.87 (14) | N4—C22—C27 | 107.3 (6) |
| O4$^{i}$—Cu1—Cu1$^{i}$ | 82.02 (10) | N4—C22—C23 | 133.0 (6) |
| O3—Cu1—Cu1$^{i}$ | 82.99 (10) | C27—C22—C23 | 119.7 (7) |
| O5—Cu1—Cu1$^{i}$ | 80.88 (10) | C24—C23—C22 | 118.4 (7) |
| O6$^{i}$—Cu1—Cu1$^{i}$ | 84.27 (11) | C24—C23—H23 | 120.8 |
| N1—Cu1—Cu1$^{i}$ | 178.75 (11) | C22—C23—H23 | 120.8 |
| O10$^{ii}$—Cu2—O9 | 165.48 (18) | C23—C24—C25 | 122.5 (7) |
| O10$^{ii}$—Cu2—O11 | 87.25 (18) | C23—C24—H24 | 118.8 |
| O9—Cu2—O11 | 88.85 (19) | C25—C24—H24 | 118.8 |
| O10$^{ii}$—Cu2—O12$^{ii}$ | 92.30 (19) | C26—C25—C24 | 120.6 (7) |
| O9—Cu2—O12$^{ii}$ | 87.95 (18) | C26—C25—H25 | 119.7 |
| O11—Cu2—O12$^{ii}$ | 165.31 (17) | C24—C25—H25 | 119.7 |
| O10$^{ii}$—Cu2—N3 | 99.22 (18) | C25—C26—C27 | 117.3 (7) |
| O9—Cu2—N3 | 95.11 (18) | C25—C26—H26 | 121.3 |
| O11—Cu2—N3 | 96.54 (17) | C27—C26—H26 | 121.3 |
| O12$^{ii}$—Cu2—N3 | 98.02 (17) | C26—C27—C22 | 121.5 (6) |
| O10$^{ii}$—Cu2—Cu2$^{ii}$ | 80.40 (13) | C26—C27—N3 | 130.8 (5) |
| O9—Cu2—Cu2$^{ii}$ | 85.37 (13) | C22—C27—N3 | 107.7 (6) |
| O11—Cu2—Cu2$^{ii}$ | 85.86 (12) | O7′—C28—C29′ | 112.0 (16) |
| O12$^{ii}$—Cu2—Cu2$^{ii}$ | 79.60 (12) | O7′—C28—O7 | 112.9 (11) |
| N3—Cu2—Cu2$^{ii}$ | 177.56 (13) | C29′—C28—O7 | 30.2 (9) |
| C1—N1—C3 | 104.9 (4) | O7′—C28—C29 | 37.5 (7) |
| C1—N1—Cu1 | 133.9 (3) | C29′—C28—C29 | 85.6 (15) |
| C3—N1—Cu1 | 121.2 (3) | O7—C28—C29 | 102.8 (11) |
| C1—N2—C2 | 106.3 (4) | O7′—C28—C21 | 116.4 (10) |
| C1—N2—C12 | 129.1 (5) | C29′—C28—C21 | 131.5 (14) |
| C2—N2—C12 | 124.2 (4) | O7—C28—C21 | 122.3 (9) |
| C21—N3—C27 | 106.2 (5) | C29—C28—C21 | 134.6 (10) |
| C21—N3—Cu2 | 134.3 (4) | C28—C29—C30 | 113.1 (16) |
| C27—N3—Cu2 | 119.5 (4) | C28—C29—H29 | 123.4 |
| C22—N4—C21 | 107.3 (5) | C30—C29—H29 | 123.4 |
| C22—N4—C32 | 123.1 (6) | C31—C30—C29 | 103 (3) |
| C21—N4—C32 | 129.5 (6) | C31—C30—H30 | 128.4 |
| C11—O1—C8 | 104.9 (5) | C29—C30—H30 | 128.4 |
| C13—O2—C16 | 104.8 (6) | O7—C31—C30 | 110 (2) |
| C17—O3—Cu1 | 123.4 (3) | O7—C31—H31 | 125.0 |
| C17—O4—Cu1$^{i}$ | 125.2 (3) | C30—C31—H31 | 125.0 |
| C19—O5—Cu1 | 126.7 (3) | C28—C29′—C30′ | 106 (2) |
| C19—O6—Cu1$^{i}$ | 122.0 (3) | C28—C29′—H29′ | 127.2 |
| C31—O7—C28 | 110.3 (14) | C30′—C29′—H29′ | 127.2 |
| C36—O8—C33 | 108 (4) | C31′—C30′—C29′ | 107 (3) |
| C31′—O7′—C28 | 104.3 (15) | C31′—C30′—H30′ | 126.6 |
| C33′—O8′—C36′ | 107 (10) | C29′—C30′—H30′ | 126.6 |
| C37—O9—Cu2 | 121.2 (4) | O7′—C31′—C30′ | 111 (3) |

| | | | |
|---|---|---|---|
| C37—O10—Cu2$^{ii}$ | 127.4 (4) | O7′—C31′—H31′ | 124.4 |
| C39—O11—Cu2 | 120.7 (4) | C30′—C31′—H31′ | 124.4 |
| C39—O12—Cu2$^{ii}$ | 127.9 (4) | N4—C32—C33′ | 115 (8) |
| N1—C1—N2 | 112.6 (5) | N4—C32—C33 | 106 (3) |
| N1—C1—C8 | 123.8 (4) | C33′—C32—C33 | 15 (5) |
| N2—C1—C8 | 123.7 (4) | N4—C32—H32A | 110.5 |
| C3—C2—N2 | 106.7 (4) | C33′—C32—H32A | 116.2 |
| C3—C2—C7 | 122.6 (5) | C33—C32—H32A | 110.5 |
| N2—C2—C7 | 130.7 (5) | N4—C32—H32B | 110.5 |
| C2—C3—C4 | 120.5 (5) | C33′—C32—H32B | 95.3 |
| C2—C3—N1 | 109.5 (4) | C33—C32—H32B | 110.5 |
| C4—C3—N1 | 130.1 (4) | H32A—C32—H32B | 108.7 |
| C5—C4—C3 | 116.6 (5) | N4—C32—H32C | 108.9 |
| C5—C4—H4 | 121.7 | C33′—C32—H32C | 108.8 |
| C3—C4—H4 | 121.7 | C33—C32—H32C | 101.3 |
| C4—C5—C6 | 121.7 (5) | H32A—C32—H32C | 10.9 |
| C4—C5—H5 | 119.1 | H32B—C32—H32C | 118.4 |
| C6—C5—H5 | 119.1 | N4—C32—H32D | 108.5 |
| C7—C6—C5 | 122.5 (5) | C33′—C32—H32D | 108.5 |
| C7—C6—H6 | 118.7 | C33—C32—H32D | 123.7 |
| C5—C6—H6 | 118.7 | H32A—C32—H32D | 96.9 |
| C6—C7—C2 | 116.1 (5) | H32B—C32—H32D | 14.5 |
| C6—C7—H7 | 121.9 | H32C—C32—H32D | 107.3 |
| C2—C7—H7 | 121.9 | O8—C33—C34 | 108 (7) |
| C9—C8—O1 | 110.2 (5) | O8—C33—C32 | 119 (6) |
| C9—C8—C1 | 133.1 (5) | C34—C33—C32 | 133 (7) |
| O1—C8—C1 | 116.6 (5) | C33—C34—C35 | 108 (4) |
| C8—C9—C10 | 106.4 (5) | C33—C34—H34 | 126.2 |
| C8—C9—H9 | 126.8 | C35—C34—H34 | 126.2 |
| C10—C9—H9 | 126.8 | C36—C35—C34 | 106 (3) |
| C11—C10—C9 | 107.4 (6) | C36—C35—H35 | 126.8 |
| C11—C10—H10 | 126.3 | C34—C35—H35 | 126.8 |
| C9—C10—H10 | 126.3 | O8—C36—C35 | 109 (2) |
| C10—C11—O1 | 111.1 (6) | O8—C36—H36 | 125.5 |
| C10—C11—H11 | 124.4 | C35—C36—H36 | 125.5 |
| O1—C11—H11 | 124.4 | O8′—C33′—C34′ | 110 (10) |
| N2—C12—C13 | 115.0 (5) | O8′—C33′—C32 | 121 (10) |
| N2—C12—H12A | 108.5 | C34′—C33′—C32 | 129 (10) |
| C13—C12—H12A | 108.5 | C33′—C34′—C35′ | 107 (9) |
| N2—C12—H12B | 108.5 | C33′—C34′—H34′ | 126.6 |
| C13—C12—H12B | 108.5 | C35′—C34′—H34′ | 126.6 |
| H12A—C12—H12B | 107.5 | C36′—C35′—C34′ | 107 (5) |
| C14—C13—O2 | 110.0 (6) | C36′—C35′—H35′ | 126.7 |
| C14—C13—C12 | 135.0 (7) | C34′—C35′—H35′ | 126.7 |
| O2—C13—C12 | 114.8 (6) | O8′—C36′—C35′ | 110 (3) |
| C13—C14—C15 | 108.3 (7) | O8′—C36′—H36′ | 125.2 |
| C13—C14—H14 | 125.8 | C35′—C36′—H36′ | 125.2 |
| C15—C14—H14 | 125.8 | O9—C37—O10 | 125.5 (6) |

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|---|---|---|---|
| C16—C15—C14 | 106.8 (7) | O9—C37—C38 | 117.5 (6) |
| C16—C15—H15 | 126.6 | O10—C37—C38 | 117.0 (6) |
| C14—C15—H15 | 126.6 | C37—C38—H38A | 109.5 |
| C15—C16—O2 | 110.1 (7) | C37—C38—H38B | 109.5 |
| C15—C16—H16 | 124.9 | H38A—C38—H38B | 109.5 |
| O2—C16—H16 | 124.9 | C37—C38—H38C | 109.5 |
| O4—C17—O3 | 126.4 (5) | H38A—C38—H38C | 109.5 |
| O4—C17—C18 | 117.2 (5) | H38B—C38—H38C | 109.5 |
| O3—C17—C18 | 116.4 (5) | O11—C39—O12 | 125.9 (6) |
| C17—C18—H18A | 109.5 | O11—C39—C40 | 117.6 (6) |
| C17—C18—H18B | 109.5 | O12—C39—C40 | 116.5 (6) |
| H18A—C18—H18B | 109.5 | C39—C40—H40A | 109.5 |
| C17—C18—H18C | 109.5 | C39—C40—H40B | 109.5 |
| H18A—C18—H18C | 109.5 | H40A—C40—H40B | 109.5 |
| H18B—C18—H18C | 109.5 | C39—C40—H40C | 109.5 |
| O6—C19—O5 | 125.7 (5) | H40A—C40—H40C | 109.5 |
| O6—C19—C20 | 118.2 (5) | H40B—C40—H40C | 109.5 |
| O5—C19—C20 | 116.1 (5) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C12—H12*B*···O3$^{iii}$ | 0.97 | 2.55 | 3.426 (7) | 151 |
| C31—H31···O6$^{iv}$ | 0.93 | 2.54 | 3.44 (3) | 166 |
| C36—H36···O4$^{i}$ | 0.93 | 2.50 | 3.371 (19) | 157 |

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