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# *trans*-Bis(*N*-{2-[2-(3-methyl-1*H*-pyrazol-5-yl-$\kappa N^2$)-acetamido-$\kappa O$]phenyl}benzamide)bis(perchlorato-$\kappa O$)copper(II)

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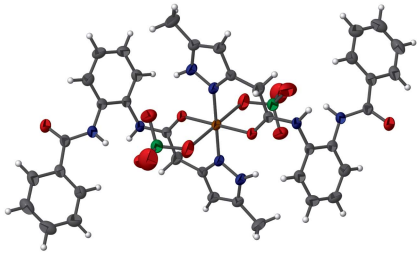
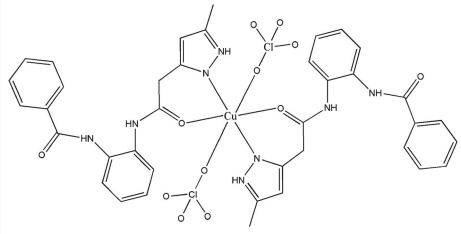
**Structural data**: full structural data are available from iucrdata.iucr.org

In the centrosymmetric title compound, $[Cu(C_{19}H_{18}N_4O_2)_2(ClO_4)_2]$, the copper ion sits at the center of an axially elongated octahedron with monodentate perchlorate ions weakly coordinated in the axial positions. In the crystal, chains running parallel to (001) are formed by N—H···O hydrogen bonds; these chains are linked into sheets parallel to (101) by C—H···O interactions.

**3D view**



**Chemical scheme**



## Structure description

Pyrazolylacetamide derivatives have been evaluated for their *in vitro* activity as anti-mycobacterial agents against *Mycobacterium smegmatis* and also as anti-tuberculosis agents with low cytotoxicity (Emmadi *et al.*, 2015). They also have therapeutic properties for the treatment of *Cryptosporidium* parasites (Sun *et al.*, 2014). Their metal complexes have proven antimicrobial activities (Dholakiya *et al.*, 2004) and may also have applications in catalysis (Jia *et al.*, 2004). Continuing our research in this field (Chkirate *et al.*, 2001), we have synthesized a copper perchlorate complex having as a ligand *trans*-bis-*N*-{2-[2-(5-methyl-1*H*-pyrazol-3-yl)acetamido]phenyl}benzamide obtained by reacting benzoyl chloride with *N*-2-aminophenyl-5-methyl-pyrazol-3-yl acetamide, the latter being obtained by the action of hydrazine on 4-(oxopropylidene)-1,5-benzodiazepin-2-one (El Abbassi *et al.*, 1989).

The title compound (Fig. 1) has crystallographically imposed inversion symmetry with the organic ligands chelating through the tertiary nitrogen of the imidazole moiety (N1) and the oxygen (O1) of the proximate carbonyl group. Weak coordination of the

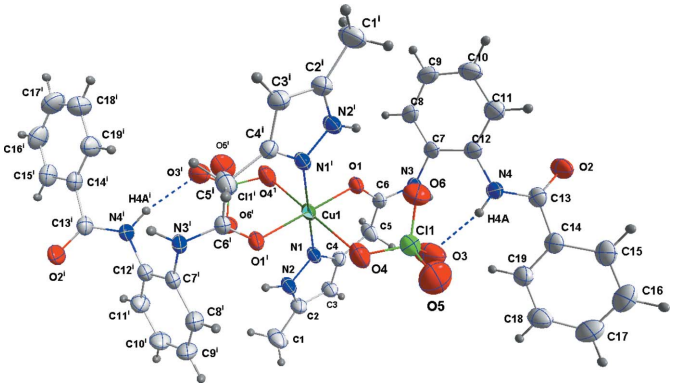



**Figure 1**
The title molecule with labeling scheme and 50% probability ellipsoids [symmetry code (i): $-x+1, -y+1, -z+1$]. Intramolecular hydrogen bonds are shown as dashed lines.

perchlorate anions completes an axially elongated octahedral environment about the copper. The axial Cu1—O4 distance of 2.505 (3) Å is considerably longer than the equatorial Cu1—O1 distance of 1.9653 (17) Å, which is consistent with the action of the Jahn–Teller effect and is within the range 2.483 (13)–2.621 (6) Å previously cited for copper-bound perchlorate ions (Hueso-Ureña *et al.*, 1999; Hong *et al.*, 1987; Lu *et al.*, 1987; Holló *et al.*, 2013).

In the crystal, pairwise N3—H3*A*···O2$^{i}$ hydrogen bonds form chains of complexes running parallel to the *c* axis, which are then associated *via* weak, pairwise C5—H5*A*···O2$^{ii}$ hydrogen bonds, forming layers parallel to (101) (Table 1 and Fig. 2).

## Synthesis and crystallization

0.125 mmol of $Cu(ClO_4)_2\cdot 6H_2O$ dissolved in 2.5 ml of ethanol were added to a solution of 5 ml of methanol containing 0.25 mmol of *trans*-bis-*N*-{2-[2-(5-methyl-1*H*-pyrazol-3-yl)-acetamido]phenyl}benzamide. The mixture was heated slightly and then left at room temperature. After filtration, blue–green single crystals were obtained.

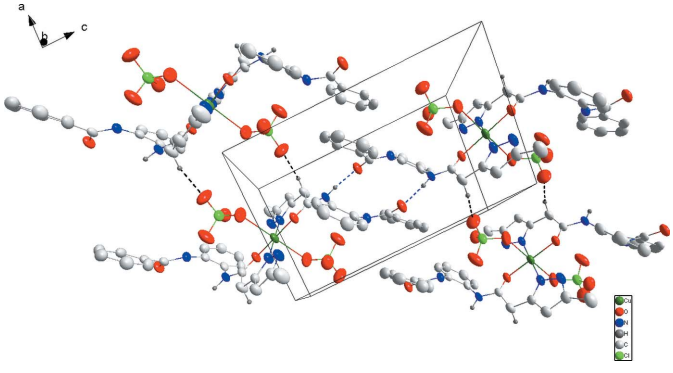



**Figure 2**
Packing diagram showing the pairwise N—H···O and C—H···O hydrogen bonds as, respectively, blue and black dashed lines.

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3*A*···O2$^{i}$ | 0.91 | 1.97 | 2.870 (3) | 171 |
| N4—H4*A*···O3 | 0.91 | 2.08 | 2.971 (3) | 166 |
| C5—H5*A*···O5$^{ii}$ | 0.99 | 2.48 | 3.358 (4) | 148 |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[Cu(C_{19}H_{18}N_4O_2)_2(ClO_4)_2]$ |
| $M_r$ | 931.19 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 298 |
| *a*, *b*, *c* (Å) | 8.6572 (2), 8.8108 (2), 14.2054 (3) |
| $\alpha, \beta, \gamma$ (°) | 79.406 (1), 86.240 (1), 67.895 (1) |
| *V* (Å$^3$) | 986.78 (4) |
| *Z* | 1 |
| Radiation type | Cu *Kα* |
| $\mu$ (mm$^{-1}$) | 2.68 |
| Crystal size (mm) | 0.24 × 0.06 × 0.02 |
| | |
| Data collection | |
| Diffractometer | Bruker D8 VENTURE PHOTON 100 CMOS |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2016) |
| $T_{min}$, $T_{max}$ | 0.77, 0.95 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 7804, 3702, 2999 |
| $R_{int}$ | 0.033 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.617 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.044, 0.118, 1.04 |
| No. of reflections | 3702 |
| No. of parameters | 278 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.41, −0.51 |

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL 2014/7* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

## Acknowledgements

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# full crystallographic data

*IUCrData* (2017). **2**, x170285 [https://doi.org/10.1107/S2414314617002851]

## *trans*-Bis(*N*-{2-[2-(3-methyl-1*H*-pyrazol-5-yl-$\kappa N^2$)acetamido-$\kappa O$]phenyl}-benzamide)bis(perchlorato-$\kappa O$)copper(II)

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*Crystal data*

$[Cu(C_{19}H_{18}N_4O_2)_2(ClO_4)_2]$
$M_r$ = 931.19
Triclinic, $P\overline{1}$
$a$ = 8.6572 (2) Å
$b$ = 8.8108 (2) Å
$c$ = 14.2054 (3) Å
$\alpha$ = 79.406 (1)°
$\beta$ = 86.240 (1)°
$\gamma$ = 67.895 (1)°
$V$ = 986.78 (4) Å$^3$
$Z$ = 1
$F(000)$ = 479
$D_x$ = 1.567 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54178 Å
Cell parameters from 5387 reflections
$\theta$ = 5.5–71.9°
$\mu$ = 2.68 mm$^{-1}$
$T$ = 298 K
Plate, pale green-blue
0.24 × 0.06 × 0.02 mm

*Data collection*

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC I$\mu$S micro–focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
$T_{min}$ = 0.77, $T_{max}$ = 0.95
7804 measured reflections
3702 independent reflections
2999 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033
$\theta_{max}$ = 71.9°, $\theta_{min}$ = 3.2°
$h$ = −10→10
$k$ = −10→10
$l$ = −17→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.118
$S$ = 1.04
3702 reflections
278 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0604P)^2 + 0.5402P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.51 e Å$^{-3}$

*Special details*

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

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on $F^2$, conventional R-factors R are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.98 Å) while those attached to nitrogen were placed in locations derived from a difference map and their parameters adjusted to give N—H = 0.91 Å. All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.5000 | 0.5000 | 0.0000 | 0.03299 (17) |
| O1 | 0.5561 (2) | 0.5620 (2) | 0.11555 (12) | 0.0359 (4) |
| O2 | 0.2816 (3) | 0.6621 (3) | 0.54249 (14) | 0.0454 (5) |
| N1 | 0.6439 (3) | 0.2722 (3) | 0.04252 (15) | 0.0348 (5) |
| N2 | 0.6726 (3) | 0.1487 (3) | −0.00892 (16) | 0.0393 (5) |
| H2 | 0.6280 | 0.1756 | −0.0688 | 0.047* |
| N3 | 0.5944 (3) | 0.5296 (3) | 0.27323 (14) | 0.0312 (5) |
| H3A | 0.6406 | 0.4602 | 0.3283 | 0.037* |
| N4 | 0.3221 (3) | 0.5880 (3) | 0.39480 (15) | 0.0331 (5) |
| H4A | 0.3106 | 0.5185 | 0.3580 | 0.040* |
| C1 | 0.8316 (5) | −0.1514 (4) | −0.0073 (3) | 0.0580 (9) |
| H1A | 0.8567 | −0.1261 | −0.0753 | 0.087* |
| H1B | 0.7407 | −0.1934 | −0.0007 | 0.087* |
| H1C | 0.9310 | −0.2360 | 0.0259 | 0.087* |
| C2 | 0.7805 (4) | 0.0020 (3) | 0.0353 (2) | 0.0388 (6) |
| C3 | 0.8220 (4) | 0.0325 (3) | 0.1198 (2) | 0.0386 (6) |
| H3 | 0.8957 | −0.0464 | 0.1676 | 0.046* |
| C4 | 0.7359 (3) | 0.2003 (3) | 0.12200 (18) | 0.0308 (5) |
| C5 | 0.7426 (4) | 0.2942 (4) | 0.1983 (2) | 0.0439 (7) |
| H5A | 0.8567 | 0.2945 | 0.1991 | 0.053* |
| H5B | 0.7253 | 0.2313 | 0.2607 | 0.053* |
| C6 | 0.6223 (3) | 0.4703 (3) | 0.19184 (17) | 0.0295 (5) |
| C7 | 0.4904 (3) | 0.6970 (3) | 0.28058 (17) | 0.0306 (5) |
| C8 | 0.5246 (4) | 0.8292 (4) | 0.2270 (2) | 0.0403 (6) |
| H8 | 0.6167 | 0.8088 | 0.1844 | 0.048* |
| C9 | 0.4245 (4) | 0.9903 (4) | 0.2358 (2) | 0.0466 (7) |
| H9 | 0.4472 | 1.0810 | 0.1990 | 0.056* |
| C10 | 0.2916 (4) | 1.0194 (4) | 0.2981 (2) | 0.0473 (7) |
| H10 | 0.2222 | 1.1304 | 0.3035 | 0.057* |
| C11 | 0.2587 (4) | 0.8881 (4) | 0.3527 (2) | 0.0414 (6) |
| H11 | 0.1683 | 0.9093 | 0.3964 | 0.050* |
| C12 | 0.3569 (3) | 0.7258 (3) | 0.34409 (18) | 0.0317 (5) |
| C13 | 0.2845 (3) | 0.5649 (3) | 0.48871 (18) | 0.0326 (6) |

| | | | | |
|---|---|---|---|---|
| C14 | 0.2482 (3) | 0.4123 (3) | 0.52507 (18) | 0.0332 (6) |
| C15 | 0.1334 (4) | 0.4169 (4) | 0.5994 (2) | 0.0414 (7) |
| H15 | 0.0806 | 0.5160 | 0.6252 | 0.050* |
| C16 | 0.0962 (4) | 0.2784 (4) | 0.6353 (2) | 0.0508 (8) |
| H16 | 0.0173 | 0.2825 | 0.6854 | 0.061* |
| C17 | 0.1736 (4) | 0.1337 (4) | 0.5985 (3) | 0.0534 (8) |
| H17 | 0.1473 | 0.0385 | 0.6229 | 0.064* |
| C18 | 0.2895 (4) | 0.1271 (4) | 0.5261 (2) | 0.0501 (8) |
| H18 | 0.3442 | 0.0266 | 0.5019 | 0.060* |
| C19 | 0.3261 (4) | 0.2659 (4) | 0.4889 (2) | 0.0427 (7) |
| H19 | 0.4048 | 0.2611 | 0.4386 | 0.051* |
| Cl1 | 0.18597 (9) | 0.49021 (9) | 0.17026 (5) | 0.04040 (19) |
| O3 | 0.3013 (4) | 0.3972 (3) | 0.24714 (19) | 0.0717 (8) |
| O4 | 0.2600 (3) | 0.4391 (3) | 0.08272 (17) | 0.0620 (7) |
| O5 | 0.0374 (4) | 0.4586 (4) | 0.1863 (2) | 0.0851 (10) |
| O6 | 0.1550 (3) | 0.6626 (3) | 0.16559 (18) | 0.0596 (6) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0478 (3) | 0.0250 (3) | 0.0209 (3) | −0.0060 (2) | −0.0055 (2) | −0.0057 (2) |
| O1 | 0.0507 (11) | 0.0292 (10) | 0.0232 (9) | −0.0084 (9) | −0.0034 (8) | −0.0060 (7) |
| O2 | 0.0662 (14) | 0.0425 (12) | 0.0283 (10) | −0.0184 (10) | −0.0031 (9) | −0.0111 (8) |
| N1 | 0.0480 (13) | 0.0280 (11) | 0.0256 (11) | −0.0087 (10) | −0.0030 (9) | −0.0087 (9) |
| N2 | 0.0564 (15) | 0.0291 (12) | 0.0289 (12) | −0.0089 (11) | −0.0070 (10) | −0.0092 (9) |
| N3 | 0.0427 (12) | 0.0303 (11) | 0.0198 (10) | −0.0117 (10) | −0.0036 (8) | −0.0051 (8) |
| N4 | 0.0434 (13) | 0.0344 (12) | 0.0246 (11) | −0.0173 (10) | 0.0019 (9) | −0.0074 (9) |
| C1 | 0.081 (3) | 0.0332 (17) | 0.054 (2) | −0.0087 (16) | −0.0120 (17) | −0.0168 (14) |
| C2 | 0.0506 (17) | 0.0272 (14) | 0.0359 (15) | −0.0106 (13) | 0.0000 (12) | −0.0071 (11) |
| C3 | 0.0479 (17) | 0.0264 (14) | 0.0352 (14) | −0.0066 (12) | −0.0067 (12) | −0.0032 (11) |
| C4 | 0.0361 (14) | 0.0270 (13) | 0.0256 (12) | −0.0083 (11) | 0.0002 (10) | −0.0032 (10) |
| C5 | 0.0532 (18) | 0.0367 (16) | 0.0332 (15) | −0.0029 (14) | −0.0118 (12) | −0.0110 (12) |
| C6 | 0.0359 (14) | 0.0306 (13) | 0.0233 (12) | −0.0132 (11) | −0.0021 (10) | −0.0049 (10) |
| C7 | 0.0417 (14) | 0.0328 (13) | 0.0209 (12) | −0.0160 (12) | −0.0037 (10) | −0.0073 (10) |
| C8 | 0.0558 (18) | 0.0401 (16) | 0.0303 (14) | −0.0235 (14) | 0.0018 (12) | −0.0071 (11) |
| C9 | 0.070 (2) | 0.0330 (15) | 0.0412 (16) | −0.0250 (15) | −0.0026 (14) | −0.0038 (12) |
| C10 | 0.063 (2) | 0.0284 (15) | 0.0489 (18) | −0.0125 (14) | −0.0039 (14) | −0.0105 (12) |
| C11 | 0.0467 (17) | 0.0371 (16) | 0.0394 (16) | −0.0128 (13) | 0.0009 (12) | −0.0103 (12) |
| C12 | 0.0410 (14) | 0.0321 (13) | 0.0250 (12) | −0.0157 (12) | −0.0045 (10) | −0.0059 (10) |
| C13 | 0.0336 (14) | 0.0356 (14) | 0.0251 (13) | −0.0086 (11) | −0.0033 (10) | −0.0048 (10) |
| C14 | 0.0349 (14) | 0.0389 (15) | 0.0246 (13) | −0.0126 (12) | −0.0043 (10) | −0.0029 (10) |
| C15 | 0.0366 (15) | 0.0518 (18) | 0.0303 (14) | −0.0113 (14) | −0.0006 (11) | −0.0046 (12) |
| C16 | 0.0439 (17) | 0.063 (2) | 0.0400 (17) | −0.0213 (16) | 0.0019 (13) | 0.0063 (15) |
| C17 | 0.0522 (19) | 0.052 (2) | 0.055 (2) | −0.0258 (17) | −0.0059 (15) | 0.0094 (15) |
| C18 | 0.059 (2) | 0.0389 (17) | 0.0511 (19) | −0.0185 (15) | −0.0025 (15) | −0.0044 (14) |
| C19 | 0.0499 (17) | 0.0412 (16) | 0.0358 (15) | −0.0161 (14) | 0.0061 (12) | −0.0071 (12) |
| Cl1 | 0.0501 (4) | 0.0418 (4) | 0.0345 (4) | −0.0215 (3) | 0.0020 (3) | −0.0100 (3) |
| O3 | 0.112 (2) | 0.0494 (15) | 0.0563 (15) | −0.0322 (15) | −0.0350 (15) | 0.0010 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O4 | 0.0802 (17) | 0.0741 (17) | 0.0506 (14) | −0.0426 (14) | 0.0204 (12) | −0.0341 (12) |
| O5 | 0.0719 (18) | 0.116 (3) | 0.098 (2) | −0.0652 (19) | 0.0271 (16) | −0.0364 (19) |
| O6 | 0.0726 (16) | 0.0368 (12) | 0.0646 (15) | −0.0147 (12) | 0.0087 (12) | −0.0122 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—N1$^{i}$ | 1.928 (2) | C5—H5B | 0.9900 |
| Cu1—N1 | 1.928 (2) | C7—C8 | 1.388 (4) |
| Cu1—O1 | 1.9652 (17) | C7—C12 | 1.393 (4) |
| Cu1—O1$^{i}$ | 1.9653 (17) | C8—C9 | 1.381 (4) |
| Cu1—O4 | 2.505 (3) | C8—H8 | 0.9500 |
| O1—C6 | 1.252 (3) | C9—C10 | 1.378 (5) |
| O2—C13 | 1.241 (3) | C9—H9 | 0.9500 |
| N1—C4 | 1.336 (3) | C10—C11 | 1.382 (4) |
| N1—N2 | 1.358 (3) | C10—H10 | 0.9500 |
| N2—C2 | 1.345 (4) | C11—C12 | 1.385 (4) |
| N2—H2 | 0.9099 | C11—H11 | 0.9500 |
| N3—C6 | 1.326 (3) | C13—C14 | 1.488 (4) |
| N3—C7 | 1.429 (3) | C14—C19 | 1.388 (4) |
| N3—H3A | 0.9099 | C14—C15 | 1.397 (4) |
| N4—C13 | 1.349 (3) | C15—C16 | 1.378 (4) |
| N4—C12 | 1.418 (3) | C15—H15 | 0.9500 |
| N4—H4A | 0.9099 | C16—C17 | 1.379 (5) |
| C1—C2 | 1.486 (4) | C16—H16 | 0.9500 |
| C1—H1A | 0.9800 | C17—C18 | 1.382 (5) |
| C1—H1B | 0.9800 | C17—H17 | 0.9500 |
| C1—H1C | 0.9800 | C18—C19 | 1.381 (4) |
| C2—C3 | 1.374 (4) | C18—H18 | 0.9500 |
| C3—C4 | 1.389 (4) | C19—H19 | 0.9500 |
| C3—H3 | 0.9500 | Cl1—O5 | 1.411 (3) |
| C4—C5 | 1.495 (4) | Cl1—O6 | 1.429 (2) |
| C5—C6 | 1.498 (4) | Cl1—O4 | 1.430 (2) |
| C5—H5A | 0.9900 | Cl1—O3 | 1.435 (3) |
| | | | |
| N1$^{i}$—Cu1—N1 | 180.0 | C8—C7—N3 | 120.4 (2) |
| N1$^{i}$—Cu1—O1 | 89.97 (8) | C12—C7—N3 | 119.1 (2) |
| N1—Cu1—O1 | 90.03 (8) | C9—C8—C7 | 119.8 (3) |
| N1$^{i}$—Cu1—O1$^{i}$ | 90.03 (8) | C9—C8—H8 | 120.1 |
| N1—Cu1—O1$^{i}$ | 89.97 (8) | C7—C8—H8 | 120.1 |
| O1—Cu1—O1$^{i}$ | 180.0 | C10—C9—C8 | 120.0 (3) |
| C6—O1—Cu1 | 129.02 (17) | C10—C9—H9 | 120.0 |
| C4—N1—N2 | 105.5 (2) | C8—C9—H9 | 120.0 |
| C4—N1—Cu1 | 130.81 (17) | C9—C10—C11 | 120.4 (3) |
| N2—N1—Cu1 | 123.71 (17) | C9—C10—H10 | 119.8 |
| C2—N2—N1 | 112.2 (2) | C11—C10—H10 | 119.8 |
| C2—N2—H2 | 128.9 | C10—C11—C12 | 120.4 (3) |
| N1—N2—H2 | 118.5 | C10—C11—H11 | 119.8 |
| C6—N3—C7 | 123.7 (2) | C12—C11—H11 | 119.8 |

| | | | |
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| C6—N3—H3A | 119.1 | C11—C12—C7 | 119.0 (3) |
| C7—N3—H3A | 117.2 | C11—C12—N4 | 122.2 (3) |
| C13—N4—C12 | 125.5 (2) | C7—C12—N4 | 118.8 (2) |
| C13—N4—H4A | 118.6 | O2—C13—N4 | 123.1 (3) |
| C12—N4—H4A | 115.3 | O2—C13—C14 | 121.4 (2) |
| C2—C1—H1A | 109.5 | N4—C13—C14 | 115.5 (2) |
| C2—C1—H1B | 109.5 | C19—C14—C15 | 119.2 (3) |
| H1A—C1—H1B | 109.5 | C19—C14—C13 | 122.4 (3) |
| C2—C1—H1C | 109.5 | C15—C14—C13 | 118.4 (3) |
| H1A—C1—H1C | 109.5 | C16—C15—C14 | 120.3 (3) |
| H1B—C1—H1C | 109.5 | C16—C15—H15 | 119.8 |
| N2—C2—C3 | 105.6 (2) | C14—C15—H15 | 119.8 |
| N2—C2—C1 | 122.0 (3) | C15—C16—C17 | 120.0 (3) |
| C3—C2—C1 | 132.4 (3) | C15—C16—H16 | 120.0 |
| C2—C3—C4 | 107.1 (2) | C17—C16—H16 | 120.0 |
| C2—C3—H3 | 126.4 | C16—C17—C18 | 120.1 (3) |
| C4—C3—H3 | 126.4 | C16—C17—H17 | 120.0 |
| N1—C4—C3 | 109.6 (2) | C18—C17—H17 | 120.0 |
| N1—C4—C5 | 122.9 (2) | C19—C18—C17 | 120.3 (3) |
| C3—C4—C5 | 127.4 (2) | C19—C18—H18 | 119.8 |
| C4—C5—C6 | 118.1 (2) | C17—C18—H18 | 119.8 |
| C4—C5—H5A | 107.8 | C18—C19—C14 | 120.0 (3) |
| C6—C5—H5A | 107.8 | C18—C19—H19 | 120.0 |
| C4—C5—H5B | 107.8 | C14—C19—H19 | 120.0 |
| C6—C5—H5B | 107.8 | O5—Cl1—O6 | 111.27 (18) |
| H5A—C5—H5B | 107.1 | O5—Cl1—O4 | 109.48 (17) |
| O1—C6—N3 | 120.3 (2) | O6—Cl1—O4 | 109.57 (15) |
| O1—C6—C5 | 124.1 (2) | O5—Cl1—O3 | 109.7 (2) |
| N3—C6—C5 | 115.5 (2) | O6—Cl1—O3 | 108.17 (15) |
| C8—C7—C12 | 120.4 (2) | O4—Cl1—O3 | 108.60 (18) |

| | | | |
|---|---|---|---|
| C4—N1—N2—C2 | −0.5 (3) | C8—C9—C10—C11 | 0.7 (5) |
| Cu1—N1—N2—C2 | 178.5 (2) | C9—C10—C11—C12 | −1.3 (5) |
| N1—N2—C2—C3 | 0.6 (3) | C10—C11—C12—C7 | 0.9 (4) |
| N1—N2—C2—C1 | −179.8 (3) | C10—C11—C12—N4 | −176.5 (3) |
| N2—C2—C3—C4 | −0.5 (3) | C8—C7—C12—C11 | 0.2 (4) |
| C1—C2—C3—C4 | −180.0 (3) | N3—C7—C12—C11 | 178.5 (2) |
| N2—N1—C4—C3 | 0.2 (3) | C8—C7—C12—N4 | 177.6 (2) |
| Cu1—N1—C4—C3 | −178.8 (2) | N3—C7—C12—N4 | −4.1 (3) |
| N2—N1—C4—C5 | 179.0 (3) | C13—N4—C12—C11 | −46.5 (4) |
| Cu1—N1—C4—C5 | 0.1 (4) | C13—N4—C12—C7 | 136.2 (3) |
| C2—C3—C4—N1 | 0.2 (3) | C12—N4—C13—O2 | −2.4 (4) |
| C2—C3—C4—C5 | −178.6 (3) | C12—N4—C13—C14 | 178.4 (2) |
| N1—C4—C5—C6 | 9.1 (4) | O2—C13—C14—C19 | −146.2 (3) |
| C3—C4—C5—C6 | −172.3 (3) | N4—C13—C14—C19 | 33.1 (4) |
| Cu1—O1—C6—N3 | −153.74 (19) | O2—C13—C14—C15 | 32.7 (4) |
| Cu1—O1—C6—C5 | 29.7 (4) | N4—C13—C14—C15 | −148.0 (3) |
| C7—N3—C6—O1 | −0.1 (4) | C19—C14—C15—C16 | −1.0 (4) |

| | | | |
|---|---|---|---|
| C7—N3—C6—C5 | 176.8 (2) | C13—C14—C15—C16 | −179.9 (2) |
| C4—C5—C6—O1 | −24.4 (4) | C14—C15—C16—C17 | 0.6 (4) |
| C4—C5—C6—N3 | 158.8 (3) | C15—C16—C17—C18 | 0.5 (5) |
| C6—N3—C7—C8 | −58.0 (3) | C16—C17—C18—C19 | −1.3 (5) |
| C6—N3—C7—C12 | 123.7 (3) | C17—C18—C19—C14 | 0.9 (5) |
| C12—C7—C8—C9 | −0.8 (4) | C15—C14—C19—C18 | 0.2 (4) |
| N3—C7—C8—C9 | −179.1 (2) | C13—C14—C19—C18 | 179.1 (3) |
| C7—C8—C9—C10 | 0.4 (4) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3*A*···O2$^{ii}$ | 0.91 | 1.97 | 2.870 (3) | 171 |
| N4—H4*A*···O3 | 0.91 | 2.08 | 2.971 (3) | 166 |
| C5—H5*A*···O5$^{iii}$ | 0.99 | 2.48 | 3.358 (4) | 148 |

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