# {μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1κ⁴O⁶,O¹,O¹′,O⁶′:2κ⁴O¹,N,N′,O¹′}-(methanol-1κO)(perchlorato-1κO)-copper(II)sodium(I)

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The molecule of the title compound, [CuNa($C_{18}H_{18}N_2O_4$)-($ClO_4$)($CH_3OH$)], is almost planar with mean deviation of 5.2 (8)°. The coordination environment of the Cu^II ion is distorted square-planar and it is $N_2O_2$-chelated by the 6,6′-dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]-diphenolate Schiff base ligand. The Na atom is chelated by the four O atoms of the Schiff base ligand, and coordinated by a methanol molecule and a perchlorate anion. The six-coordinate Na atom adopts a distorted octahedral coordination geometry. The O atoms of the perchlorate anion are disordered over two sites with site-occupancy factors of 0.697 (5) and 0.303 (5). O—H⋯O hydrogen bonding occurs.

## Related literature

For chemical background, see: Lindoy et al. (1976). For related structures, see: Correia et al. (2005). For bond-length data, see: Allen et al. (1987).
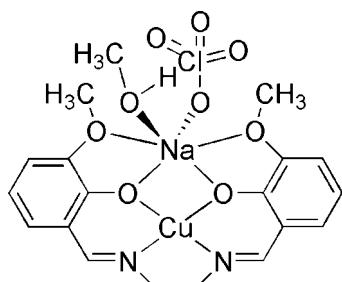


## Experimental

### Crystal data

| | |
|---|---|
| [CuNa($C_{18}H_{18}N_2O_4$)($ClO_4$)($CH_4O$)] | $\beta$ = 104.273 (3)° |
| $M_r$ = 544.38 | $V$ = 2220.1 (7) Å³ |
| Monoclinic, $P2_1/n$ | $Z$ = 4 |
| $a$ = 12.030 (2) Å | Mo $K\alpha$ radiation |
| $b$ = 8.1444 (14) Å | $\mu$ = 1.18 mm⁻¹ |
| $c$ = 23.381 (4) Å | $T$ = 273 K |
| | 0.17 × 0.15 × 0.11 mm |

### Data collection

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 10424 measured reflections |
| Absorption correction: multi-scan (SADABS; Sheldrick, 2003) | 3843 independent reflections |
| $T_{min}$ = 0.825, $T_{max}$ = 0.881 | 2651 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.039 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.048 | 148 restraints |
| $wR(F^2)$ = 0.131 | H-atom parameters constrained |
| $S$ = 1.03 | $\Delta\rho_{max}$ = 0.56 e Å⁻³ |
| 3843 reflections | $\Delta\rho_{min}$ = −0.68 e Å⁻³ |
| 339 parameters | |

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

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| O9—H9A⋯O7[i] | 0.82 | 2.11 | 2.912 (8) | 164 |
| O9—H9A⋯O5′[i] | 0.82 | 1.99 | 2.761 (13) | 156 |
| O9—H9A⋯O5′[i] | 0.82 | 1.99 | 2.761 (13) | 156 |
| O9—H9A⋯O7[i] | 0.82 | 2.11 | 2.912 (8) | 164 |

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: XP in SHELXTL (Sheldrick, 2008); software used to prepare material for publication: XP in SHELXTL.

## References

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Lindoy, L. F., Lip, H. C., Power, L. F. & Rea, T. H. (1976). Inorg. Chem. 15, 1724–1727.
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# supporting information

# {µ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^6,O^1,O^{1\prime},O^{6\prime}$:2$\kappa^4O^1,N,N\prime,O^{1\prime}$}(methanol-1$\kappa O$)(perchlorato-1$\kappa O$)copper(II)sodium(I)

**Hui-Quan Xiao and Hua Zhang**

### S1. Comment

The schiff bases have been known as effective ligands for metal ions and used in the mechanism of many biochemical processes (Lindoy *et al.*, 1976). *N,N*-Disalicylideneethylenediamine type schiff bases present versatile steric, electronic and lipophilic properties. The synthesis, characterization and solution studies of *N,N*′-disalicylideneethylenediamine type complexes have been reported recently (Correia *et al.*, 2005). We report here the synthesis and crystal structure of the title compound, (I). The molecular structure of (I) is shown in Fig. 1. The values of the geometric parameters in (I) are normal (Allen *et al.*, 1987). Cu(II) and Na(I) are connected *via* two bridging oxygen atoms of the ligand. The coordination environment of the Cu$^{2+}$ ion is distorted square-planar and it is coordinated by N$_2$O$_2$ of the Schiff base ligand. The Na atom is chelated by the four O atoms of the 6,6′-dimethoxy-2,2′-(ethane-1,2-diyldiiminodimethylene)diphenol ligand, a methanol and a perchlorate anion. The six-coordinate Na atom adopts a distorted octahedral coordination geometry.

### S2. Experimental

A mixture of 6,6′-dimethoxy-2,2′-(ethane-1,2-diyldiiminodimethylene)diphenol (1 mmol) and copper chloride (1 mmol) in absolute ethanol (15 ml) was stirred for 30 min and sodium perchlorate (1 mmol) was added, stirred for another 15 min and then filtered. The resulting clear orange solution was allowed to evaporate at room temperature for 7 days, after which large orange block-shaped crystals of the title complex suitable for X-ray diffraction analysis were obtained.

### S3. Refinement

The H atoms were fixed geometrically and were treated as riding on their parent atoms, with C—H distances 0.93, 0.96 and 0.97 Å for aryl, methyl and methylene type H-atoms, respectively, and O—H = 0.85 Å. The H-atoms were allowed $U_{iso}(H) = 1.2U_{eq}$(parent aryl and methylene C atoms), or $U_{iso}(H) = 1.5U_{eq}$(methyl C and hydroxyl O atoms). The O-atoms of the perchlorate anion are disordered over two sites with unequal site occupancy factors 0.697 (5) and 0.303 (5).
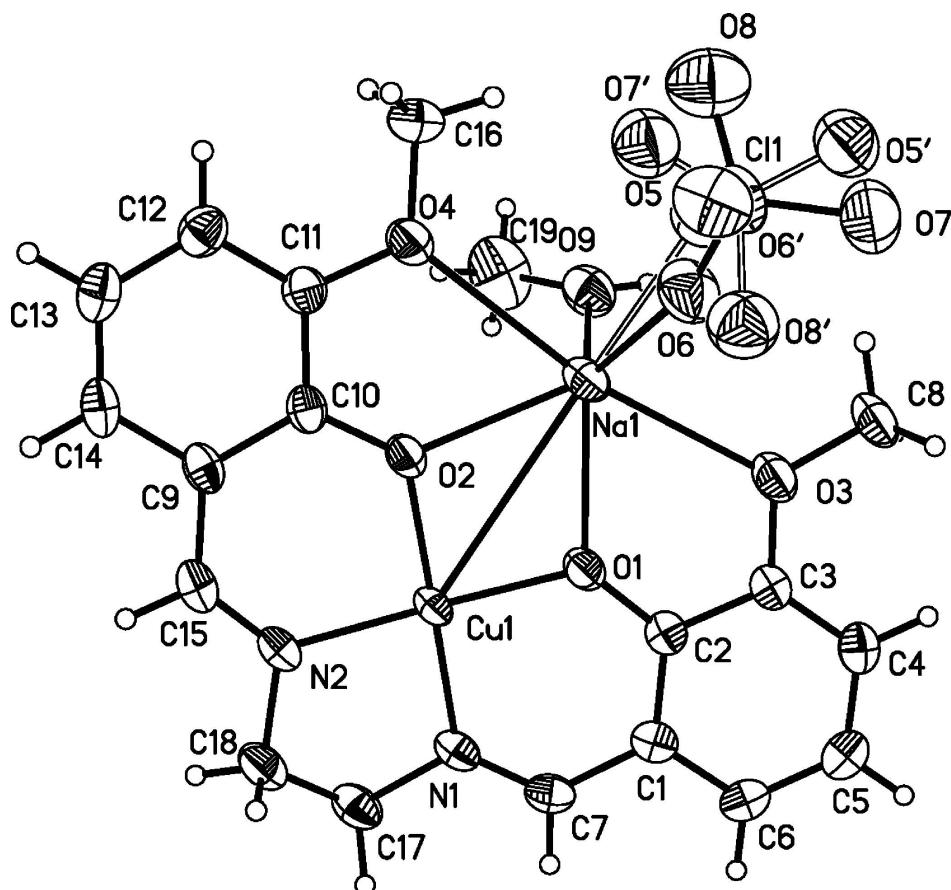
**Figure 1**

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

**{$\mu$-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato- $1\kappa^4O^6,O^1,O^{1\prime},O^{6\prime}$: $2\kappa^4O^1,N,N′,O^{1\prime}$} (methanol-$1\kappa O$)(perchlorato- $1\kappa O$)copper(II)sodium(I)**

*Crystal data*

| | |
|---|---|
| [CuNa($C_{18}H_{18}N_2O_4$)($ClO_4$)($CH_4O$)] | $F(000) = 1116$ |
| $M_r = 544.38$ | $D_x = 1.629$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2yn | Cell parameters from 2083 reflections |
| $a = 12.030$ (2) Å | $\theta = 2.7$–21.2° |
| $b = 8.1444$ (14) Å | $\mu = 1.18$ mm$^{-1}$ |
| $c = 23.381$ (4) Å | $T = 273$ K |
| $\beta = 104.273$ (3)° | Block, blue |
| $V = 2220.1$ (7) Å$^3$ | $0.17 \times 0.15 \times 0.11$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003) |
| Radiation source: fine-focus sealed tube | $T_{min} = 0.825$, $T_{max} = 0.881$ |
| Graphite monochromator | 10424 measured reflections |
| $\varphi$ and $\omega$ scans | 3843 independent reflections |

| | | | | |
|---|---|---|---|---|
| 2651 reflections with $I > 2\sigma(I)$ | | | $h = -14 \rightarrow 10$ | |
| $R_{int} = 0.039$ | | | $k = -9 \rightarrow 9$ | |
| $\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$ | | | $l = -27 \rightarrow 26$ | |

*Refinement*

| | | |
|---|---|---|
| Refinement on $F^2$ | | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | | |
| $R[F^2 > 2\sigma(F^2)] = 0.048$ | | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.131$ | | |
| $S = 1.03$ | | H-atom parameters constrained |
| 3843 reflections | | $w = 1/[\sigma^2(F_o^2) + (0.0701P)^2 + 0.3025P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 339 parameters | | |
| 148 restraints | | $(\Delta/\sigma)_{max} = 0.002$ |
| Primary atom site location: structure-invariant direct methods | | $\Delta\rho_{max} = 0.56$ e Å$^{-3}$ |
| | | $\Delta\rho_{min} = -0.68$ 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Cu1 | 0.67526 (4) | 0.41736 (7) | 1.00850 (2) | 0.0401 (2) | |
| Cl1 | 0.50250 (12) | 0.6363 (2) | 0.73548 (7) | 0.0739 (4) | |
| Na1 | 0.64991 (14) | 0.4180 (2) | 0.86447 (7) | 0.0487 (5) | |
| O1 | 0.7475 (2) | 0.5185 (4) | 0.95491 (12) | 0.0450 (7) | |
| O2 | 0.5730 (2) | 0.3261 (4) | 0.94164 (12) | 0.0469 (8) | |
| O3 | 0.8214 (3) | 0.6120 (4) | 0.86695 (14) | 0.0586 (9) | |
| O4 | 0.4620 (3) | 0.2267 (4) | 0.83993 (13) | 0.0551 (8) | |
| O5 | 0.4054 (5) | 0.7314 (9) | 0.7368 (3) | 0.0941 (18) | 0.697 (5) |
| O6 | 0.5622 (6) | 0.5794 (11) | 0.7907 (3) | 0.107 (2) | 0.697 (5) |
| O7 | 0.5660 (5) | 0.7560 (8) | 0.7127 (3) | 0.1002 (19) | 0.697 (5) |
| O8 | 0.4583 (6) | 0.5066 (8) | 0.6955 (3) | 0.121 (2) | 0.697 (5) |
| O5′ | 0.5499 (13) | 0.648 (2) | 0.6860 (5) | 0.102 (3) | 0.303 (5) |
| O6′ | 0.5809 (11) | 0.5076 (15) | 0.7574 (8) | 0.095 (3) | 0.303 (5) |
| O7′ | 0.3899 (7) | 0.596 (2) | 0.7381 (8) | 0.106 (3) | 0.303 (5) |
| O8′ | 0.5499 (14) | 0.683 (2) | 0.7956 (3) | 0.100 (3) | 0.303 (5) |
| O9 | 0.7367 (4) | 0.1937 (5) | 0.8355 (2) | 0.0792 (12) | |
| H9A | 0.7905 | 0.1921 | 0.8198 | 0.119* | |
| N1 | 0.7854 (3) | 0.4916 (5) | 1.07680 (15) | 0.0450 (9) | |
| N2 | 0.5934 (3) | 0.3323 (5) | 1.06299 (15) | 0.0461 (9) | |
| C1 | 0.9026 (4) | 0.6473 (5) | 1.0254 (2) | 0.0438 (11) | |
| C2 | 0.8414 (3) | 0.6065 (5) | 0.9680 (2) | 0.0400 (10) | |
| C3 | 0.8843 (4) | 0.6644 (5) | 0.92130 (19) | 0.0433 (11) | |

| C4 | 0.9803 (4) | 0.7612 (6) | 0.9308 (2) | 0.0533 (12) |
| H4 | 1.0059 | 0.7997 | 0.8988 | 0.064* |
| C5 | 1.0398 (4) | 0.8024 (6) | 0.9880 (3) | 0.0583 (13) |
| H5 | 1.1046 | 0.8689 | 0.9944 | 0.070* |
| C6 | 1.0018 (4) | 0.7438 (6) | 1.0342 (2) | 0.0549 (12) |
| H6 | 1.0424 | 0.7684 | 1.0725 | 0.066* |
| C7 | 0.8704 (4) | 0.5871 (6) | 1.0767 (2) | 0.0476 (11) |
| H7 | 0.9152 | 0.6201 | 1.1132 | 0.057* |
| C8 | 0.8646 (5) | 0.6465 (8) | 0.8172 (2) | 0.0694 (15) |
| H8A | 0.8684 | 0.7632 | 0.8122 | 0.104* |
| H8B | 0.8147 | 0.5994 | 0.7826 | 0.104* |
| H8C | 0.9399 | 0.6003 | 0.8229 | 0.104* |
| C9 | 0.4421 (4) | 0.1995 (5) | 0.9915 (2) | 0.0449 (11) |
| C10 | 0.4820 (4) | 0.2381 (5) | 0.94127 (19) | 0.0404 (10) |
| C11 | 0.4171 (4) | 0.1799 (6) | 0.8863 (2) | 0.0455 (11) |
| C12 | 0.3175 (4) | 0.0908 (6) | 0.8808 (2) | 0.0559 (13) |
| H12 | 0.2759 | 0.0549 | 0.8440 | 0.067* |
| C13 | 0.2806 (4) | 0.0556 (6) | 0.9310 (3) | 0.0639 (15) |
| H13 | 0.2136 | −0.0043 | 0.9278 | 0.077* |
| C14 | 0.3411 (4) | 0.1075 (6) | 0.9848 (2) | 0.0545 (13) |
| H14 | 0.3151 | 0.0814 | 1.0180 | 0.065* |
| C15 | 0.5014 (4) | 0.2496 (6) | 1.0498 (2) | 0.0501 (12) |
| H15 | 0.4695 | 0.2188 | 1.0806 | 0.060* |
| C16 | 0.4046 (5) | 0.1701 (8) | 0.7830 (2) | 0.0810 (18) |
| H16A | 0.4001 | 0.0525 | 0.7833 | 0.122* |
| H16B | 0.4462 | 0.2042 | 0.7549 | 0.122* |
| H16C | 0.3286 | 0.2154 | 0.7723 | 0.122* |
| C17 | 0.7679 (5) | 0.4219 (7) | 1.1319 (2) | 0.0614 (14) |
| H17A | 0.7920 | 0.5000 | 1.1639 | 0.074* |
| H17B | 0.8132 | 0.3227 | 1.1420 | 0.074* |
| C18 | 0.6426 (5) | 0.3831 (7) | 1.1231 (2) | 0.0619 (14) |
| H18A | 0.6334 | 0.2961 | 1.1499 | 0.074* |
| H18B | 0.6026 | 0.4795 | 1.1320 | 0.074* |
| C19 | 0.7189 (7) | 0.0396 (9) | 0.8542 (3) | 0.107 (2) |
| H19A | 0.6615 | 0.0434 | 0.8763 | 0.161* |
| H19B | 0.7892 | −0.0022 | 0.8788 | 0.161* |
| H19C | 0.6935 | −0.0309 | 0.8206 | 0.161* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0401 (3) | 0.0532 (4) | 0.0286 (3) | 0.0046 (2) | 0.0112 (2) | 0.0037 (2) |
| Cl1 | 0.0659 (9) | 0.0907 (10) | 0.0711 (9) | 0.0173 (7) | 0.0283 (7) | 0.0296 (8) |
| Na1 | 0.0491 (10) | 0.0658 (12) | 0.0315 (9) | 0.0029 (8) | 0.0108 (8) | 0.0001 (8) |
| O1 | 0.0392 (17) | 0.066 (2) | 0.0297 (16) | −0.0046 (15) | 0.0077 (13) | 0.0015 (14) |
| O2 | 0.0442 (18) | 0.067 (2) | 0.0328 (17) | −0.0092 (15) | 0.0147 (14) | 0.0002 (14) |
| O3 | 0.0522 (19) | 0.089 (3) | 0.0370 (19) | −0.0065 (17) | 0.0157 (15) | 0.0078 (17) |
| O4 | 0.0504 (19) | 0.079 (2) | 0.0386 (18) | −0.0120 (16) | 0.0158 (15) | −0.0082 (16) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O5 | 0.082 (3) | 0.100 (3) | 0.099 (3) | 0.023 (3) | 0.022 (3) | 0.000 (3) |
| O6 | 0.103 (3) | 0.110 (3) | 0.099 (3) | 0.015 (3) | 0.011 (3) | 0.029 (3) |
| O7 | 0.100 (3) | 0.105 (3) | 0.102 (3) | −0.007 (3) | 0.038 (3) | 0.024 (3) |
| O8 | 0.122 (3) | 0.114 (3) | 0.119 (3) | 0.012 (3) | 0.014 (3) | −0.007 (3) |
| O5′ | 0.101 (4) | 0.110 (4) | 0.099 (4) | 0.005 (3) | 0.030 (3) | 0.008 (3) |
| O6′ | 0.094 (4) | 0.096 (4) | 0.093 (4) | 0.009 (4) | 0.019 (4) | 0.013 (4) |
| O7′ | 0.098 (4) | 0.114 (4) | 0.105 (4) | 0.006 (3) | 0.022 (3) | 0.008 (4) |
| O8′ | 0.096 (4) | 0.101 (4) | 0.101 (4) | 0.007 (4) | 0.018 (4) | 0.016 (4) |
| O9 | 0.084 (3) | 0.082 (3) | 0.080 (3) | 0.017 (2) | 0.038 (2) | −0.005 (2) |
| N1 | 0.052 (2) | 0.057 (2) | 0.0242 (19) | 0.010 (2) | 0.0073 (16) | 0.0034 (17) |
| N2 | 0.055 (2) | 0.053 (2) | 0.033 (2) | 0.0042 (19) | 0.0157 (18) | 0.0058 (17) |
| C1 | 0.044 (3) | 0.044 (3) | 0.042 (3) | 0.008 (2) | 0.007 (2) | −0.004 (2) |
| C2 | 0.033 (2) | 0.044 (3) | 0.044 (3) | 0.0067 (19) | 0.0110 (19) | 0.000 (2) |
| C3 | 0.042 (3) | 0.048 (3) | 0.042 (3) | 0.008 (2) | 0.015 (2) | 0.007 (2) |
| C4 | 0.052 (3) | 0.051 (3) | 0.063 (3) | 0.001 (2) | 0.023 (2) | 0.009 (2) |
| C5 | 0.055 (3) | 0.046 (3) | 0.073 (4) | −0.007 (2) | 0.014 (3) | −0.004 (3) |
| C6 | 0.050 (3) | 0.050 (3) | 0.061 (3) | −0.003 (2) | 0.006 (2) | −0.011 (2) |
| C7 | 0.048 (3) | 0.052 (3) | 0.039 (3) | 0.009 (2) | 0.002 (2) | −0.004 (2) |
| C8 | 0.073 (4) | 0.098 (4) | 0.043 (3) | 0.000 (3) | 0.025 (3) | 0.015 (3) |
| C9 | 0.047 (3) | 0.046 (3) | 0.047 (3) | 0.012 (2) | 0.023 (2) | 0.009 (2) |
| C10 | 0.038 (2) | 0.042 (3) | 0.043 (3) | 0.0073 (19) | 0.015 (2) | 0.004 (2) |
| C11 | 0.042 (3) | 0.049 (3) | 0.049 (3) | 0.002 (2) | 0.016 (2) | −0.002 (2) |
| C12 | 0.044 (3) | 0.059 (3) | 0.063 (3) | −0.003 (2) | 0.011 (2) | −0.004 (3) |
| C13 | 0.048 (3) | 0.062 (3) | 0.088 (5) | −0.008 (2) | 0.030 (3) | 0.003 (3) |
| C14 | 0.051 (3) | 0.052 (3) | 0.071 (4) | 0.005 (2) | 0.036 (3) | 0.013 (3) |
| C15 | 0.059 (3) | 0.050 (3) | 0.049 (3) | 0.013 (2) | 0.028 (2) | 0.014 (2) |
| C16 | 0.080 (4) | 0.117 (5) | 0.046 (3) | −0.026 (4) | 0.015 (3) | −0.022 (3) |
| C17 | 0.068 (3) | 0.083 (4) | 0.030 (3) | 0.007 (3) | 0.006 (2) | 0.005 (2) |
| C18 | 0.087 (4) | 0.068 (4) | 0.037 (3) | 0.002 (3) | 0.026 (3) | 0.004 (2) |
| C19 | 0.127 (6) | 0.090 (5) | 0.110 (6) | 0.039 (5) | 0.038 (5) | 0.022 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—O1 | 1.881 (3) | C4—H4 | 0.9300 |
| Cu1—O2 | 1.887 (3) | C5—C6 | 1.360 (7) |
| Cu1—N1 | 1.905 (4) | C5—H5 | 0.9300 |
| Cu1—N2 | 1.922 (4) | C6—H6 | 0.9300 |
| Cl1—O6 | 1.394 (4) | C7—H7 | 0.9300 |
| Cl1—O5 | 1.408 (4) | C8—H8A | 0.9600 |
| Cl1—O7′ | 1.410 (5) | C8—H8B | 0.9600 |
| Cl1—O5′ | 1.413 (5) | C8—H8C | 0.9600 |
| Cl1—O6′ | 1.418 (5) | C9—C14 | 1.403 (6) |
| Cl1—O7 | 1.421 (4) | C9—C10 | 1.410 (6) |
| Cl1—O8 | 1.424 (5) | C9—C15 | 1.432 (7) |
| Cl1—O8′ | 1.432 (5) | C10—C11 | 1.411 (6) |
| O1—C2 | 1.309 (5) | C11—C12 | 1.380 (6) |
| O2—C10 | 1.308 (5) | C12—C13 | 1.382 (7) |
| O3—C3 | 1.377 (5) | C12—H12 | 0.9300 |

| | | | |
|---|---|---|---|
| O3—C8 | 1.415 (5) | C13—C14 | 1.357 (7) |
| O4—C11 | 1.378 (5) | C13—H13 | 0.9300 |
| O4—C16 | 1.417 (6) | C14—H14 | 0.9300 |
| O9—C19 | 1.362 (8) | C15—H15 | 0.9300 |
| O9—H9A | 0.8200 | C16—H16A | 0.9600 |
| N1—C7 | 1.285 (6) | C16—H16B | 0.9600 |
| N1—C17 | 1.470 (6) | C16—H16C | 0.9600 |
| N2—C15 | 1.267 (6) | C17—C18 | 1.504 (7) |
| N2—C18 | 1.444 (6) | C17—H17A | 0.9700 |
| C1—C6 | 1.400 (7) | C17—H17B | 0.9700 |
| C1—C2 | 1.402 (6) | C18—H18A | 0.9700 |
| C1—C7 | 1.435 (6) | C18—H18B | 0.9700 |
| C2—C3 | 1.400 (6) | C19—H19A | 0.9600 |
| C3—C4 | 1.370 (6) | C19—H19B | 0.9600 |
| C4—C5 | 1.393 (7) | C19—H19C | 0.9600 |
| | | | |
| O1—Cu1—O2 | 86.23 (12) | O3—C8—H8B | 109.5 |
| O1—Cu1—N1 | 94.56 (15) | H8A—C8—H8B | 109.5 |
| O2—Cu1—N1 | 174.99 (15) | O3—C8—H8C | 109.5 |
| O1—Cu1—N2 | 174.73 (15) | H8A—C8—H8C | 109.5 |
| O2—Cu1—N2 | 94.09 (15) | H8B—C8—H8C | 109.5 |
| N1—Cu1—N2 | 85.58 (16) | C14—C9—C10 | 119.2 (4) |
| O6—Cl1—O5 | 113.8 (5) | C14—C9—C15 | 118.2 (4) |
| O7′—Cl1—O5′ | 129.6 (11) | C10—C9—C15 | 122.5 (4) |
| O7′—Cl1—O6′ | 111.9 (10) | O2—C10—C9 | 125.0 (4) |
| O5′—Cl1—O6′ | 88.9 (10) | O2—C10—C11 | 117.6 (4) |
| O6—Cl1—O7 | 112.0 (5) | C9—C10—C11 | 117.4 (4) |
| O5—Cl1—O7 | 99.0 (5) | O4—C11—C12 | 124.9 (4) |
| O6—Cl1—O8 | 112.6 (5) | O4—C11—C10 | 112.8 (4) |
| O5—Cl1—O8 | 104.2 (4) | C12—C11—C10 | 122.2 (4) |
| O7—Cl1—O8 | 114.3 (5) | C11—C12—C13 | 118.9 (5) |
| O7′—Cl1—O8′ | 100.0 (10) | C11—C12—H12 | 120.5 |
| O5′—Cl1—O8′ | 129.9 (11) | C13—C12—H12 | 120.5 |
| O6′—Cl1—O8′ | 76.9 (10) | C14—C13—C12 | 120.8 (5) |
| C2—O1—Cu1 | 126.7 (3) | C14—C13—H13 | 119.6 |
| C10—O2—Cu1 | 126.5 (3) | C12—C13—H13 | 119.6 |
| C3—O3—C8 | 117.9 (4) | C13—C14—C9 | 121.5 (4) |
| C11—O4—C16 | 117.0 (4) | C13—C14—H14 | 119.3 |
| C19—O9—H9A | 109.5 | C9—C14—H14 | 119.3 |
| C7—N1—C17 | 121.4 (4) | N2—C15—C9 | 125.7 (4) |
| C7—N1—Cu1 | 125.4 (3) | N2—C15—H15 | 117.2 |
| C17—N1—Cu1 | 113.1 (3) | C9—C15—H15 | 117.2 |
| C15—N2—C18 | 120.9 (4) | O4—C16—H16A | 109.5 |
| C15—N2—Cu1 | 126.2 (3) | O4—C16—H16B | 109.5 |
| C18—N2—Cu1 | 112.8 (3) | H16A—C16—H16B | 109.5 |
| C6—C1—C2 | 120.1 (4) | O4—C16—H16C | 109.5 |
| C6—C1—C7 | 117.7 (4) | H16A—C16—H16C | 109.5 |
| C2—C1—C7 | 122.2 (4) | H16B—C16—H16C | 109.5 |

| | | | |
|---|---|---|---|
| O1—C2—C3 | 117.7 (4) | N1—C17—C18 | 108.4 (4) |
| O1—C2—C1 | 125.0 (4) | N1—C17—H17A | 110.0 |
| C3—C2—C1 | 117.3 (4) | C18—C17—H17A | 110.0 |
| C4—C3—O3 | 125.3 (4) | N1—C17—H17B | 110.0 |
| C4—C3—C2 | 121.7 (4) | C18—C17—H17B | 110.0 |
| O3—C3—C2 | 113.0 (4) | H17A—C17—H17B | 108.4 |
| C3—C4—C5 | 120.4 (5) | N2—C18—C17 | 110.5 (4) |
| C3—C4—H4 | 119.8 | N2—C18—H18A | 109.5 |
| C5—C4—H4 | 119.8 | C17—C18—H18A | 109.5 |
| C6—C5—C4 | 119.0 (5) | N2—C18—H18B | 109.5 |
| C6—C5—H5 | 120.5 | C17—C18—H18B | 109.5 |
| C4—C5—H5 | 120.5 | H18A—C18—H18B | 108.1 |
| C5—C6—C1 | 121.4 (5) | O9—C19—H19A | 109.5 |
| C5—C6—H6 | 119.3 | O9—C19—H19B | 109.5 |
| C1—C6—H6 | 119.3 | H19A—C19—H19B | 109.5 |
| N1—C7—C1 | 126.0 (4) | O9—C19—H19C | 109.5 |
| N1—C7—H7 | 117.0 | H19A—C19—H19C | 109.5 |
| C1—C7—H7 | 117.0 | H19B—C19—H19C | 109.5 |
| O3—C8—H8A | 109.5 | | |
| | | | |
| O2—Cu1—O1—C2 | −175.3 (3) | C2—C1—C6—C5 | 1.2 (7) |
| N1—Cu1—O1—C2 | −0.2 (3) | C7—C1—C6—C5 | 178.4 (4) |
| N2—Cu1—O1—C2 | 91.1 (16) | C17—N1—C7—C1 | 172.8 (4) |
| O1—Cu1—O2—C10 | −174.8 (4) | Cu1—N1—C7—C1 | −4.1 (7) |
| N1—Cu1—O2—C10 | 86.0 (17) | C6—C1—C7—N1 | −176.8 (4) |
| N2—Cu1—O2—C10 | 0.0 (4) | C2—C1—C7—N1 | 0.3 (7) |
| O1—Cu1—N1—C7 | 3.7 (4) | Cu1—O2—C10—C9 | 1.9 (6) |
| O2—Cu1—N1—C7 | 102.6 (16) | Cu1—O2—C10—C11 | −179.5 (3) |
| N2—Cu1—N1—C7 | −171.1 (4) | C14—C9—C10—O2 | 178.3 (4) |
| O1—Cu1—N1—C17 | −173.5 (3) | C15—C9—C10—O2 | −2.3 (7) |
| O2—Cu1—N1—C17 | −74.6 (17) | C14—C9—C10—C11 | −0.4 (6) |
| N2—Cu1—N1—C17 | 11.8 (3) | C15—C9—C10—C11 | 179.1 (4) |
| O1—Cu1—N2—C15 | 91.5 (16) | C16—O4—C11—C12 | −3.9 (7) |
| O2—Cu1—N2—C15 | −1.8 (4) | C16—O4—C11—C10 | 178.3 (4) |
| N1—Cu1—N2—C15 | −176.8 (4) | O2—C10—C11—O4 | 0.1 (6) |
| O1—Cu1—N2—C18 | −83.8 (16) | C9—C10—C11—O4 | 178.8 (4) |
| O2—Cu1—N2—C18 | −177.1 (3) | O2—C10—C11—C12 | −177.8 (4) |
| N1—Cu1—N2—C18 | 7.9 (3) | C9—C10—C11—C12 | 1.0 (7) |
| Cu1—O1—C2—C3 | 176.9 (3) | O4—C11—C12—C13 | −178.4 (4) |
| Cu1—O1—C2—C1 | −3.1 (6) | C10—C11—C12—C13 | −0.8 (7) |
| C6—C1—C2—O1 | −179.4 (4) | C11—C12—C13—C14 | 0.0 (8) |
| C7—C1—C2—O1 | 3.6 (7) | C12—C13—C14—C9 | 0.6 (8) |
| C6—C1—C2—C3 | 0.7 (6) | C10—C9—C14—C13 | −0.4 (7) |
| C7—C1—C2—C3 | −176.4 (4) | C15—C9—C14—C13 | −179.9 (4) |
| C8—O3—C3—C4 | 6.6 (7) | C18—N2—C15—C9 | 176.8 (4) |
| C8—O3—C3—C2 | −172.6 (4) | Cu1—N2—C15—C9 | 1.9 (7) |
| O1—C2—C3—C4 | 178.1 (4) | C14—C9—C15—N2 | 179.7 (4) |
| C1—C2—C3—C4 | −1.9 (6) | C10—C9—C15—N2 | 0.2 (7) |

| O1—C2—C3—O3 | −2.7 (6) | C7—N1—C17—C18 | 154.9 (4) |
| O1—C2—C3—O3 | 177.3 (4) | Cu1—N1—C17—C18 | −27.8 (5) |
| O3—C3—C4—C5 | −177.8 (4) | C15—N2—C18—C17 | 159.2 (4) |
| C2—C3—C4—C5 | 1.3 (7) | Cu1—N2—C18—C17 | −25.3 (5) |
| C3—C4—C5—C6 | 0.6 (7) | N1—C17—C18—N2 | 33.7 (6) |
| C4—C5—C6—C1 | −1.8 (7) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
| --- | --- | --- | --- | --- |
| O9—H9*A*···O7$^i$ | 0.82 | 2.11 | 2.912 (8) | 164 |
| O9—H9*A*···O5$^{ri}$ | 0.82 | 1.99 | 2.761 (13) | 156 |
| O9—H9*A*···O5$^{ri}$ | 0.82 | 1.99 | 2.761 (13) | 156 |
| O9—H9*A*···O7$^i$ | 0.82 | 2.11 | 2.912 (8) | 164 |

Symmetry code: (i) −*x*+3/2, *y*−1/2, −*z*+3/2.