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# Di-$\mu$-perchlorato-bis{$\mu$-2-[(2-pyridyl)-methylaminomethyl]phenolato)-dicopper(II) acetonitrile disolvate

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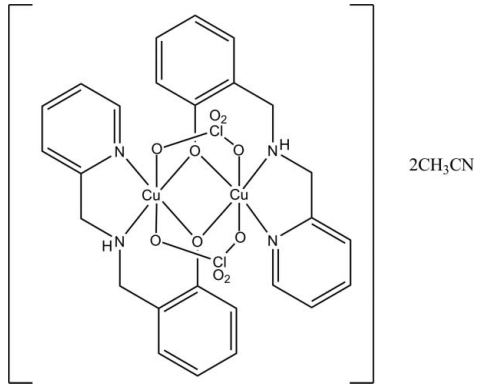
Key indicators: single-crystal X-ray study; $T$ = 200 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.078; $wR$ factor = 0.199; data-to-parameter ratio = 31.4.

In the crystal of the dinuclear title compound, $[Cu_2(C_{13}H_{13}N_2O)_2(ClO_4)_2]\cdot 2CH_3CN$, the two bridging perchlorate ions chelate to the two $Cu^{II}$ atoms in a $\mu$-$O$:$O'$ fashion on opposite sides of the equatorial plane. The $Cu^{II}$ ions display a distorted octahedral coordination geometry (in the usual 4 + 2 Jahn–Teller arrangement), each being coordinated by two O atoms from the two perchlorate ligands, and two N and O atoms from the reduced Schiff base ligand. The asymmetric unit contains two acetonitrile solvent molecules. In the crystal structure, in addition to N—H···O hydrogen bonds, there are weak C—H···O interactions between the perchlorate O atoms and the reduced Schiff base ligand. C—H···N interactions are also present.

## Related literature

For related structures containing bridging perchlorate anions, see: Sony *et al.* (2006); Sarkar *et al.* (2004); Neves *et al.* (2001); Torelli *et al.* (2000); O'Connor *et al.* (1986). For the synthesis, see: Yisgedu (2001).




## Experimental

### Crystal data

$[Cu_2(C_{13}H_{13}N_2O)_2(ClO_4)_2]\cdot 2C_2H_3N$
$M_r$ = 834.60
Monoclinic, $P2_1/n$
$a$ = 16.0285 (4) Å
$b$ = 9.4062 (3) Å
$c$ = 24.7097 (10) Å
$\beta$ = 102.665 (3)°
$V$ = 3634.8 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.38 mm$^{-1}$
$T$ = 200 K
0.53 × 0.46 × 0.39 mm

### Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2008)
$T_{min}$ = 0.848, $T_{max}$ = 1.000 (expected range = 0.495–0.584)
33853 measured reflections
14212 independent reflections
8089 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.036

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.078
$wR(F^2)$ = 0.199
$S$ = 1.19
14212 reflections
453 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −2.24 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Cu1—O1*B* | 1.9410 (18) | Cu2—O1*A* | 1.9440 (18) |
| Cu1—O1*A* | 1.942 (2) | Cu2—O1*B* | 1.952 (2) |
| Cu1—N2*A* | 1.972 (3) | Cu2—N2*B* | 1.971 (3) |
| Cu1—N1*A* | 1.974 (2) | Cu2—N1*B* | 1.973 (2) |
| Cu1—O21 | 2.494 (2) | Cu2—O12 | 2.489 (2) |
| Cu1—O11 | 2.706 (2) | Cu2—O22 | 2.670 (2) |
| Cu1—Cu2 | 2.9543 (5) | | |

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1*A*—H1*AA*···O23$^{i}$ | 0.93 | 2.05 | 2.913 (4) | 154 |
| N1*B*—H1*BA*···O14$^{ii}$ | 0.93 | 2.09 | 2.943 (4) | 152 |
| C7*B*—H7*BA*···O14$^{iii}$ | 0.99 | 2.53 | 3.167 (4) | 122 |
| C22*S*—H22*H*···O13$^{iv}$ | 0.98 | 2.47 | 3.264 (8) | 138 |
| C7*A*—H7*AB*···O23$^{v}$ | 0.99 | 2.48 | 3.143 (4) | 124 |
| C4*A*—H4*AA*···N1*S* | 0.95 | 2.69 | 3.643 (7) | 175 |
| C12*B*—H12*B*···N2*S* | 0.95 | 2.67 | 3.616 (9) | 171 |

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2008) ; cell refinement: *CrysAlis RED* (Oxford Diffraction, 2008); data reduction: *CrysAlis RED*; 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: NG2609).

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# supporting information

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# Di-$\mu$-perchlorato-bis{$\mu$-2-[(2-pyridyl)methylaminomethyl]phenolato)dicopper(II) acetonitrile disolvate

**Gervas E. Assey, Teshome Yisgedu, Yilma Gultneh, Ray J. Butcher and Yohannes Tesema**

## S1. Comment

Dinucleating metal centers in protein complexes play important roles in biology such as dioxygen transport or activation, electron transfer, hydrolytic chemistry and nitrogen oxide reduction (Torelli *et al.* 2000). Many of the copper enzymes have oxidase or oxygenase activities. In order to model dinuclear copper enzymes, copper complexes containing binucleating ligands with bridging phenoxo groups have to be synthesized. In biological systems, type 3 copper enzymes tyrosinase and catechol oxidase contain similar dinuclear copper active sites and are responsible for hydroxylation of monophenols and/or oxidation of catechols (Neves *et al.* 2001).

We report here the synthesis and crystal structure determination of binuclear copper complex $C_{30}H_{32}Cl_2Cu_2N_6O_{10}$ for which the molecular structure is shown in Fig.1. The geometry around the $Cu^{II}$ ions in Fig. 1 of the title compound can be described as that of distorted octahedral (with the usual tetragonal distortion seen in 6-coordinate Cu complexes) with each $Cu^{II}$ ion coordinated to one pyridine N atom, a secondary amine N atom, two O atoms from the perchlorate groups and two bridging O atoms from the salicylaldamine groups. The Cu—$N_{py}$ bond distances are; Cu(1)—N(2 A) 1.973 (3) Å and Cu(2)—N(2B) 1.971 (3) Å. The Cu—$N_{amine}$ bond distances are: Cu(1)—N(1 A) 1.975 (2) Å and Cu(2)—N(1B) 1.974 (2) Å. Having two copper centers bridged by a perchlorate ion has been previously observed (Sony *et al.*, 2006; O′Connor *et al.*, 1986). However, in this instance, the two copper centers are bridged by two perchlorate ions on opposite sides of the equatorial plane. The Cu—$O_{perchlorate}$ distances range from 2.489 (2) to 2.707 (3) Å. The Cu—Cu distance is 2.9542 (5) Å.

The crystals contain two molecules of acetonitrile as solvate. In the crystal structure, in addition to N—H···O hydrogen bonds, there are C—H···O interactions between the perchlorate O atoms and the reduced Schiff base ligand.

## S2. Experimental

The ligand (2-pyridylmethyl)(2-hydroxybenzyl)amine ($L^1$H) was synthesized as described below (Yisgedu, 2001). To 5.4 g (50 mmol) of 2-(2-aminomethyl)pyridine in 10 ml of ethanol was added 6.1 g (50 mmol) of salicylaldehyde in 15 ml of ethanol which resulted in a deep yellow color. The solution was left to stir for 30 minutes. A sodium borohydride solution (3 g $NaBH_4$, 0.4 g NaOH, and 40.0 ml of $H_2O$) were added dropwise. The solution changed to colorless and was left to stir for one hour after adding all the $NaBH_4$ solution. The volume of the solution was reduced to 20 ml after extracting three times with chloroform (3 *x* 40 ml). The extracts were combined and dried in anhydrous $Na_2SO_4$ overnight. The $Na_2SO_4$ was filtered and the filtrate concentrated to give a colorless oil (9.3 g, 87%).

The metal complex was synthesized as described below (Yisgedu, 2001). 1.64 g (7.65 mmol) of $L^1$H was mixed with 2.86 g (7.65 mmol) of $Cu(ClO_4)_2.6H_2O$ in 25 ml MeOH and 1.75 ml $NaOCH_3$. The solution mixture was stirred overnight, filtered, washed with 1:1 mixture of ether and methanol and dried to give 2.3 g (80%). Crystals suitable for X-ray diffraction were obtained by layering a solution of the complex in acetonitrile with diethyl ether.

### S3. Refinement

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with a C—H distance of 0.95 and 0.99 Å $U_{iso}$(H) = 1.2$U_{eq}$(C). The H atoms attached to N were idealized with an N–H distance of 0.93 Å. The highest peak and lowest peaks in the final difference Fourier were 1.29 and -2.24 e/Å$^3$ [0.71 and 0.70 Å from Cu1].

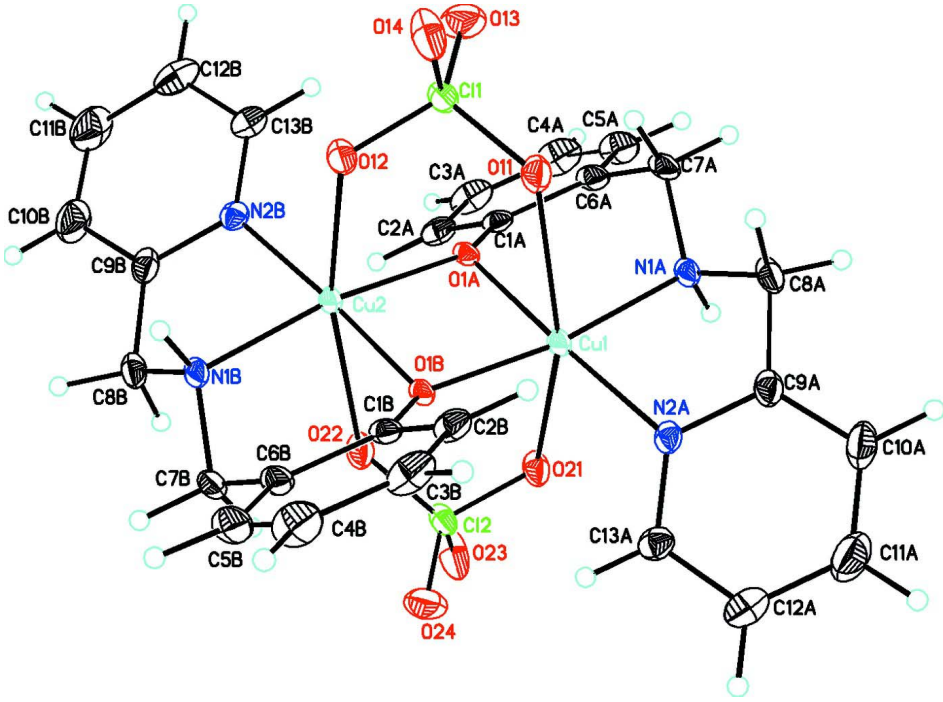


**Figure 1**

The molecular structure of the dinuclear complex, $C_{26}H_{26}Cl_2Cu_2N_4O_{10}$ showing the atom numbering scheme and 50% probability displacement ellipsoids.

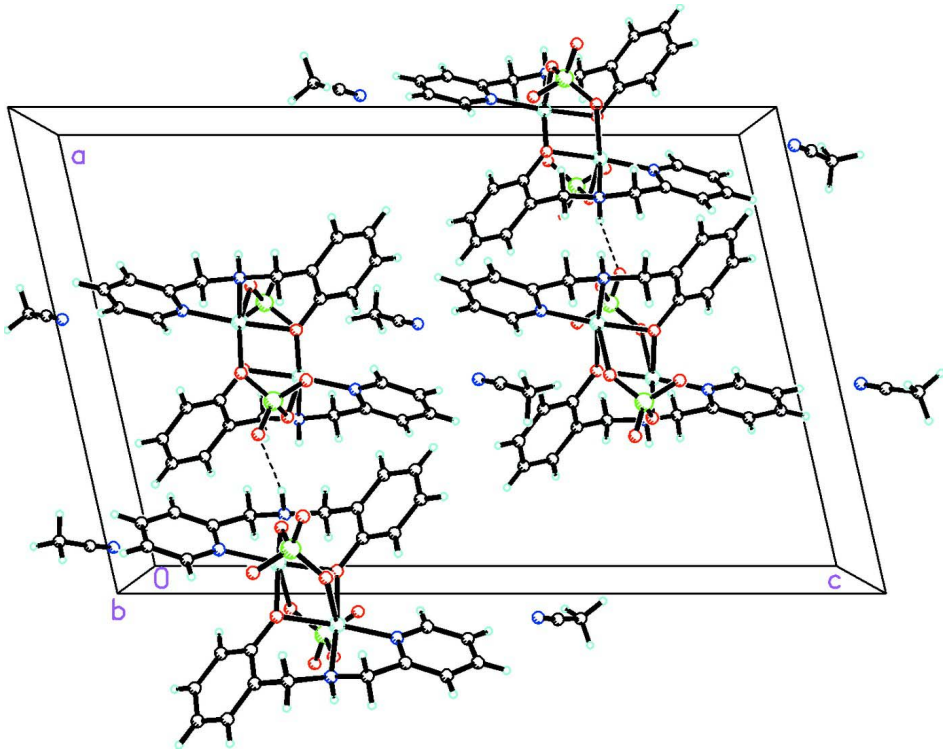


**Figure 2**

The molecular packing for $C_{26}H_{26}Cl_2Cu_2N_4O_{10}$, $2(C_2H_3N)$ viewed down the *b* axis showing the intermolecular N—H···O, C—H···O and C–H···N interactions.

**Di-*μ*-perchlorato-bis{*μ*-2-[(2-pyridyl)methylaminomethyl]phenolato)dicopper(II) acetonitrile disolvate**

*Crystal data*

$[Cu_2(C_{13}H_{13}N_2O)_2(ClO_4)_2]\cdot 2C_2H_3N$
$M_r = 834.60$
Monoclinic, $P2_1/n$
$a = 16.0285$ (4) Å
$b = 9.4062$ (3) Å
$c = 24.7097$ (10) Å
$\beta = 102.665$ (3)°
$V = 3634.8$ (2) Å$^3$
$Z = 4$
$F(000) = 1704$
$D_x = 1.525$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 11642 reflections
$\theta = 4.7$–$34.7°$
$\mu = 1.38$ mm$^{-1}$
$T = 200$ K
Chunk, dark green
0.53 × 0.46 × 0.39 mm

*Data collection*

Oxford Diffraction Gemini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.5081 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2008)
$T_{min} = 0.848$, $T_{max} = 1.000$
33853 measured reflections
14212 independent reflections
8089 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 34.8°$, $\theta_{min} = 4.7°$
$h = -25 \rightarrow 25$
$k = -14 \rightarrow 11$
$l = -39 \rightarrow 38$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.078$
$wR(F^2) = 0.199$
$S = 1.19$
14212 reflections
453 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.0713P)^2 + 3.514P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.29$ e Å$^{-3}$
$\Delta\rho_{min} = -2.24$ e Å$^{-3}$

*Special details*

**Experimental**. CrysAlis RED, Oxford Diffraction Ltd., Version 1.171.32.15 (release 10-01-2008 CrysAlis171 .NET) (compiled Jan 10 2008,16:37:18) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm (Oxford Diffraction, 2008).

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.05889 (2) | 0.91878 (4) | 0.214778 (15) | 0.02910 (8) |
| Cu2 | −0.06076 (2) | 1.04142 (4) | 0.277641 (15) | 0.02901 (8) |
| Cl1 | −0.10838 (4) | 0.68198 (8) | 0.24709 (4) | 0.03933 (18) |
| Cl2 | 0.10650 (4) | 1.27847 (8) | 0.24782 (4) | 0.0440 (2) |
| O11 | −0.05145 (14) | 0.6989 (3) | 0.20982 (10) | 0.0450 (6) |
| O12 | −0.14408 (13) | 0.8171 (2) | 0.25739 (10) | 0.0425 (6) |
| O13 | −0.06250 (19) | 0.6237 (3) | 0.29860 (13) | 0.0743 (9) |
| O14 | −0.17758 (15) | 0.5894 (3) | 0.22222 (15) | 0.0730 (10) |
| O21 | 0.14267 (14) | 1.1426 (2) | 0.23742 (11) | 0.0443 (6) |
| O22 | 0.04757 (14) | 1.2593 (3) | 0.28331 (11) | 0.0483 (6) |
| O23 | 0.17503 (16) | 1.3695 (3) | 0.27486 (17) | 0.0819 (11) |
| O24 | 0.0624 (2) | 1.3376 (4) | 0.19615 (15) | 0.0843 (10) |
| O1A | 0.04239 (11) | 0.9262 (2) | 0.29027 (8) | 0.0264 (4) |
| O1B | −0.04444 (11) | 1.0330 (2) | 0.20172 (8) | 0.0262 (4) |
| N1A | 0.15385 (15) | 0.7811 (3) | 0.23295 (11) | 0.0347 (6) |
| H1AA | 0.2049 | 0.8316 | 0.2381 | 0.042* |
| N2A | 0.08589 (15) | 0.9092 (3) | 0.14074 (11) | 0.0332 (6) |
| N1B | −0.15526 (15) | 1.1796 (3) | 0.25897 (11) | 0.0347 (6) |
| H1BA | −0.2064 | 1.1300 | 0.2551 | 0.042* |
| N2B | −0.08647 (15) | 1.0555 (3) | 0.35188 (10) | 0.0333 (6) |
| C1A | 0.11031 (17) | 0.9121 (3) | 0.33359 (12) | 0.0328 (6) |
| C2A | 0.1249 (2) | 1.0062 (4) | 0.37820 (13) | 0.0432 (8) |

| | | | | |
|---|---|---|---|---|
| H2AA | 0.0877 | 1.0847 | 0.3784 | 0.052* |
| C3A | 0.1937 (2) | 0.9851 (5) | 0.42218 (15) | 0.0599 (11) |
| H3AA | 0.2019 | 1.0478 | 0.4530 | 0.072* |
| C4A | 0.2502 (3) | 0.8764 (6) | 0.42243 (17) | 0.0730 (14) |
| H4AA | 0.2973 | 0.8640 | 0.4529 | 0.088* |
| C5A | 0.2379 (2) | 0.7856 (5) | 0.37814 (18) | 0.0617 (12) |
| H5AA | 0.2780 | 0.7114 | 0.3779 | 0.074* |
| C6A | 0.16741 (19) | 0.7989 (4) | 0.33285 (14) | 0.0408 (8) |
| C7A | 0.15409 (19) | 0.7000 (3) | 0.28532 (15) | 0.0441 (8) |
| H7AA | 0.0989 | 0.6498 | 0.2820 | 0.053* |
| H7AB | 0.2003 | 0.6281 | 0.2914 | 0.053* |
| C8A | 0.1471 (2) | 0.6924 (3) | 0.18345 (16) | 0.0449 (8) |
| H8AA | 0.0998 | 0.6232 | 0.1807 | 0.054* |
| H8AB | 0.2009 | 0.6392 | 0.1852 | 0.054* |
| C9A | 0.1302 (2) | 0.7899 (4) | 0.13437 (15) | 0.0422 (8) |
| C10A | 0.1570 (3) | 0.7668 (5) | 0.08580 (19) | 0.0721 (13) |
| H10A | 0.1873 | 0.6826 | 0.0810 | 0.087* |
| C11A | 0.1395 (3) | 0.8674 (6) | 0.0441 (2) | 0.0800 (14) |
| H11A | 0.1568 | 0.8517 | 0.0102 | 0.096* |
| C12A | 0.0973 (3) | 0.9893 (5) | 0.05174 (16) | 0.0597 (11) |
| H12A | 0.0867 | 1.0606 | 0.0238 | 0.072* |
| C13A | 0.0704 (2) | 1.0075 (4) | 0.10056 (14) | 0.0414 (8) |
| H13A | 0.0402 | 1.0915 | 0.1058 | 0.050* |
| C1B | −0.11278 (17) | 1.0433 (3) | 0.15872 (12) | 0.0329 (6) |
| C2B | −0.1271 (2) | 0.9480 (4) | 0.11472 (13) | 0.0404 (8) |
| H2BA | −0.0887 | 0.8711 | 0.1146 | 0.048* |
| C3B | −0.1972 (2) | 0.9648 (5) | 0.07100 (15) | 0.0583 (11) |
| H3BA | −0.2054 | 0.9006 | 0.0406 | 0.070* |
| C4B | −0.2548 (3) | 1.0718 (6) | 0.07082 (17) | 0.0659 (13) |
| H4BA | −0.3028 | 1.0817 | 0.0408 | 0.079* |
| C5B | −0.2424 (2) | 1.1645 (5) | 0.11447 (17) | 0.0593 (11) |
| H5BA | −0.2833 | 1.2375 | 0.1147 | 0.071* |
| C6B | −0.17098 (19) | 1.1552 (4) | 0.15908 (14) | 0.0417 (8) |
| C7B | −0.1574 (2) | 1.2582 (3) | 0.20605 (15) | 0.0413 (8) |
| H7BA | −0.2043 | 1.3288 | 0.1998 | 0.050* |
| H7BB | −0.1028 | 1.3095 | 0.2084 | 0.050* |
| C8B | −0.1461 (2) | 1.2726 (3) | 0.30813 (15) | 0.0430 (8) |
| H8BA | −0.1995 | 1.3268 | 0.3068 | 0.052* |
| H8BB | −0.0987 | 1.3409 | 0.3094 | 0.052* |
| C9B | −0.1276 (2) | 1.1781 (4) | 0.35779 (15) | 0.0433 (8) |
| C10B | −0.1509 (3) | 1.2083 (5) | 0.40691 (19) | 0.0734 (13) |
| H10B | −0.1796 | 1.2946 | 0.4112 | 0.088* |
| C11B | −0.1321 (4) | 1.1125 (6) | 0.4497 (2) | 0.0852 (16) |
| H11B | −0.1458 | 1.1342 | 0.4842 | 0.102* |
| C12B | −0.0936 (3) | 0.9851 (6) | 0.44275 (17) | 0.0684 (13) |
| H12B | −0.0829 | 0.9162 | 0.4715 | 0.082* |
| C13B | −0.0707 (2) | 0.9600 (4) | 0.39270 (14) | 0.0473 (9) |
| H13B | −0.0433 | 0.8732 | 0.3874 | 0.057* |

| | | | | |
|---|---|---|---|---|
| N1S | 0.4394 (4) | 0.8308 (7) | 0.5336 (2) | 0.129 (2) |
| C11S | 0.4318 (6) | 0.9186 (8) | 0.5605 (3) | 0.124 (3) |
| C12S | 0.4157 (9) | 1.0326 (9) | 0.5941 (3) | 0.191 (5) |
| H12C | 0.4518 | 1.1138 | 0.5895 | 0.287* |
| H12D | 0.4287 | 1.0028 | 0.6331 | 0.287* |
| H12E | 0.3554 | 1.0602 | 0.5831 | 0.287* |
| N2S | −0.0703 (6) | 0.6977 (8) | 0.5421 (3) | 0.175 (3) |
| C21S | −0.0794 (5) | 0.6218 (9) | 0.5687 (2) | 0.125 (3) |
| C22S | −0.0856 (7) | 0.5063 (9) | 0.6015 (3) | 0.159 (4) |
| H22F | −0.0700 | 0.4201 | 0.5837 | 0.238* |
| H22G | −0.1444 | 0.4976 | 0.6063 | 0.238* |
| H22H | −0.0468 | 0.5185 | 0.6378 | 0.238* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.02109 (14) | 0.02713 (17) | 0.03988 (18) | 0.00594 (13) | 0.00843 (13) | 0.00543 (14) |
| Cu2 | 0.02246 (15) | 0.02678 (17) | 0.03891 (18) | 0.00478 (13) | 0.00915 (13) | 0.00460 (14) |
| Cl1 | 0.0237 (3) | 0.0266 (3) | 0.0693 (5) | −0.0011 (3) | 0.0136 (3) | 0.0037 (3) |
| Cl2 | 0.0232 (3) | 0.0261 (3) | 0.0851 (6) | −0.0005 (3) | 0.0166 (3) | 0.0049 (4) |
| O11 | 0.0344 (11) | 0.0397 (12) | 0.0651 (15) | 0.0012 (10) | 0.0203 (11) | −0.0048 (11) |
| O12 | 0.0290 (10) | 0.0281 (11) | 0.0729 (15) | −0.0041 (9) | 0.0165 (10) | −0.0073 (10) |
| O13 | 0.0604 (17) | 0.079 (2) | 0.0856 (19) | 0.0134 (15) | 0.0201 (15) | 0.0459 (16) |
| O14 | 0.0306 (11) | 0.0388 (14) | 0.153 (3) | −0.0105 (10) | 0.0276 (15) | −0.0308 (16) |
| O21 | 0.0327 (10) | 0.0316 (11) | 0.0726 (15) | −0.0027 (9) | 0.0198 (11) | −0.0094 (11) |
| O22 | 0.0330 (11) | 0.0421 (13) | 0.0728 (16) | −0.0001 (10) | 0.0181 (11) | −0.0070 (12) |
| O23 | 0.0329 (12) | 0.0408 (14) | 0.174 (3) | −0.0134 (11) | 0.0275 (16) | −0.0393 (17) |
| O24 | 0.0676 (19) | 0.081 (2) | 0.110 (2) | 0.0226 (16) | 0.0311 (17) | 0.0583 (18) |
| O1A | 0.0194 (8) | 0.0242 (9) | 0.0333 (9) | 0.0033 (7) | 0.0009 (7) | 0.0083 (7) |
| O1B | 0.0179 (8) | 0.0263 (9) | 0.0325 (9) | 0.0049 (7) | 0.0016 (7) | 0.0068 (7) |
| N1A | 0.0231 (10) | 0.0268 (12) | 0.0568 (15) | 0.0031 (9) | 0.0141 (11) | 0.0034 (11) |
| N2A | 0.0239 (10) | 0.0333 (13) | 0.0444 (13) | −0.0014 (10) | 0.0117 (10) | −0.0027 (11) |
| N1B | 0.0215 (10) | 0.0281 (12) | 0.0563 (15) | 0.0017 (9) | 0.0124 (10) | 0.0035 (11) |
| N2B | 0.0287 (11) | 0.0344 (13) | 0.0374 (12) | −0.0059 (10) | 0.0084 (10) | −0.0017 (10) |
| C1A | 0.0208 (11) | 0.0384 (15) | 0.0387 (14) | −0.0040 (11) | 0.0054 (11) | 0.0161 (12) |
| C2A | 0.0340 (15) | 0.055 (2) | 0.0394 (16) | −0.0127 (15) | 0.0065 (13) | 0.0070 (14) |
| C3A | 0.0455 (19) | 0.091 (3) | 0.0385 (18) | −0.022 (2) | −0.0004 (16) | 0.0096 (19) |
| C4A | 0.042 (2) | 0.116 (4) | 0.050 (2) | −0.011 (2) | −0.0129 (18) | 0.028 (2) |
| C5A | 0.0308 (16) | 0.078 (3) | 0.071 (2) | 0.0094 (18) | −0.0007 (17) | 0.036 (2) |
| C6A | 0.0263 (13) | 0.0437 (17) | 0.0500 (17) | 0.0037 (13) | 0.0034 (13) | 0.0219 (14) |
| C7A | 0.0256 (13) | 0.0325 (15) | 0.074 (2) | 0.0097 (12) | 0.0116 (14) | 0.0224 (15) |
| C8A | 0.0322 (15) | 0.0291 (15) | 0.076 (2) | 0.0055 (13) | 0.0183 (16) | −0.0042 (15) |
| C9A | 0.0342 (14) | 0.0363 (17) | 0.061 (2) | −0.0026 (13) | 0.0206 (14) | −0.0079 (15) |
| C10A | 0.083 (3) | 0.063 (3) | 0.086 (3) | 0.007 (2) | 0.052 (2) | −0.017 (2) |
| C11A | 0.100 (3) | 0.085 (3) | 0.069 (3) | −0.006 (3) | 0.051 (2) | −0.016 (2) |
| C12A | 0.062 (2) | 0.072 (3) | 0.049 (2) | −0.016 (2) | 0.0207 (18) | 0.0019 (19) |
| C13A | 0.0349 (15) | 0.0461 (18) | 0.0434 (17) | −0.0056 (14) | 0.0093 (13) | 0.0036 (14) |
| C1B | 0.0227 (12) | 0.0354 (15) | 0.0401 (14) | −0.0012 (11) | 0.0056 (11) | 0.0160 (12) |

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|---|---|---|---|---|---|---|
| C2B | 0.0304 (14) | 0.0536 (19) | 0.0375 (15) | −0.0065 (14) | 0.0081 (12) | 0.0085 (14) |
| C3B | 0.0408 (18) | 0.094 (3) | 0.0380 (17) | −0.014 (2) | 0.0050 (15) | 0.0084 (19) |
| C4B | 0.0387 (19) | 0.104 (3) | 0.048 (2) | 0.001 (2) | −0.0067 (16) | 0.023 (2) |
| C5B | 0.0313 (16) | 0.076 (3) | 0.067 (2) | 0.0151 (17) | 0.0027 (16) | 0.035 (2) |
| C6B | 0.0260 (13) | 0.0445 (18) | 0.0539 (18) | 0.0072 (13) | 0.0074 (13) | 0.0220 (15) |
| C7B | 0.0300 (14) | 0.0312 (15) | 0.064 (2) | 0.0091 (12) | 0.0140 (14) | 0.0167 (14) |
| C8B | 0.0357 (15) | 0.0305 (16) | 0.067 (2) | 0.0030 (13) | 0.0192 (15) | −0.0096 (14) |
| C9B | 0.0326 (14) | 0.0417 (18) | 0.060 (2) | −0.0050 (13) | 0.0195 (14) | −0.0122 (15) |
| C10B | 0.085 (3) | 0.068 (3) | 0.081 (3) | 0.000 (2) | 0.047 (2) | −0.021 (2) |
| C11B | 0.113 (4) | 0.089 (4) | 0.068 (3) | −0.009 (3) | 0.052 (3) | −0.021 (3) |
| C12B | 0.076 (3) | 0.087 (3) | 0.046 (2) | −0.026 (3) | 0.022 (2) | 0.003 (2) |
| C13B | 0.0449 (18) | 0.053 (2) | 0.0460 (18) | −0.0111 (16) | 0.0133 (15) | 0.0022 (16) |
| N1S | 0.159 (6) | 0.107 (4) | 0.106 (4) | 0.031 (4) | −0.002 (4) | −0.003 (3) |
| C11S | 0.171 (7) | 0.097 (5) | 0.077 (4) | 0.021 (5) | −0.034 (4) | −0.004 (3) |
| C12S | 0.354 (15) | 0.108 (6) | 0.093 (5) | 0.047 (8) | 0.011 (7) | −0.014 (5) |
| N2S | 0.225 (8) | 0.136 (6) | 0.135 (6) | −0.078 (6) | −0.022 (5) | 0.019 (5) |
| C21S | 0.160 (6) | 0.125 (5) | 0.063 (3) | −0.062 (5) | −0.035 (4) | 0.025 (3) |
| C22S | 0.221 (10) | 0.130 (6) | 0.099 (5) | −0.043 (6) | −0.022 (6) | 0.044 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—O1B | 1.9410 (18) | C8A—C9A | 1.497 (5) |
| Cu1—O1A | 1.942 (2) | C8A—H8AA | 0.9900 |
| Cu1—N2A | 1.972 (3) | C8A—H8AB | 0.9900 |
| Cu1—N1A | 1.974 (2) | C9A—C10A | 1.378 (6) |
| Cu1—O21 | 2.494 (2) | C10A—C11A | 1.381 (7) |
| Cu1—O11 | 2.706 (2) | C10A—H10A | 0.9500 |
| Cu1—Cu2 | 2.9543 (5) | C11A—C12A | 1.365 (7) |
| Cu2—O1A | 1.9440 (18) | C11A—H11A | 0.9500 |
| Cu2—O1B | 1.952 (2) | C12A—C13A | 1.378 (5) |
| Cu2—N2B | 1.971 (3) | C12A—H12A | 0.9500 |
| Cu2—N1B | 1.973 (2) | C13A—H13A | 0.9500 |
| Cu2—O12 | 2.489 (2) | C1B—C2B | 1.389 (5) |
| Cu2—O22 | 2.670 (2) | C1B—C6B | 1.408 (4) |
| Cl1—O13 | 1.432 (3) | C2B—C3B | 1.387 (4) |
| Cl1—O14 | 1.438 (3) | C2B—H2BA | 0.9500 |
| Cl1—O12 | 1.439 (2) | C3B—C4B | 1.365 (6) |
| Cl1—O11 | 1.440 (3) | C3B—H3BA | 0.9500 |
| Cl2—O24 | 1.429 (3) | C4B—C5B | 1.367 (6) |
| Cl2—O22 | 1.434 (3) | C4B—H4BA | 0.9500 |
| Cl2—O23 | 1.437 (3) | C5B—C6B | 1.407 (5) |
| Cl2—O21 | 1.449 (2) | C5B—H5BA | 0.9500 |
| O1A—C1A | 1.356 (3) | C6B—C7B | 1.490 (5) |
| O1B—C1B | 1.352 (3) | C7B—H7BA | 0.9900 |
| N1A—C8A | 1.465 (4) | C7B—H7BB | 0.9900 |
| N1A—C7A | 1.502 (4) | C8B—C9B | 1.492 (5) |
| N1A—H1AA | 0.9300 | C8B—H8BA | 0.9900 |
| N2A—C13A | 1.339 (4) | C8B—H8BB | 0.9900 |

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|---|---|---|---|
| N2A—C9A | 1.355 (4) | C9B—C10B | 1.375 (6) |
| N1B—C8B | 1.478 (4) | C10B—C11B | 1.371 (7) |
| N1B—C7B | 1.496 (4) | C10B—H10B | 0.9500 |
| N1B—H1BA | 0.9300 | C11B—C12B | 1.376 (7) |
| N2B—C13B | 1.333 (4) | C11B—H11B | 0.9500 |
| N2B—C9B | 1.352 (4) | C12B—C13B | 1.385 (6) |
| C1A—C2A | 1.393 (5) | C12B—H12B | 0.9500 |
| C1A—C6A | 1.407 (4) | C13B—H13B | 0.9500 |
| C2A—C3A | 1.383 (5) | N1S—C11S | 1.083 (8) |
| C2A—H2AA | 0.9500 | C11S—C12S | 1.416 (11) |
| C3A—C4A | 1.364 (7) | C12S—H12C | 0.9800 |
| C3A—H3AA | 0.9500 | C12S—H12D | 0.9800 |
| C4A—C5A | 1.368 (7) | C12S—H12E | 0.9800 |
| C4A—H4AA | 0.9500 | N2S—C21S | 1.003 (9) |
| C5A—C6A | 1.410 (5) | C21S—C22S | 1.371 (10) |
| C5A—H5AA | 0.9500 | C22S—H22F | 0.9800 |
| C6A—C7A | 1.476 (5) | C22S—H22G | 0.9800 |
| C7A—H7AA | 0.9900 | C22S—H22H | 0.9800 |
| C7A—H7AB | 0.9900 | | |

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|---|---|---|---|
| O1B—Cu1—O1A | 81.30 (8) | C5A—C4A—H4AA | 120.5 |
| O1B—Cu1—N2A | 102.94 (9) | C4A—C5A—C6A | 122.0 (4) |
| O1A—Cu1—N2A | 175.24 (8) | C4A—C5A—H5AA | 119.0 |
| O1B—Cu1—N1A | 171.26 (9) | C6A—C5A—H5AA | 119.0 |
| O1A—Cu1—N1A | 93.77 (10) | C1A—C6A—C5A | 117.8 (3) |
| N2A—Cu1—N1A | 82.30 (11) | C1A—C6A—C7A | 120.4 (3) |
| O1B—Cu1—O21 | 88.16 (7) | C5A—C6A—C7A | 121.8 (3) |
| O1A—Cu1—O21 | 86.22 (8) | C6A—C7A—N1A | 109.7 (3) |
| N2A—Cu1—O21 | 91.71 (9) | C6A—C7A—H7AA | 109.7 |
| N1A—Cu1—O21 | 98.77 (9) | N1A—C7A—H7AA | 109.7 |
| O1B—Cu1—O11 | 83.69 (7) | C6A—C7A—H7AB | 109.7 |
| O1A—Cu1—O11 | 81.12 (8) | N1A—C7A—H7AB | 109.7 |
| N2A—Cu1—O11 | 101.38 (9) | H7AA—C7A—H7AB | 108.2 |
| N1A—Cu1—O11 | 88.43 (9) | N1A—C8A—C9A | 107.1 (3) |
| O21—Cu1—O11 | 165.84 (8) | N1A—C8A—H8AA | 110.3 |
| O1B—Cu1—Cu2 | 40.76 (6) | C9A—C8A—H8AA | 110.3 |
| O1A—Cu1—Cu2 | 40.54 (5) | N1A—C8A—H8AB | 110.3 |
| N2A—Cu1—Cu2 | 143.65 (7) | C9A—C8A—H8AB | 110.3 |
| N1A—Cu1—Cu2 | 133.92 (8) | H8AA—C8A—H8AB | 108.5 |
| O21—Cu1—Cu2 | 86.10 (6) | N2A—C9A—C10A | 120.2 (4) |
| O11—Cu1—Cu2 | 80.16 (5) | N2A—C9A—C8A | 114.8 (3) |
| O1A—Cu2—O1B | 80.98 (8) | C10A—C9A—C8A | 125.0 (3) |
| O1A—Cu2—N2B | 103.41 (9) | C9A—C10A—C11A | 119.4 (4) |
| O1B—Cu2—N2B | 175.47 (9) | C9A—C10A—H10A | 120.3 |
| O1A—Cu2—N1B | 170.89 (10) | C11A—C10A—H10A | 120.3 |
| O1B—Cu2—N1B | 93.43 (10) | C12A—C11A—C10A | 119.9 (4) |
| N2B—Cu2—N1B | 82.36 (11) | C12A—C11A—H11A | 120.0 |
| O1A—Cu2—O12 | 87.68 (7) | C10A—C11A—H11A | 120.0 |

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| O1B—Cu2—O12 | 87.22 (8) | C11A—C12A—C13A | 119.0 (4) |
| N2B—Cu2—O12 | 91.81 (9) | C11A—C12A—H12A | 120.5 |
| N1B—Cu2—O12 | 99.28 (9) | C13A—C12A—H12A | 120.5 |
| O1A—Cu2—O22 | 84.20 (7) | N2A—C13A—C12A | 121.4 (4) |
| O1B—Cu2—O22 | 81.88 (8) | N2A—C13A—H13A | 119.3 |
| N2B—Cu2—O22 | 99.55 (9) | C12A—C13A—H13A | 119.3 |
| N1B—Cu2—O22 | 87.91 (9) | O1B—C1B—C2B | 122.4 (3) |
| O12—Cu2—O22 | 167.30 (8) | O1B—C1B—C6B | 118.2 (3) |
| O1A—Cu2—Cu1 | 40.49 (6) | C2B—C1B—C6B | 119.5 (3) |
| O1B—Cu2—Cu1 | 40.49 (5) | C3B—C2B—C1B | 120.2 (4) |
| N2B—Cu2—Cu1 | 143.89 (7) | C3B—C2B—H2BA | 119.9 |
| N1B—Cu2—Cu1 | 133.48 (8) | C1B—C2B—H2BA | 119.9 |
| O12—Cu2—Cu1 | 86.83 (6) | C4B—C3B—C2B | 121.2 (4) |
| O22—Cu2—Cu1 | 80.65 (5) | C4B—C3B—H3BA | 119.4 |
| O13—Cl1—O14 | 110.2 (2) | C2B—C3B—H3BA | 119.4 |
| O13—Cl1—O12 | 109.12 (18) | C3B—C4B—C5B | 119.1 (3) |
| O14—Cl1—O12 | 108.11 (14) | C3B—C4B—H4BA | 120.4 |
| O13—Cl1—O11 | 109.68 (16) | C5B—C4B—H4BA | 120.4 |
| O14—Cl1—O11 | 109.34 (18) | C4B—C5B—C6B | 122.1 (4) |
| O12—Cl1—O11 | 110.34 (14) | C4B—C5B—H5BA | 119.0 |
| O24—Cl2—O22 | 109.42 (17) | C6B—C5B—H5BA | 119.0 |
| O24—Cl2—O23 | 111.2 (2) | C5B—C6B—C1B | 117.9 (3) |
| O22—Cl2—O23 | 109.24 (19) | C5B—C6B—C7B | 121.6 (3) |
| O24—Cl2—O21 | 108.87 (19) | C1B—C6B—C7B | 120.5 (3) |
| O22—Cl2—O21 | 109.87 (15) | C6B—C7B—N1B | 109.4 (3) |
| O23—Cl2—O21 | 108.26 (14) | C6B—C7B—H7BA | 109.8 |
| Cl1—O11—Cu1 | 123.70 (13) | N1B—C7B—H7BA | 109.8 |
| Cl1—O12—Cu2 | 124.58 (12) | C6B—C7B—H7BB | 109.8 |
| Cl2—O21—Cu1 | 124.58 (12) | N1B—C7B—H7BB | 109.8 |
| Cl2—O22—Cu2 | 124.93 (14) | H7BA—C7B—H7BB | 108.3 |
| C1A—O1A—Cu1 | 120.01 (18) | N1B—C8B—C9B | 106.8 (3) |
| C1A—O1A—Cu2 | 133.53 (19) | N1B—C8B—H8BA | 110.4 |
| Cu1—O1A—Cu2 | 98.98 (8) | C9B—C8B—H8BA | 110.4 |
| C1B—O1B—Cu1 | 133.25 (19) | N1B—C8B—H8BB | 110.4 |
| C1B—O1B—Cu2 | 119.75 (17) | C9B—C8B—H8BB | 110.4 |
| Cu1—O1B—Cu2 | 98.74 (8) | H8BA—C8B—H8BB | 108.6 |
| C8A—N1A—C7A | 114.6 (3) | N2B—C9B—C10B | 120.3 (4) |
| C8A—N1A—Cu1 | 105.76 (18) | N2B—C9B—C8B | 115.7 (3) |
| C7A—N1A—Cu1 | 112.68 (19) | C10B—C9B—C8B | 124.0 (3) |
| C8A—N1A—H1AA | 107.9 | C11B—C10B—C9B | 119.2 (4) |
| C7A—N1A—H1AA | 107.9 | C11B—C10B—H10B | 120.4 |
| Cu1—N1A—H1AA | 107.9 | C9B—C10B—H10B | 120.4 |
| C13A—N2A—C9A | 120.2 (3) | C10B—C11B—C12B | 120.4 (4) |
| C13A—N2A—Cu1 | 127.8 (2) | C10B—C11B—H11B | 119.8 |
| C9A—N2A—Cu1 | 111.9 (2) | C12B—C11B—H11B | 119.8 |
| C8B—N1B—C7B | 113.9 (3) | C11B—C12B—C13B | 118.2 (4) |
| C8B—N1B—Cu2 | 105.36 (18) | C11B—C12B—H12B | 120.9 |
| C7B—N1B—Cu2 | 113.53 (19) | C13B—C12B—H12B | 120.9 |

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|---|---|---|---|
| C8B—N1B—H1BA | 107.9 | N2B—C13B—C12B | 121.2 (4) |
| C7B—N1B—H1BA | 107.9 | N2B—C13B—H13B | 119.4 |
| Cu2—N1B—H1BA | 107.9 | C12B—C13B—H13B | 119.4 |
| C13B—N2B—C9B | 120.6 (3) | N1S—C11S—C12S | 176.0 (11) |
| C13B—N2B—Cu2 | 128.0 (2) | C11S—C12S—H12C | 109.5 |
| C9B—N2B—Cu2 | 111.4 (2) | C11S—C12S—H12D | 109.5 |
| O1A—C1A—C2A | 122.0 (3) | H12C—C12S—H12D | 109.5 |
| O1A—C1A—C6A | 118.4 (3) | C11S—C12S—H12E | 109.5 |
| C2A—C1A—C6A | 119.7 (3) | H12C—C12S—H12E | 109.5 |
| C3A—C2A—C1A | 119.8 (4) | H12D—C12S—H12E | 109.5 |
| C3A—C2A—H2AA | 120.1 | N2S—C21S—C22S | 172.2 (12) |
| C1A—C2A—H2AA | 120.1 | C21S—C22S—H22F | 109.5 |
| C4A—C3A—C2A | 121.7 (4) | C21S—C22S—H22G | 109.5 |
| C4A—C3A—H3AA | 119.1 | H22F—C22S—H22G | 109.5 |
| C2A—C3A—H3AA | 119.1 | C21S—C22S—H22H | 109.5 |
| C3A—C4A—C5A | 119.0 (3) | H22F—C22S—H22H | 109.5 |
| C3A—C4A—H4AA | 120.5 | H22G—C22S—H22H | 109.5 |

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|---|---|---|---|
| O1B—Cu1—Cu2—O1A | 179.56 (12) | O1A—Cu1—N1A—C8A | 146.8 (2) |
| N2A—Cu1—Cu2—O1A | −176.33 (15) | N2A—Cu1—N1A—C8A | −35.8 (2) |
| N1A—Cu1—Cu2—O1A | 9.69 (13) | O21—Cu1—N1A—C8A | −126.4 (2) |
| O21—Cu1—Cu2—O1A | −88.74 (10) | O11—Cu1—N1A—C8A | 65.9 (2) |
| O11—Cu1—Cu2—O1A | 87.82 (10) | Cu2—Cu1—N1A—C8A | 140.56 (17) |
| O1A—Cu1—Cu2—O1B | −179.56 (12) | O1B—Cu1—N1A—C7A | −34.4 (7) |
| N2A—Cu1—Cu2—O1B | 4.11 (15) | O1A—Cu1—N1A—C7A | 21.0 (2) |
| N1A—Cu1—Cu2—O1B | −169.88 (13) | N2A—Cu1—N1A—C7A | −161.7 (2) |
| O21—Cu1—Cu2—O1B | 91.70 (10) | O21—Cu1—N1A—C7A | 107.7 (2) |
| O11—Cu1—Cu2—O1B | −91.74 (10) | O11—Cu1—N1A—C7A | −60.0 (2) |
| O1B—Cu1—Cu2—N2B | 178.15 (15) | Cu2—Cu1—N1A—C7A | 14.7 (2) |
| O1A—Cu1—Cu2—N2B | −1.41 (15) | O1B—Cu1—N2A—C13A | 31.6 (3) |
| N2A—Cu1—Cu2—N2B | −177.74 (17) | O1A—Cu1—N2A—C13A | −121.0 (11) |
| N1A—Cu1—Cu2—N2B | 8.28 (16) | N1A—Cu1—N2A—C13A | −155.5 (3) |
| O21—Cu1—Cu2—N2B | −90.15 (14) | O21—Cu1—N2A—C13A | −56.9 (3) |
| O11—Cu1—Cu2—N2B | 86.41 (13) | O11—Cu1—N2A—C13A | 117.7 (2) |
| O1B—Cu1—Cu2—N1B | −10.37 (13) | Cu2—Cu1—N2A—C13A | 28.9 (3) |
| O1A—Cu1—Cu2—N1B | 170.07 (13) | O1B—Cu1—N2A—C9A | −152.9 (2) |
| N2A—Cu1—Cu2—N1B | −6.26 (16) | O1A—Cu1—N2A—C9A | 54.4 (12) |
| N1A—Cu1—Cu2—N1B | 179.75 (14) | N1A—Cu1—N2A—C9A | 20.0 (2) |
| O21—Cu1—Cu2—N1B | 81.33 (12) | O21—Cu1—N2A—C9A | 118.6 (2) |
| O11—Cu1—Cu2—N1B | −102.11 (11) | O11—Cu1—N2A—C9A | −66.8 (2) |
| O1B—Cu1—Cu2—O12 | 89.42 (10) | Cu2—Cu1—N2A—C9A | −155.63 (16) |
| O1A—Cu1—Cu2—O12 | −90.14 (10) | O1A—Cu2—N1B—C8B | −93.2 (6) |
| N2A—Cu1—Cu2—O12 | 93.53 (13) | O1B—Cu2—N1B—C8B | −144.97 (19) |
| N1A—Cu1—Cu2—O12 | −80.45 (11) | N2B—Cu2—N1B—C8B | 36.7 (2) |
| O21—Cu1—Cu2—O12 | −178.88 (8) | O12—Cu2—N1B—C8B | 127.29 (19) |
| O11—Cu1—Cu2—O12 | −2.32 (8) | O22—Cu2—N1B—C8B | −63.2 (2) |
| O1B—Cu1—Cu2—O22 | −88.43 (10) | Cu1—Cu2—N1B—C8B | −138.24 (17) |
| O1A—Cu1—Cu2—O22 | 92.01 (10) | O1A—Cu2—N1B—C7B | 32.1 (7) |

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|---|---|---|---|
| N2A—Cu1—Cu2—O22 | −84.31 (13) | O1B—Cu2—N1B—C7B | −19.6 (2) |
| N1A—Cu1—Cu2—O22 | 101.70 (12) | N2B—Cu2—N1B—C7B | 162.0 (2) |
| O21—Cu1—Cu2—O22 | 3.27 (8) | O12—Cu2—N1B—C7B | −107.4 (2) |
| O11—Cu1—Cu2—O22 | 179.83 (7) | O22—Cu2—N1B—C7B | 62.1 (2) |
| O13—Cl1—O11—Cu1 | −79.9 (2) | Cu1—Cu2—N1B—C7B | −12.9 (2) |
| O14—Cl1—O11—Cu1 | 159.15 (15) | O1A—Cu2—N2B—C13B | −31.5 (3) |
| O12—Cl1—O11—Cu1 | 40.37 (19) | O1B—Cu2—N2B—C13B | 134.0 (11) |
| O1B—Cu1—O11—Cl1 | −60.39 (16) | N1B—Cu2—N2B—C13B | 155.6 (3) |
| O1A—Cu1—O11—Cl1 | 21.75 (15) | O12—Cu2—N2B—C13B | 56.5 (3) |
| N2A—Cu1—O11—Cl1 | −162.37 (16) | O22—Cu2—N2B—C13B | −117.8 (3) |
| N1A—Cu1—O11—Cl1 | 115.81 (17) | Cu1—Cu2—N2B—C13B | −30.6 (3) |
| O21—Cu1—O11—Cl1 | −5.2 (4) | O1A—Cu2—N2B—C9B | 150.9 (2) |
| Cu2—Cu1—O11—Cl1 | −19.35 (14) | O1B—Cu2—N2B—C9B | −43.5 (13) |
| O13—Cl1—O12—Cu2 | 76.0 (2) | N1B—Cu2—N2B—C9B | −21.9 (2) |
| O14—Cl1—O12—Cu2 | −164.11 (19) | O12—Cu2—N2B—C9B | −121.1 (2) |
| O11—Cl1—O12—Cu2 | −44.6 (2) | O22—Cu2—N2B—C9B | 64.6 (2) |
| O1A—Cu2—O12—Cl1 | −14.02 (18) | Cu1—Cu2—N2B—C9B | 151.84 (17) |
| O1B—Cu2—O12—Cl1 | 67.05 (18) | Cu1—O1A—C1A—C2A | 131.2 (3) |
| N2B—Cu2—O12—Cl1 | −117.38 (18) | Cu2—O1A—C1A—C2A | −11.7 (4) |
| N1B—Cu2—O12—Cl1 | 160.07 (18) | Cu1—O1A—C1A—C6A | −48.6 (3) |
| O22—Cu2—O12—Cl1 | 36.2 (5) | Cu2—O1A—C1A—C6A | 168.5 (2) |
| Cu1—Cu2—O12—Cl1 | 26.51 (17) | O1A—C1A—C2A—C3A | 178.1 (3) |
| O24—Cl2—O21—Cu1 | −75.8 (2) | C6A—C1A—C2A—C3A | −2.1 (5) |
| O22—Cl2—O21—Cu1 | 44.1 (2) | C1A—C2A—C3A—C4A | 2.3 (6) |
| O23—Cl2—O21—Cu1 | 163.3 (2) | C2A—C3A—C4A—C5A | −0.5 (7) |
| O1B—Cu1—O21—Cl2 | 13.46 (18) | C3A—C4A—C5A—C6A | −1.6 (7) |
| O1A—Cu1—O21—Cl2 | −67.94 (18) | O1A—C1A—C6A—C5A | 179.9 (3) |
| N2A—Cu1—O21—Cl2 | 116.36 (18) | C2A—C1A—C6A—C5A | 0.1 (5) |
| N1A—Cu1—O21—Cl2 | −161.18 (18) | O1A—C1A—C6A—C7A | 1.2 (4) |
| O11—Cu1—O21—Cl2 | −41.3 (4) | C2A—C1A—C6A—C7A | −178.6 (3) |
| Cu2—Cu1—O21—Cl2 | −27.31 (17) | C4A—C5A—C6A—C1A | 1.7 (6) |
| O24—Cl2—O22—Cu2 | 80.6 (2) | C4A—C5A—C6A—C7A | −179.6 (4) |
| O23—Cl2—O22—Cu2 | −157.54 (17) | C1A—C6A—C7A—N1A | 58.6 (4) |
| O21—Cl2—O22—Cu2 | −38.9 (2) | C5A—C6A—C7A—N1A | −120.1 (3) |
| O1A—Cu2—O22—Cl2 | 58.62 (17) | C8A—N1A—C7A—C6A | 175.9 (2) |
| O1B—Cu2—O22—Cl2 | −23.06 (16) | Cu1—N1A—C7A—C6A | −63.1 (3) |
| N2B—Cu2—O22—Cl2 | 161.29 (17) | C7A—N1A—C8A—C9A | 168.9 (2) |
| N1B—Cu2—O22—Cl2 | −116.82 (18) | Cu1—N1A—C8A—C9A | 44.1 (3) |
| O12—Cu2—O22—Cl2 | 8.1 (5) | C13A—N2A—C9A—C10A | −2.1 (5) |
| Cu1—Cu2—O22—Cl2 | 17.91 (15) | Cu1—N2A—C9A—C10A | −178.0 (3) |
| O1B—Cu1—O1A—C1A | −154.0 (2) | C13A—N2A—C9A—C8A | 176.9 (3) |
| N2A—Cu1—O1A—C1A | −0.9 (12) | Cu1—N2A—C9A—C8A | 1.0 (3) |
| N1A—Cu1—O1A—C1A | 33.3 (2) | N1A—C8A—C9A—N2A | −30.5 (4) |
| O21—Cu1—O1A—C1A | −65.3 (2) | N1A—C8A—C9A—C10A | 148.5 (4) |
| O11—Cu1—O1A—C1A | 121.1 (2) | N2A—C9A—C10A—C11A | 1.0 (6) |
| Cu2—Cu1—O1A—C1A | −153.7 (2) | C8A—C9A—C10A—C11A | −178.0 (4) |
| O1B—Cu1—O1A—Cu2 | −0.29 (8) | C9A—C10A—C11A—C12A | 1.2 (7) |
| N2A—Cu1—O1A—Cu2 | 152.8 (11) | C10A—C11A—C12A—C13A | −2.1 (7) |

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|---|---|---|---|
| N1A—Cu1—O1A—Cu2 | −173.02 (9) | C9A—N2A—C13A—C12A | 1.2 (5) |
| O21—Cu1—O1A—Cu2 | 88.42 (8) | Cu1—N2A—C13A—C12A | 176.3 (3) |
| O11—Cu1—O1A—Cu2 | −85.20 (8) | C11A—C12A—C13A—N2A | 1.0 (6) |
| O1B—Cu2—O1A—C1A | 148.3 (2) | Cu1—O1B—C1B—C2B | 10.3 (4) |
| N2B—Cu2—O1A—C1A | −32.8 (3) | Cu2—O1B—C1B—C2B | −130.8 (3) |
| N1B—Cu2—O1A—C1A | 95.8 (6) | Cu1—O1B—C1B—C6B | −169.7 (2) |
| O12—Cu2—O1A—C1A | −124.1 (2) | Cu2—O1B—C1B—C6B | 49.2 (3) |
| O22—Cu2—O1A—C1A | 65.7 (2) | O1B—C1B—C2B—C3B | −178.7 (3) |
| Cu1—Cu2—O1A—C1A | 148.0 (3) | C6B—C1B—C2B—C3B | 1.3 (5) |
| O1B—Cu2—O1A—Cu1 | 0.29 (8) | C1B—C2B—C3B—C4B | −1.9 (6) |
| N2B—Cu2—O1A—Cu1 | 179.15 (9) | C2B—C3B—C4B—C5B | 0.5 (6) |
| N1B—Cu2—O1A—Cu1 | −52.3 (6) | C3B—C4B—C5B—C6B | 1.5 (7) |
| O12—Cu2—O1A—Cu1 | 87.84 (9) | C4B—C5B—C6B—C1B | −2.1 (6) |
| O22—Cu2—O1A—Cu1 | −82.38 (9) | C4B—C5B—C6B—C7B | 179.1 (4) |
| O1A—Cu1—O1B—C1B | −146.2 (2) | O1B—C1B—C6B—C5B | −179.4 (3) |
| N2A—Cu1—O1B—C1B | 36.0 (3) | C2B—C1B—C6B—C5B | 0.6 (5) |
| N1A—Cu1—O1B—C1B | −90.1 (7) | O1B—C1B—C6B—C7B | −0.5 (4) |
| O21—Cu1—O1B—C1B | 127.3 (2) | C2B—C1B—C6B—C7B | 179.5 (3) |
| O11—Cu1—O1B—C1B | −64.3 (2) | C5B—C6B—C7B—N1B | 119.9 (3) |
| Cu2—Cu1—O1B—C1B | −146.5 (3) | C1B—C6B—C7B—N1B | −58.9 (4) |
| O1A—Cu1—O1B—Cu2 | 0.29 (8) | C8B—N1B—C7B—C6B | −177.3 (2) |
| N2A—Cu1—O1B—Cu2 | −177.50 (9) | Cu2—N1B—C7B—C6B | 62.1 (3) |
| N1A—Cu1—O1B—Cu2 | 56.4 (7) | C7B—N1B—C8B—C9B | −168.9 (2) |
| O21—Cu1—O1B—Cu2 | −86.17 (9) | Cu2—N1B—C8B—C9B | −43.9 (3) |
| O11—Cu1—O1B—Cu2 | 82.23 (8) | C13B—N2B—C9B—C10B | 2.6 (5) |
| O1A—Cu2—O1B—C1B | 152.1 (2) | Cu2—N2B—C9B—C10B | −179.7 (3) |
| N2B—Cu2—O1B—C1B | −13.7 (13) | C13B—N2B—C9B—C8B | −176.6 (3) |
| N1B—Cu2—O1B—C1B | −35.1 (2) | Cu2—N2B—C9B—C8B | 1.2 (3) |
| O12—Cu2—O1B—C1B | 64.0 (2) | N1B—C8B—C9B—N2B | 28.9 (4) |
| O22—Cu2—O1B—C1B | −122.5 (2) | N1B—C8B—C9B—C10B | −150.3 (4) |
| Cu1—Cu2—O1B—C1B | 152.4 (2) | N2B—C9B—C10B—C11B | −0.3 (6) |
| O1A—Cu2—O1B—Cu1 | −0.29 (8) | C8B—C9B—C10B—C11B | 178.8 (4) |
| N2B—Cu2—O1B—Cu1 | −166.1 (11) | C9B—C10B—C11B—C12B | −2.6 (8) |
| N1B—Cu2—O1B—Cu1 | 172.48 (9) | C10B—C11B—C12B—C13B | 3.1 (8) |
| O12—Cu2—O1B—Cu1 | −88.38 (8) | C9B—N2B—C13B—C12B | −2.0 (5) |
| O22—Cu2—O1B—Cu1 | 85.08 (8) | Cu2—N2B—C13B—C12B | −179.4 (3) |
| O1B—Cu1—N1A—C8A | 91.5 (7) | C11B—C12B—C13B—N2B | −0.9 (6) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1*A*—H1*AA*···O23$^{i}$ | 0.93 | 2.05 | 2.913 (4) | 154 |
| N1*B*—H1*BA*···O14$^{ii}$ | 0.93 | 2.09 | 2.943 (4) | 152 |
| C7*B*—H7*BA*···O14$^{iii}$ | 0.99 | 2.53 | 3.167 (4) | 122 |
| C22*S*—H22*H*···O13$^{iv}$ | 0.98 | 2.47 | 3.264 (8) | 138 |
| C7*A*—H7*AB*···O23$^{v}$ | 0.99 | 2.48 | 3.143 (4) | 124 |

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|---|---|---|---|---|
| C4*A*—H4*AA*···N1*S* | 0.95 | 2.69 | 3.643 (7) | 175 |
| C12*B*—H12*B*···N2*S* | 0.95 | 2.67 | 3.616 (9) | 171 |

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