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# Di-$\mu$-nicotinamide-$\kappa^2O$:$N^1$;$\kappa^2N^1$:$O$-bis[aquabis(4-methoxybenzoato-$\kappa O$)-copper(II)]

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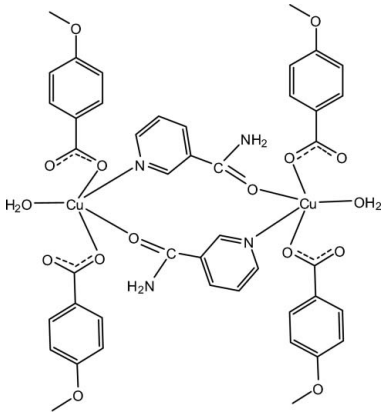
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.026; $wR$ factor = 0.072; data-to-parameter ratio = 17.1.

The asymmetric unit of the centrosymmetric dinuclear title compound, $[Cu_2(C_8H_7O_3)_4(C_6H_6N_2O)_2(H_2O)_2]$, contains one half of the complex molecule. Each $Cu^{II}$ atom is five-coordinated by one N atom from one bridging nicotinamide ligand and one O atom from another symmetry-related bridging nicotinamide ligand, two O atoms from two 4-methoxybenzoate ligands, and one water molecule, forming a distorted square-pyramidal geometry. Intermolecular O—H···O and N—H···O hydrogen bonds link the molecules into layers parallel to $(\bar{1}01)$. $\pi$–$\pi$ interactions, indicated by short intermolecular distances of 3.801 (1) Å between the centroids of the benzene rings and 3.653 (1) Å between the centroids of the pyridine rings, further stabilize the structure.

## Related literature

For related structures, see: Hökelek & Necefoğlu (1996); Hökelek *et al.* (2009*a*,*b*,*c*,*d*).



## Experimental

### Crystal data

$[Cu_2(C_8H_7O_3)_4(C_6H_6N_2O)_2(H_2O)_2]$
$M_r$ = 1011.93
Monoclinic, $P2_1/n$
$a$ = 14.1707 (3) Å
$b$ = 8.4319 (2) Å
$c$ = 18.0225 (3) Å
$\beta$ = 95.847 (2)°
$V$ = 2142.23 (8) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.07 mm$^{-1}$
$T$ = 100 K
0.37 × 0.37 × 0.23 mm

### Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.678, $T_{max}$ = 0.781
20329 measured reflections
5403 independent reflections
4813 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.072
$S$ = 1.05
5403 reflections
316 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.47 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2$A$···O1$^{i}$ | 0.86 (2) | 2.03 (2) | 2.8407 (18) | 158 (2) |
| N2—H2$B$···O4$^{ii}$ | 0.83 (2) | 2.29 (2) | 2.9897 (17) | 141.4 (18) |
| O8—H81···O1$^{iii}$ | 0.79 (3) | 1.97 (3) | 2.7236 (15) | 159 (3) |
| O8—H82···O4$^{iii}$ | 0.825 (18) | 1.803 (18) | 2.6052 (16) | 163.9 (18) |

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

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: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2731).

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# supporting information

*Acta Cryst.* (2010). E**66**, m807–m808 [doi:10.1107/S1600536810022415]

# Di-$\mu$-nicotinamide-$\kappa^2O$:$N^1$;$\kappa^2N^1$:$O$-bis[aquabis(4-methoxybenzoato-$\kappa O$)copper(II)]

**Tuncer Hökelek, Yasemin Süzen, Barış Tercan, Erdinç Tenlik and Hacali Necefoğlu**

## S1. Comment

As a part of our ongoing study of transition metal complexes of nicotinamide (Hökelek & Necefoğlu, 1996; Hökelek *et al.*, 2009*a, b, c, d*), herein we report the crystal structure of the title dinuclear complex.

The title compound, (I), consists of dimeric units located around a crystallographic symmetry centre and made up of two Cu cations, four 4-methoxybenzoate (MB) anions, two nicotinamide (NA) ligands and two water molecules (Fig. 1). Both of the $Cu^{II}$ centres are five-coordinated with distorted square-pyramidal environments, and the two monomeric units are bridged through the two nicotinamide (NA) ligands about an inversion center. The Cu1···Cu1$^{i}$ (symmetry code: (i) 2 - *x*, -*y*, 1 - *z*) distance is 7.1368 (3) Å. The average Cu—O bond length is 2.0626 (10) Å, and the Cu atom is displaced out of the least-squares planes of the carboxylate groups (O1/C1/O2) and (O4/C9/O5) by 0.0015 (2) and -0.2589 (2) Å, respectively.

The dihedral angles between the planar carboxylate groups and the adjacent benzene rings A (C2—C7) and B (C10—C15) are 1.85 (5) and 10.16 (7) °, respectively, while those between rings A, B and C (N1/C17—C21) are A/B = 28.50 (4), A/C = 81.64 (4), B/C = 58.50 (4) °.

In the crystal structure, intermolecular O—H···O and N—H···O hydrogen bonds (Table 1) link the molecules into layers. The $\pi$–$\pi$ contacts between the benzene rings and between the pyridine rings, *Cg*2—*Cg*2$^{i}$ and *Cg*3—*Cg*3$^{ii}$ [symmetry codes: (i) 2 - *x*, 2 - *y*, -*z*; (ii) 1 - *x*, 2 - *y*, -*z*, where *Cg*2 and *Cg*3 are the centroids of the rings B (C10—C15) and C (N1/C17—C21)] may further stabilize the structure, with centroid-centroid distances of 3.801 (1) and 3.653 (1) Å, respectively.

## S2. Experimental

The title compound was prepared by the reaction of $CuSO_4.5H_2O$ (2.50 g, 10 mmol) in $H_2O$ (50 ml) and NA (2.44 g, 20 mmol) in $H_2O$ (50 ml) with sodium 4-methoxybenzoate (3.48 g, 20 mmol) in $H_2O$ (100 ml). The mixture was filtered and set aside to crystallize at ambient temperature for one week, giving blue single crystals.

## S3. Refinement

Atoms H81, H82 (for $H_2O$) and H2A, H2B (for $NH_2$) were located in difference Fourier maps and refined isotropically. The remaining H atoms were positioned geometrically with C—H = 0.93 and 0.96 Å for aromatic and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}$(H) = $xU_{eq}$(C), where $x$ = 1.5 for methyl H and $x$ = 1.2 for aromatic H atoms.

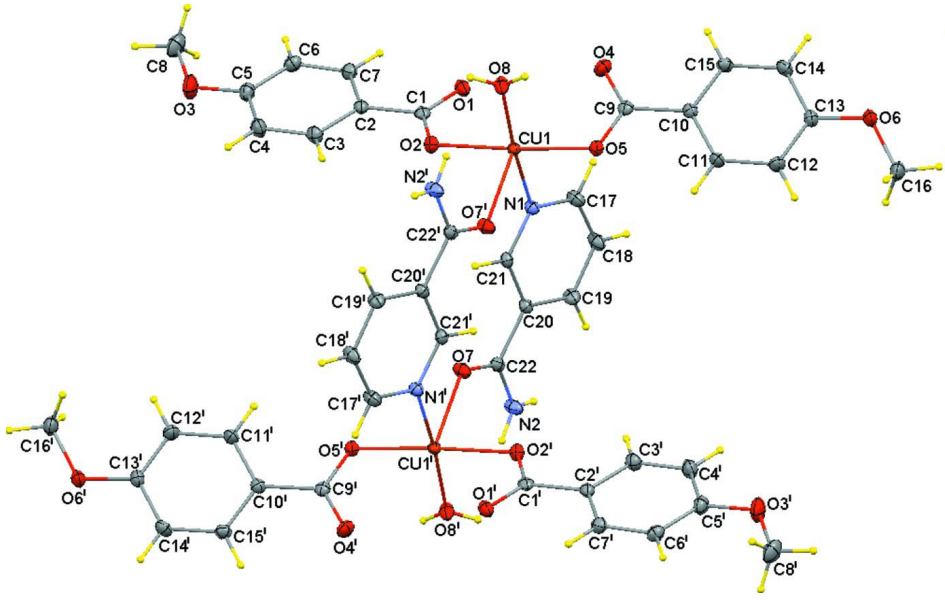


**Figure 1**

The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry code: (′) 2 - *x*, -*y*, 1 - *z*].

**Di-*μ*-nicotinamide-$\kappa^2O$:$N^1$;$\kappa^2N^1$:*O*- bis[aquabis(4-methoxybenzoato-$\kappa O$)copper(II)]**

*Crystal data*

$[Cu_2(C_8H_7O_3)_4(C_6H_6N_2O)_2(H_2O)_2]$
$M_r$ = 1011.93
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a$ = 14.1707 (3) Å
$b$ = 8.4319 (2) Å
$c$ = 18.0225 (3) Å
$\beta$ = 95.847 (2)°
$V$ = 2142.23 (8) Å$^3$
$Z$ = 2
$F(000)$ = 1044
$D_x$ = 1.569 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9977 reflections
$\theta$ = 2.7–28.5°
$\mu$ = 1.07 mm$^{-1}$
$T$ = 100 K
Block, blue
0.37 × 0.37 × 0.23 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)
$T_{min}$ = 0.678, $T_{max}$ = 0.781
20329 measured reflections
5403 independent reflections
4813 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021
$\theta_{max}$ = 28.5°, $\theta_{min}$ = 1.7°
$h$ = −18→18
$k$ = −10→11
$l$ = −24→24

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.072
$S$ = 1.05
5403 reflections
316 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

| | |
|---|---|
| Secondary atom site location: difference Fourier map | $w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 1.1134P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| Hydrogen site location: inferred from neighbouring sites | $(\Delta/\sigma)_{max} = 0.001$ |
| H atoms treated by a mixture of independent and constrained refinement | $\Delta\rho_{max} = 0.47$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.29$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.832076 (11) | 0.152692 (19) | 0.356751 (8) | 0.00986 (6) |
| O1 | 0.89942 (7) | 0.40998 (13) | 0.27780 (5) | 0.0155 (2) |
| O2 | 0.94951 (7) | 0.16598 (12) | 0.30792 (5) | 0.01368 (19) |
| O3 | 1.28693 (8) | 0.39532 (15) | 0.12796 (7) | 0.0251 (2) |
| O4 | 0.66614 (8) | 0.34649 (13) | 0.32513 (6) | 0.0181 (2) |
| O5 | 0.71138 (7) | 0.14541 (12) | 0.40038 (5) | 0.01317 (19) |
| O6 | 0.32798 (7) | 0.34252 (13) | 0.52920 (6) | 0.0170 (2) |
| O7 | 1.10015 (7) | 0.07805 (12) | 0.58526 (5) | 0.0153 (2) |
| O8 | 0.77027 (8) | 0.04960 (14) | 0.26669 (6) | 0.0167 (2) |
| H81 | 0.7200 (18) | 0.008 (3) | 0.2652 (13) | 0.047 (7)* |
| H82 | 0.7977 (13) | −0.001 (2) | 0.2360 (10) | 0.017 (4)* |
| N1 | 0.88593 (8) | 0.27822 (14) | 0.44653 (6) | 0.0118 (2) |
| N2 | 1.09767 (9) | 0.27022 (17) | 0.67244 (7) | 0.0171 (3) |
| H2A | 1.0823 (15) | 0.365 (3) | 0.6840 (12) | 0.029 (5)* |
| H2B | 1.1375 (14) | 0.224 (2) | 0.7019 (11) | 0.022 (5)* |
| C1 | 0.95896 (9) | 0.30016 (17) | 0.27686 (7) | 0.0125 (3) |
| C2 | 1.04648 (9) | 0.32640 (17) | 0.23831 (7) | 0.0125 (3) |
| C3 | 1.11660 (10) | 0.20966 (18) | 0.23693 (8) | 0.0152 (3) |
| H3 | 1.1096 | 0.1132 | 0.2608 | 0.018* |
| C4 | 1.19625 (10) | 0.23685 (19) | 0.20030 (8) | 0.0187 (3) |
| H4 | 1.2429 | 0.1594 | 0.2003 | 0.022* |
| C5 | 1.20666 (10) | 0.38071 (19) | 0.16333 (8) | 0.0173 (3) |
| C6 | 1.13758 (10) | 0.49779 (18) | 0.16412 (8) | 0.0166 (3) |
| H6 | 1.1442 | 0.5936 | 0.1396 | 0.020* |
| C7 | 1.05849 (10) | 0.46977 (18) | 0.20197 (7) | 0.0153 (3) |
| H7 | 1.0126 | 0.5484 | 0.2031 | 0.018* |
| C8 | 1.29541 (12) | 0.5321 (2) | 0.08255 (9) | 0.0254 (3) |
| H8A | 1.3544 | 0.5279 | 0.0607 | 0.038* |
| H8B | 1.2938 | 0.6258 | 0.1126 | 0.038* |

| | | | | |
|---|---|---|---|---|
| H8C | 1.2437 | 0.5346 | 0.0437 | 0.038* |
| C9 | 0.65288 (9) | 0.25480 (17) | 0.37733 (7) | 0.0123 (3) |
| C10 | 0.56660 (9) | 0.27358 (16) | 0.41748 (7) | 0.0121 (2) |
| C11 | 0.55839 (10) | 0.19292 (18) | 0.48349 (8) | 0.0148 (3) |
| H11 | 0.6064 | 0.1240 | 0.5019 | 0.018* |
| C12 | 0.47980 (10) | 0.21312 (18) | 0.52268 (8) | 0.0159 (3) |
| H12 | 0.4753 | 0.1586 | 0.5670 | 0.019* |
| C13 | 0.40798 (10) | 0.31546 (17) | 0.49503 (8) | 0.0134 (3) |
| C14 | 0.41505 (10) | 0.39815 (18) | 0.42856 (8) | 0.0156 (3) |
| H14 | 0.3669 | 0.4669 | 0.4102 | 0.019* |
| C15 | 0.49373 (10) | 0.37730 (17) | 0.39027 (8) | 0.0142 (3) |
| H15 | 0.4985 | 0.4324 | 0.3461 | 0.017* |
| C16 | 0.32415 (10) | 0.26991 (19) | 0.60087 (8) | 0.0190 (3) |
| H16A | 0.2661 | 0.2992 | 0.6205 | 0.028* |
| H16B | 0.3771 | 0.3052 | 0.6343 | 0.028* |
| H16C | 0.3267 | 0.1567 | 0.5958 | 0.028* |
| C17 | 0.83872 (10) | 0.40389 (17) | 0.47003 (8) | 0.0152 (3) |
| H17 | 0.7874 | 0.4437 | 0.4394 | 0.018* |
| C18 | 0.86367 (10) | 0.47614 (18) | 0.53812 (8) | 0.0169 (3) |
| H18 | 0.8306 | 0.5645 | 0.5524 | 0.020* |
| C19 | 0.93883 (10) | 0.41469 (17) | 0.58490 (8) | 0.0153 (3) |
| H19 | 0.9555 | 0.4591 | 0.6316 | 0.018* |
| C20 | 0.98863 (9) | 0.28598 (16) | 0.56074 (7) | 0.0114 (2) |
| C21 | 0.96065 (9) | 0.22322 (16) | 0.49060 (7) | 0.0117 (2) |
| H21 | 0.9953 | 0.1395 | 0.4735 | 0.014* |
| C22 | 1.06782 (9) | 0.20324 (17) | 0.60760 (7) | 0.0120 (2) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.00880 (8) | 0.01102 (9) | 0.00963 (8) | 0.00027 (6) | 0.00037 (6) | −0.00144 (6) |
| O1 | 0.0127 (4) | 0.0164 (5) | 0.0175 (5) | 0.0029 (4) | 0.0014 (4) | −0.0019 (4) |
| O2 | 0.0120 (4) | 0.0141 (5) | 0.0153 (4) | −0.0002 (4) | 0.0033 (4) | −0.0005 (4) |
| O3 | 0.0202 (5) | 0.0259 (6) | 0.0315 (6) | −0.0008 (5) | 0.0141 (5) | 0.0034 (5) |
| O4 | 0.0195 (5) | 0.0198 (6) | 0.0158 (5) | −0.0003 (4) | 0.0055 (4) | 0.0042 (4) |
| O5 | 0.0114 (4) | 0.0150 (5) | 0.0133 (4) | 0.0011 (4) | 0.0024 (3) | −0.0006 (4) |
| O6 | 0.0133 (5) | 0.0200 (5) | 0.0183 (5) | 0.0049 (4) | 0.0049 (4) | 0.0030 (4) |
| O7 | 0.0165 (5) | 0.0120 (5) | 0.0168 (5) | 0.0028 (4) | −0.0017 (4) | −0.0015 (4) |
| O8 | 0.0116 (5) | 0.0229 (6) | 0.0154 (5) | −0.0010 (4) | 0.0013 (4) | −0.0084 (4) |
| N1 | 0.0112 (5) | 0.0113 (6) | 0.0128 (5) | 0.0002 (4) | 0.0002 (4) | −0.0008 (4) |
| N2 | 0.0184 (6) | 0.0162 (7) | 0.0155 (6) | 0.0042 (5) | −0.0048 (5) | −0.0034 (5) |
| C1 | 0.0118 (6) | 0.0150 (6) | 0.0102 (5) | −0.0009 (5) | −0.0017 (5) | −0.0029 (5) |
| C2 | 0.0113 (6) | 0.0147 (7) | 0.0113 (6) | −0.0004 (5) | 0.0001 (5) | −0.0018 (5) |
| C3 | 0.0154 (6) | 0.0133 (7) | 0.0171 (6) | 0.0007 (5) | 0.0025 (5) | 0.0006 (5) |
| C4 | 0.0154 (6) | 0.0186 (7) | 0.0224 (7) | 0.0039 (6) | 0.0042 (5) | 0.0005 (6) |
| C5 | 0.0139 (6) | 0.0213 (7) | 0.0172 (6) | −0.0031 (6) | 0.0046 (5) | −0.0014 (6) |
| C6 | 0.0191 (7) | 0.0153 (7) | 0.0155 (6) | −0.0014 (5) | 0.0025 (5) | 0.0012 (5) |
| C7 | 0.0156 (6) | 0.0156 (7) | 0.0147 (6) | 0.0013 (5) | 0.0010 (5) | −0.0008 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8 | 0.0256 (8) | 0.0279 (9) | 0.0243 (7) | −0.0082 (7) | 0.0101 (6) | 0.0011 (7) |
| C9 | 0.0124 (6) | 0.0130 (6) | 0.0112 (6) | −0.0021 (5) | 0.0001 (5) | −0.0027 (5) |
| C10 | 0.0117 (6) | 0.0118 (6) | 0.0128 (6) | −0.0004 (5) | 0.0009 (5) | −0.0007 (5) |
| C11 | 0.0139 (6) | 0.0156 (7) | 0.0149 (6) | 0.0048 (5) | 0.0021 (5) | 0.0026 (5) |
| C12 | 0.0175 (7) | 0.0165 (7) | 0.0141 (6) | 0.0036 (5) | 0.0037 (5) | 0.0038 (5) |
| C13 | 0.0117 (6) | 0.0136 (7) | 0.0153 (6) | 0.0005 (5) | 0.0028 (5) | −0.0015 (5) |
| C14 | 0.0140 (6) | 0.0141 (7) | 0.0184 (6) | 0.0033 (5) | −0.0005 (5) | 0.0024 (5) |
| C15 | 0.0149 (6) | 0.0137 (7) | 0.0138 (6) | 0.0005 (5) | 0.0002 (5) | 0.0031 (5) |
| C16 | 0.0178 (7) | 0.0209 (8) | 0.0194 (7) | 0.0025 (6) | 0.0079 (5) | 0.0020 (6) |
| C17 | 0.0131 (6) | 0.0132 (7) | 0.0186 (6) | 0.0019 (5) | −0.0024 (5) | −0.0015 (5) |
| C18 | 0.0151 (6) | 0.0146 (7) | 0.0205 (7) | 0.0045 (5) | −0.0013 (5) | −0.0051 (5) |
| C19 | 0.0146 (6) | 0.0155 (7) | 0.0153 (6) | 0.0000 (5) | −0.0011 (5) | −0.0053 (5) |
| C20 | 0.0100 (6) | 0.0110 (6) | 0.0132 (6) | −0.0010 (5) | 0.0006 (5) | 0.0001 (5) |
| C21 | 0.0106 (6) | 0.0111 (6) | 0.0136 (6) | −0.0005 (5) | 0.0019 (5) | −0.0002 (5) |
| C22 | 0.0108 (6) | 0.0121 (6) | 0.0131 (6) | −0.0005 (5) | 0.0006 (5) | 0.0018 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—O2 | 1.9634 (10) | C6—H6 | 0.9300 |
| Cu1—O5 | 1.9548 (10) | C7—H7 | 0.9300 |
| Cu1—O7$^{i}$ | 2.3655 (10) | C8—H8A | 0.9600 |
| Cu1—O8 | 1.9667 (10) | C8—H8B | 0.9600 |
| Cu1—N1 | 2.0171 (11) | C8—H8C | 0.9600 |
| O1—C1 | 1.2540 (17) | C9—C10 | 1.4912 (18) |
| O2—C1 | 1.2754 (17) | C10—C15 | 1.4030 (19) |
| O3—C8 | 1.426 (2) | C11—C10 | 1.3856 (19) |
| O4—C9 | 1.2466 (17) | C11—C12 | 1.3886 (19) |
| O5—C9 | 1.2808 (17) | C11—H11 | 0.9300 |
| O6—C13 | 1.3634 (17) | C12—C13 | 1.3876 (19) |
| O6—C16 | 1.4355 (17) | C12—H12 | 0.9300 |
| O7—Cu1$^{i}$ | 2.3655 (10) | C13—C14 | 1.399 (2) |
| O8—H81 | 0.79 (3) | C14—C15 | 1.381 (2) |
| O8—H82 | 0.83 (2) | C14—H14 | 0.9300 |
| N1—C17 | 1.3444 (18) | C15—H15 | 0.9300 |
| N1—C21 | 1.3401 (17) | C16—H16A | 0.9600 |
| N2—C22 | 1.3278 (18) | C16—H16B | 0.9600 |
| N2—H2A | 0.86 (2) | C16—H16C | 0.9600 |
| N2—H2B | 0.83 (2) | C17—H17 | 0.9300 |
| C1—C2 | 1.4985 (19) | C18—C17 | 1.3833 (19) |
| C2—C7 | 1.394 (2) | C18—C19 | 1.3895 (19) |
| C3—C2 | 1.4007 (19) | C18—H18 | 0.9300 |
| C3—C4 | 1.383 (2) | C19—H19 | 0.9300 |
| C3—H3 | 0.9300 | C20—C19 | 1.3886 (19) |
| C4—H4 | 0.9300 | C20—C21 | 1.3903 (18) |
| C5—O3 | 1.3650 (17) | C21—H21 | 0.9300 |
| C5—C4 | 1.399 (2) | C22—O7 | 1.2345 (17) |
| C5—C6 | 1.391 (2) | C22—C20 | 1.5053 (18) |
| C6—C7 | 1.390 (2) | | |

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|---|---|---|---|
| O2—Cu1—O7$^{i}$ | 85.44 (4) | H8A—C8—H8B | 109.5 |
| O2—Cu1—O8 | 88.96 (4) | H8A—C8—H8C | 109.5 |
| O2—Cu1—N1 | 93.49 (4) | H8B—C8—H8C | 109.5 |
| O5—Cu1—O2 | 176.73 (4) | O4—C9—O5 | 123.30 (13) |
| O5—Cu1—O7$^{i}$ | 97.41 (4) | O4—C9—C10 | 119.63 (12) |
| O5—Cu1—O8 | 89.07 (4) | O5—C9—C10 | 117.05 (12) |
| O5—Cu1—N1 | 88.22 (4) | C11—C10—C9 | 120.61 (12) |
| O8—Cu1—O7$^{i}$ | 97.34 (4) | C11—C10—C15 | 118.88 (13) |
| O8—Cu1—N1 | 173.84 (5) | C15—C10—C9 | 120.48 (12) |
| N1—Cu1—O7$^{i}$ | 88.50 (4) | C10—C11—C12 | 121.22 (13) |
| C1—O2—Cu1 | 112.27 (9) | C10—C11—H11 | 119.4 |
| C5—O3—C8 | 117.64 (13) | C12—C11—H11 | 119.4 |
| C9—O5—Cu1 | 114.26 (9) | C11—C12—H12 | 120.3 |
| C13—O6—C16 | 116.39 (11) | C13—C12—C11 | 119.38 (13) |
| C22—O7—Cu1$^{i}$ | 134.96 (9) | C13—C12—H12 | 120.3 |
| Cu1—O8—H82 | 125.4 (12) | O6—C13—C12 | 123.72 (13) |
| Cu1—O8—H81 | 123.2 (18) | O6—C13—C14 | 116.04 (12) |
| H82—O8—H81 | 103 (2) | C12—C13—C14 | 120.24 (13) |
| C17—N1—Cu1 | 120.44 (9) | C13—C14—H14 | 120.1 |
| C21—N1—Cu1 | 120.36 (9) | C15—C14—C13 | 119.77 (13) |
| C21—N1—C17 | 118.32 (12) | C15—C14—H14 | 120.1 |
| C22—N2—H2A | 122.8 (14) | C10—C15—H15 | 119.7 |
| C22—N2—H2B | 120.0 (14) | C14—C15—C10 | 120.51 (13) |
| H2B—N2—H2A | 116.8 (19) | C14—C15—H15 | 119.7 |
| O1—C1—O2 | 123.25 (13) | O6—C16—H16A | 109.5 |
| O1—C1—C2 | 119.15 (13) | O6—C16—H16B | 109.5 |
| O2—C1—C2 | 117.60 (12) | O6—C16—H16C | 109.5 |
| C3—C2—C1 | 121.78 (13) | H16A—C16—H16B | 109.5 |
| C7—C2—C1 | 119.50 (12) | H16A—C16—H16C | 109.5 |
| C7—C2—C3 | 118.72 (13) | H16B—C16—H16C | 109.5 |
| C2—C3—H3 | 119.8 | N1—C17—C18 | 122.43 (12) |
| C4—C3—C2 | 120.44 (14) | N1—C17—H17 | 118.8 |
| C4—C3—H3 | 119.8 | C18—C17—H17 | 118.8 |
| C3—C4—C5 | 120.11 (14) | C17—C18—C19 | 119.00 (13) |
| C3—C4—H4 | 119.9 | C17—C18—H18 | 120.5 |
| C5—C4—H4 | 119.9 | C19—C18—H18 | 120.5 |
| O3—C5—C4 | 115.72 (14) | C18—C19—H19 | 120.5 |
| O3—C5—C6 | 124.15 (14) | C20—C19—C18 | 118.94 (12) |
| C6—C5—C4 | 120.13 (13) | C20—C19—H19 | 120.5 |
| C5—C6—H6 | 120.4 | C19—C20—C21 | 118.40 (12) |
| C7—C6—C5 | 119.18 (14) | C19—C20—C22 | 124.05 (12) |
| C7—C6—H6 | 120.4 | C21—C20—C22 | 117.45 (12) |
| C2—C7—H7 | 119.3 | N1—C21—C20 | 122.83 (13) |
| C6—C7—C2 | 121.41 (13) | N1—C21—H21 | 118.6 |
| C6—C7—H7 | 119.3 | C20—C21—H21 | 118.6 |
| O3—C8—H8A | 109.5 | O7—C22—N2 | 123.72 (13) |
| O3—C8—H8B | 109.5 | O7—C22—C20 | 119.57 (12) |

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|---|---|---|---|
| O3—C8—H8C | 109.5 | N2—C22—C20 | 116.69 (12) |
| | | | |
| O7$^{i}$—Cu1—O2—C1 | −166.69 (9) | C6—C5—O3—C8 | −6.9 (2) |
| O8—Cu1—O2—C1 | 95.87 (9) | O3—C5—C4—C3 | −179.07 (13) |
| N1—Cu1—O2—C1 | −78.48 (9) | C6—C5—C4—C3 | 0.9 (2) |
| O7$^{i}$—Cu1—O5—C9 | −177.06 (9) | O3—C5—C6—C7 | 179.92 (13) |
| O8—Cu1—O5—C9 | −79.78 (9) | C4—C5—C6—C7 | 0.0 (2) |
| N1—Cu1—O5—C9 | 94.69 (9) | C5—C6—C7—C2 | −0.8 (2) |
| O2—Cu1—N1—C17 | 128.61 (11) | O4—C9—C10—C11 | −168.45 (13) |
| O2—Cu1—N1—C21 | −62.33 (11) | O4—C9—C10—C15 | 9.4 (2) |
| O5—Cu1—N1—C17 | −48.59 (11) | O5—C9—C10—C11 | 9.80 (19) |
| O5—Cu1—N1—C21 | 120.47 (11) | O5—C9—C10—C15 | −172.30 (12) |
| O7$^{i}$—Cu1—N1—C17 | −146.05 (11) | C9—C10—C15—C14 | −178.15 (13) |
| O7$^{i}$—Cu1—N1—C21 | 23.01 (10) | C11—C10—C15—C14 | −0.2 (2) |
| Cu1—O2—C1—O1 | −0.05 (16) | C12—C11—C10—C9 | 177.95 (13) |
| Cu1—O2—C1—C2 | 179.28 (9) | C12—C11—C10—C15 | 0.0 (2) |
| Cu1—O5—C9—O4 | 8.36 (17) | C10—C11—C12—C13 | 0.3 (2) |
| Cu1—O5—C9—C10 | −169.82 (9) | C11—C12—C13—O6 | 179.65 (13) |
| C16—O6—C13—C12 | 5.6 (2) | C11—C12—C13—C14 | −0.4 (2) |
| C16—O6—C13—C14 | −174.33 (13) | O6—C13—C14—C15 | −179.84 (13) |
| Cu1—N1—C17—C18 | 168.29 (11) | C12—C13—C14—C15 | 0.2 (2) |
| C21—N1—C17—C18 | −1.0 (2) | C13—C14—C15—C10 | 0.1 (2) |
| Cu1—N1—C21—C20 | −166.33 (10) | C19—C18—C17—N1 | −1.6 (2) |
| C17—N1—C21—C20 | 3.0 (2) | C17—C18—C19—C20 | 2.2 (2) |
| O1—C1—C2—C3 | 178.44 (12) | C21—C20—C19—C18 | −0.4 (2) |
| O1—C1—C2—C7 | −2.31 (19) | C22—C20—C19—C18 | −176.58 (13) |
| O2—C1—C2—C3 | −0.91 (19) | C19—C20—C21—N1 | −2.3 (2) |
| O2—C1—C2—C7 | 178.33 (12) | C22—C20—C21—N1 | 174.18 (12) |
| C1—C2—C7—C6 | −178.58 (12) | O7—C22—C20—C19 | 170.96 (14) |
| C3—C2—C7—C6 | 0.7 (2) | O7—C22—C20—C21 | −5.28 (19) |
| C4—C3—C2—C1 | 179.42 (13) | N2—C22—O7—Cu1$^{i}$ | 29.9 (2) |
| C4—C3—C2—C7 | 0.2 (2) | N2—C22—C20—C19 | −7.8 (2) |
| C2—C3—C4—C5 | −0.9 (2) | N2—C22—C20—C21 | 175.94 (13) |
| C4—C5—O3—C8 | 173.01 (14) | C20—C22—O7—Cu1$^{i}$ | −148.77 (10) |

Symmetry code: (i) −*x*+2, −*y*, −*z*+1.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*A*···O1$^{ii}$ | 0.86 (2) | 2.03 (2) | 2.8407 (18) | 158 (2) |
| N2—H2*B*···O4$^{iii}$ | 0.83 (2) | 2.29 (2) | 2.9897 (17) | 141.4 (18) |
| O8—H81···O1$^{iv}$ | 0.79 (3) | 1.97 (3) | 2.7236 (15) | 159 (3) |
| O8—H82···O4$^{iv}$ | 0.825 (18) | 1.803 (18) | 2.6052 (16) | 163.9 (18) |

Symmetry codes: (ii) −*x*+2, −*y*+1, −*z*+1; (iii) *x*+1/2, −*y*+1/2, *z*+1/2; (iv) −*x*+3/2, *y*−1/2, −*z*+1/2.