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Chlorido(1,10-phenanthroline)(1*H*-1,2,4-triazole-3-carboxylato)copper(II)

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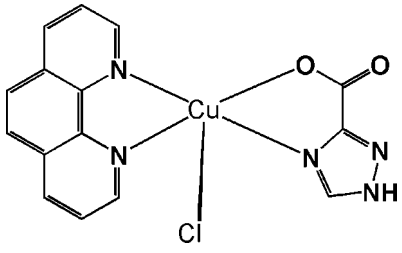
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.034; wR factor = 0.096; data-to-parameter ratio = 11.9.

The title complex, $[Cu(C_3H_2N_3O_2)Cl(C_{12}H_8N_2)]$, crystallizes with two independent molecules in the asymmetric unit. Each Cu^{II} atom is coordinated by an N atom and an O atom from the bidentate 1*H*-1,2,4-triazole-3-carboxylate ligand, two N atoms from the 1,10-phenanthroline ligand, and the Cl atom. The coordination geometry is based on a ClN_3O square pyramid. In the crystal structure, the molecules are linked by intermolecular N—H···O hydrogen bonds.

Related literature

For related literature, see: Guo & Wang (2005); Zhao *et al.* (2008).



Experimental

Crystal data

$[Cu(C_3H_2N_3O_2)Cl(C_{12}H_8N_2)]$
M_r = 391.27
Monoclinic, $P2_1/c$
a = 12.7302 (16) Å
b = 17.562 (3) Å
c = 14.299 (2) Å
β = 113.836 (2)°
V = 2924.2 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.70 mm^{-1}
T = 298 (2) K
0.53 × 0.49 × 0.47 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.467, T_{max} = 0.503
(expected range = 0.418–0.451)
14193 measured reflections
5142 independent reflections
3277 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.096
S = 1.04
5142 reflections
433 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O4^{i}	0.86	1.99	2.835 (4)	166
N7—H7···O2^{ii}	0.86	1.94	2.797 (4)	172

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: TK2217).

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Chlorido(1,10-phenanthroline)(1*H*-1,2,4-triazole-3-carboxylato)copper(II)

Jie Zhu, Xian-Hong Yin, Yu Feng, Shan-Shan Zhang, Kai Zhao and Cui-Wu Lin

S1. Comment

In connection with on-going studies in coordination chemistry (Zhao *et al.*, 2008) and the biological importance of triazole molecules (Guo & Wang, 2005), the crystal structure of a new ternary Cu(II) complex with 1*H*-1,2,4-triazole-3-carboxylate (TRIA), 1,10-phenanthroline (phen) and Cl is described.

Two independent mononuclear complex molecules, Cu(TRIA)(phen)Cl, comprise the asymmetric unit of (I), Fig. 1. Each Cu atom is chelated by a N atom and a O atom, derived from the TRIA anion, two N atoms from the chelating phen ligand, and the penta-coordinated coordination geometry is completed by a Cl atom. The latter atom occupies an axial position in the approximately square-pyramidal N_3OCl coordination geometry; the angles around the Cu(II) atom range from 81.66 (12) to 166.88 (12)°.

The primary intermolecular contacts in the crystal structure are of the type N—H···O and involve both amines and both of the non-coordinating carbonyls of the TRIA anions (Table 1).

S2. Experimental

$CuCl_2.2H_2O$ (0.5 mmol, 85.2 mg) dissolved in distilled water (15 ml) was added with stirring at 323 K to 1*H*-1,2,4-triazole-3-carboxylic acid (1 mmol, 113 mg) also dissolved in distilled water (5 ml). The resulting blue solution was allowed to react for 30 min and 1,10-phenanthroline (0.5 mmol, 99.1 mg) dissolved in ethanol (5 ml) was added. Dark-blue crystals suitable for X-ray analysis were obtained by slow evaporation over a period of one month (yield 85%). Analysis. Found: C 46.08, H 2.52, Cl 9.00, Cu 16.29, N 17.83, O 8.23%. $C_{15}H_{10}ClCuN_5O_2$ requires: C 46.04, H 2.58, Cl 9.06, Cu 16.24, N 17.90, O 8.18%.

S3. Refinement

The C– and N-bound H atoms were placed in calculated positions and included in the refinement in the riding-model approximation with N—H = 0.86 Å and C—H = 0.93 Å, and with U_{iso}(H) 1.2U_{eq}(C,*N*).

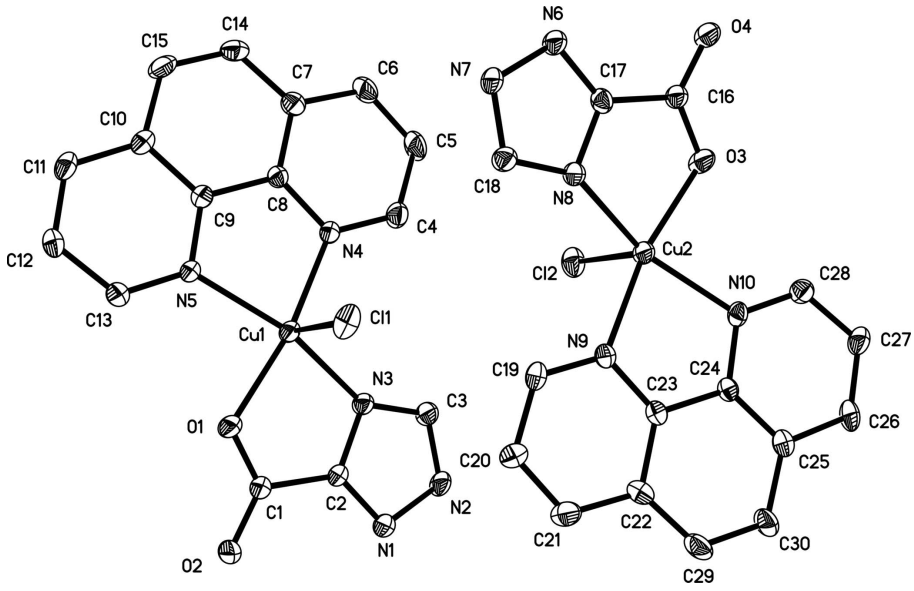

Figure 1

The molecular structures of the two independent molecules in (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme. The H atoms are omitted for clarity.

Chlorido(1,10-phenanthroline)(1*H*-1,2,4-triazole-3-carboxylato)copper(II)

Crystal data

$[Cu(C_3H_2N_3O_2)Cl(C_{12}H_8N_2)]$
$M_r = 391.27$
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Hall symbol: -P 2ybc
$a = 12.7302\ (16)$ Å
$b = 17.562\ (3)$ Å
$c = 14.299\ (2)$ Å
$\beta = 113.836\ (2)°$
$V = 2924.2\ (7)$ Å^3
$Z = 8$
$F(000) = 1576$
$D_x = 1.777$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4070 reflections
$\theta = 2.8–26.9°$
$\mu = 1.70$ mm^{-1}
$T = 298$ K
Prism, dark-blue
0.53 × 0.49 × 0.47 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.467$, $T_{max} = 0.503$
14193 measured reflections
5142 independent reflections
3277 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.8°$
$h = -9\rightarrow15$
$k = -20\rightarrow20$
$l = -17\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.096$
$S = 1.04$
5142 reflections
433 parameters
2 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

$w = 1/[\sigma^2(F_o^2) + (0.0357P)^2 + 2.079P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ 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	0.40914 (4)	0.59579 (2)	0.14980 (4)	0.03021 (14)
Cu2	0.09358 (4)	0.44546 (2)	0.35025 (4)	0.03027 (14)
Cl1	0.47137 (8)	0.60210 (6)	0.33526 (8)	0.0430 (3)
Cl2	0.02771 (8)	0.43345 (6)	0.16237 (8)	0.0435 (3)
N1	0.1523 (3)	0.75001 (18)	0.0769 (2)	0.0363 (8)
N2	0.0815 (3)	0.69152 (17)	0.0746 (2)	0.0344 (8)
H2	0.0109	0.6965	0.0657	0.041*
N3	0.2440 (2)	0.63748 (17)	0.1008 (2)	0.0289 (7)
N4	0.3832 (2)	0.48281 (16)	0.1427 (2)	0.0273 (7)
N5	0.5511 (2)	0.56362 (16)	0.1292 (2)	0.0259 (7)
N6	0.3479 (3)	0.29065 (17)	0.4200 (2)	0.0342 (8)
N7	0.4151 (3)	0.34806 (17)	0.4121 (2)	0.0336 (8)
H7	0.4843	0.3424	0.4171	0.040*
N8	0.2549 (2)	0.40305 (16)	0.3910 (2)	0.0290 (7)
N9	0.1178 (2)	0.55924 (16)	0.3493 (2)	0.0287 (7)
N10	−0.0475 (2)	0.47917 (17)	0.3696 (2)	0.0278 (7)
O1	0.4428 (2)	0.70196 (14)	0.1296 (2)	0.0413 (7)
O2	0.3680 (2)	0.81737 (15)	0.0851 (2)	0.0466 (8)
O3	0.0617 (2)	0.34048 (14)	0.3793 (2)	0.0399 (7)
O4	0.1371 (2)	0.22583 (14)	0.4277 (2)	0.0392 (7)
C1	0.3611 (3)	0.7493 (2)	0.1033 (3)	0.0322 (9)
C2	0.2492 (3)	0.7149 (2)	0.0931 (3)	0.0290 (9)
C3	0.1364 (3)	0.6260 (2)	0.0879 (3)	0.0329 (9)
H3	0.1041	0.5786	0.0882	0.039*
C4	0.2961 (3)	0.4431 (2)	0.1466 (3)	0.0375 (10)
H4	0.2342	0.4694	0.1497	0.045*
C5	0.2937 (4)	0.3643 (2)	0.1461 (3)	0.0473 (12)
H5	0.2307	0.3389	0.1485	0.057*
C6	0.3838 (4)	0.3233 (2)	0.1422 (3)	0.0436 (11)
H6	0.3830	0.2704	0.1429	0.052*

C7	0.4772 (3)	0.3632 (2)	0.1371 (3)	0.0341 (10)
C8	0.4721 (3)	0.4430 (2)	0.1373 (3)	0.0256 (9)
C9	0.5629 (3)	0.4865 (2)	0.1295 (3)	0.0251 (8)
C10	0.6570 (3)	0.4505 (2)	0.1219 (3)	0.0309 (9)
C11	0.7427 (3)	0.4971 (2)	0.1136 (3)	0.0365 (10)
H11	0.8074	0.4758	0.1090	0.044*
C12	0.7291 (3)	0.5749 (2)	0.1124 (3)	0.0353 (10)
H12	0.7844	0.6066	0.1061	0.042*
C13	0.6325 (3)	0.6063 (2)	0.1207 (3)	0.0319 (9)
H13	0.6250	0.6590	0.1201	0.038*
C14	0.5729 (4)	0.3277 (2)	0.1292 (3)	0.0427 (11)
H14	0.5765	0.2748	0.1288	0.051*
C15	0.6596 (3)	0.3685 (2)	0.1222 (3)	0.0422 (11)
H15	0.7216	0.3434	0.1176	0.051*
C16	0.1432 (3)	0.2929 (2)	0.4052 (3)	0.0295 (9)
C17	0.2519 (3)	0.3259 (2)	0.4067 (3)	0.0292 (9)
C18	0.3601 (3)	0.4141 (2)	0.3956 (3)	0.0319 (9)
H18	0.3904	0.4608	0.3883	0.038*
C19	0.2018 (3)	0.5979 (2)	0.3396 (3)	0.0366 (10)
H19	0.2658	0.5715	0.3412	0.044*
C20	0.1980 (4)	0.6772 (2)	0.3269 (3)	0.0417 (11)
H20	0.2584	0.7025	0.3197	0.050*
C21	0.1050 (3)	0.7171 (2)	0.3251 (3)	0.0408 (11)
H21	0.1012	0.7696	0.3159	0.049*
C22	0.0151 (3)	0.6776 (2)	0.3375 (3)	0.0326 (9)
C23	0.0260 (3)	0.5985 (2)	0.3494 (3)	0.0268 (9)
C24	−0.0622 (3)	0.5555 (2)	0.3619 (3)	0.0247 (8)
C25	−0.1584 (3)	0.5917 (2)	0.3659 (3)	0.0317 (9)
C26	−0.2413 (3)	0.5454 (2)	0.3793 (3)	0.0367 (10)
H26	−0.3067	0.5671	0.3819	0.044*
C27	−0.2255 (3)	0.4686 (2)	0.3884 (3)	0.0378 (10)
H27	−0.2793	0.4376	0.3984	0.045*
C28	−0.1272 (3)	0.4369 (2)	0.3826 (3)	0.0330 (9)
H28	−0.1174	0.3844	0.3880	0.040*
C29	−0.0847 (4)	0.7134 (2)	0.3396 (3)	0.0428 (11)
H29	−0.0931	0.7659	0.3310	0.051*
C30	−0.1669 (3)	0.6726 (2)	0.3536 (3)	0.0409 (10)
H30	−0.2305	0.6976	0.3554	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0245 (3)	0.0246 (3)	0.0455 (3)	0.0001 (2)	0.0183 (2)	−0.0029 (2)
Cu2	0.0238 (3)	0.0244 (3)	0.0463 (3)	0.0038 (2)	0.0181 (2)	0.0024 (2)
Cl1	0.0310 (6)	0.0590 (7)	0.0408 (5)	−0.0006 (5)	0.0164 (5)	−0.0093 (5)
Cl2	0.0323 (6)	0.0566 (7)	0.0420 (5)	0.0026 (5)	0.0154 (5)	−0.0063 (5)
N1	0.0269 (18)	0.0319 (18)	0.054 (2)	0.0027 (15)	0.0201 (17)	0.0032 (16)
N2	0.0201 (17)	0.038 (2)	0.047 (2)	−0.0001 (15)	0.0148 (16)	−0.0030 (16)

N3	0.0234 (17)	0.0262 (17)	0.0378 (18)	−0.0006 (14)	0.0130 (15)	−0.0029 (15)
N4	0.0262 (18)	0.0264 (17)	0.0327 (18)	−0.0003 (14)	0.0154 (15)	−0.0008 (14)
N5	0.0227 (17)	0.0260 (17)	0.0309 (17)	0.0020 (14)	0.0128 (14)	0.0000 (14)
N6	0.0255 (18)	0.0291 (18)	0.050 (2)	0.0013 (15)	0.0180 (16)	0.0002 (16)
N7	0.0213 (17)	0.0344 (19)	0.048 (2)	0.0020 (14)	0.0167 (16)	−0.0018 (15)
N8	0.0211 (17)	0.0271 (18)	0.0391 (19)	0.0017 (13)	0.0124 (15)	−0.0017 (14)
N9	0.0251 (18)	0.0280 (18)	0.0356 (19)	0.0035 (14)	0.0152 (15)	−0.0011 (14)
N10	0.0218 (17)	0.0322 (18)	0.0319 (18)	0.0043 (14)	0.0135 (15)	0.0030 (15)
O1	0.0275 (15)	0.0283 (15)	0.073 (2)	0.0034 (12)	0.0251 (15)	0.0005 (14)
O2	0.0346 (16)	0.0296 (16)	0.085 (2)	0.0021 (13)	0.0337 (16)	0.0087 (15)
O3	0.0246 (15)	0.0268 (15)	0.073 (2)	0.0052 (12)	0.0245 (14)	0.0081 (14)
O4	0.0314 (15)	0.0267 (15)	0.0655 (19)	0.0031 (12)	0.0259 (15)	0.0054 (14)
C1	0.030 (2)	0.027 (2)	0.045 (2)	−0.0003 (19)	0.021 (2)	−0.0012 (19)
C2	0.025 (2)	0.028 (2)	0.038 (2)	0.0031 (17)	0.0168 (18)	0.0014 (18)
C3	0.026 (2)	0.030 (2)	0.042 (2)	−0.0045 (18)	0.0141 (19)	−0.0057 (18)
C4	0.034 (2)	0.034 (2)	0.052 (3)	−0.0056 (19)	0.024 (2)	−0.007 (2)
C5	0.046 (3)	0.037 (2)	0.070 (3)	−0.018 (2)	0.034 (2)	−0.005 (2)
C6	0.051 (3)	0.026 (2)	0.061 (3)	−0.012 (2)	0.031 (2)	−0.004 (2)
C7	0.035 (2)	0.028 (2)	0.040 (2)	−0.0036 (18)	0.015 (2)	−0.0022 (18)
C8	0.025 (2)	0.025 (2)	0.028 (2)	−0.0019 (16)	0.0112 (17)	−0.0008 (16)
C9	0.0227 (19)	0.028 (2)	0.0230 (19)	−0.0008 (16)	0.0073 (16)	−0.0019 (16)
C10	0.026 (2)	0.037 (2)	0.029 (2)	0.0059 (17)	0.0110 (18)	−0.0001 (17)
C11	0.023 (2)	0.048 (3)	0.039 (2)	0.0042 (19)	0.0131 (19)	0.002 (2)
C12	0.029 (2)	0.038 (2)	0.041 (2)	−0.0078 (19)	0.017 (2)	0.0002 (19)
C13	0.030 (2)	0.028 (2)	0.038 (2)	−0.0020 (17)	0.0146 (19)	0.0009 (18)
C14	0.046 (3)	0.023 (2)	0.060 (3)	0.006 (2)	0.023 (2)	0.001 (2)
C15	0.035 (2)	0.037 (2)	0.056 (3)	0.014 (2)	0.019 (2)	0.001 (2)
C16	0.025 (2)	0.028 (2)	0.037 (2)	0.0012 (18)	0.0139 (18)	0.0003 (18)
C17	0.025 (2)	0.030 (2)	0.033 (2)	0.0050 (18)	0.0125 (18)	−0.0008 (18)
C18	0.028 (2)	0.029 (2)	0.039 (2)	0.0000 (18)	0.0139 (19)	0.0014 (18)
C19	0.027 (2)	0.042 (3)	0.047 (3)	0.0003 (19)	0.022 (2)	−0.001 (2)
C20	0.041 (3)	0.034 (2)	0.055 (3)	−0.009 (2)	0.025 (2)	−0.004 (2)
C21	0.041 (3)	0.032 (2)	0.048 (3)	−0.004 (2)	0.017 (2)	0.0029 (19)
C22	0.034 (2)	0.026 (2)	0.033 (2)	0.0037 (18)	0.0091 (19)	−0.0034 (17)
C23	0.027 (2)	0.029 (2)	0.024 (2)	0.0034 (17)	0.0104 (17)	−0.0016 (16)
C24	0.0201 (19)	0.028 (2)	0.025 (2)	0.0048 (16)	0.0073 (17)	0.0003 (16)
C25	0.029 (2)	0.037 (2)	0.030 (2)	0.0057 (18)	0.0124 (18)	−0.0016 (18)
C26	0.023 (2)	0.052 (3)	0.039 (2)	0.0104 (19)	0.0153 (19)	−0.003 (2)
C27	0.028 (2)	0.048 (3)	0.042 (2)	−0.003 (2)	0.020 (2)	−0.001 (2)
C28	0.031 (2)	0.032 (2)	0.036 (2)	0.0001 (18)	0.0142 (19)	0.0017 (18)
C29	0.046 (3)	0.028 (2)	0.056 (3)	0.013 (2)	0.022 (2)	−0.001 (2)
C30	0.036 (2)	0.036 (2)	0.056 (3)	0.011 (2)	0.023 (2)	−0.003 (2)

Geometric parameters (Å, º)

Cu1—O1	1.960 (3)	C5—H5	0.9300
Cu1—N4	2.007 (3)	C6—C7	1.407 (5)
Cu1—N5	2.026 (3)	C6—H6	0.9300

Cu1—N3	2.063 (3)	C7—C8	1.404 (5)
Cu1—Cl1	2.4443 (12)	C7—C14	1.414 (5)
Cu2—O3	1.968 (3)	C8—C9	1.427 (5)
Cu2—N10	2.014 (3)	C9—C10	1.396 (5)
Cu2—N9	2.023 (3)	C10—C11	1.407 (5)
Cu2—N8	2.036 (3)	C10—C15	1.440 (5)
Cu2—Cl2	2.4788 (12)	C11—C12	1.376 (5)
N1—C2	1.313 (4)	C11—H11	0.9300
N1—N2	1.359 (4)	C12—C13	1.396 (5)
N2—C3	1.320 (5)	C12—H12	0.9300
N2—H2	0.8600	C13—H13	0.9300
N3—C3	1.321 (5)	C14—C15	1.353 (6)
N3—C2	1.368 (4)	C14—H14	0.9300
N4—C4	1.330 (5)	C15—H15	0.9300
N4—C8	1.359 (4)	C16—C17	1.493 (5)
N5—C13	1.323 (5)	C18—H18	0.9300
N5—C9	1.363 (4)	C19—C20	1.403 (5)
N6—C17	1.313 (4)	C19—H19	0.9300
N6—N7	1.357 (4)	C20—C21	1.367 (5)
N7—C18	1.326 (4)	C20—H20	0.9300
N7—H7	0.8600	C21—C22	1.410 (5)
N8—C18	1.328 (5)	C21—H21	0.9300
N8—C17	1.376 (4)	C22—C23	1.401 (5)
N9—C19	1.320 (5)	C22—C29	1.428 (5)
N9—C23	1.357 (4)	C23—C24	1.422 (5)
N10—C28	1.329 (5)	C24—C25	1.402 (5)
N10—C24	1.352 (4)	C25—C26	1.405 (5)
O1—C1	1.265 (4)	C25—C30	1.431 (5)
O2—C1	1.233 (4)	C26—C27	1.362 (5)
O3—C16	1.265 (4)	C26—H26	0.9300
O4—C16	1.232 (4)	C27—C28	1.402 (5)
C1—C2	1.499 (5)	C27—H27	0.9300
C3—H3	0.9300	C28—H28	0.9300
C4—C5	1.385 (5)	C29—C30	1.349 (6)
C4—H4	0.9300	C29—H29	0.9300
C5—C6	1.374 (6)	C30—H30	0.9300

O1—Cu1—N4	166.89 (12)	N4—C8—C7	123.7 (3)
O1—Cu1—N5	89.02 (11)	N4—C8—C9	116.7 (3)
N4—Cu1—N5	81.67 (12)	C7—C8—C9	119.7 (3)
O1—Cu1—N3	82.28 (11)	N5—C9—C10	123.1 (3)
N4—Cu1—N3	102.10 (12)	N5—C9—C8	116.1 (3)
N5—Cu1—N3	153.69 (12)	C10—C9—C8	120.8 (3)
O1—Cu1—Cl1	97.04 (9)	C9—C10—C11	117.5 (4)
N4—Cu1—Cl1	94.25 (9)	C9—C10—C15	118.1 (3)
N5—Cu1—Cl1	104.68 (9)	C11—C10—C15	124.3 (4)
N3—Cu1—Cl1	101.02 (9)	C12—C11—C10	118.7 (4)
O3—Cu2—N10	88.58 (11)	C12—C11—H11	120.6

O3—Cu2—N9	166.41 (12)	C10—C11—H11	120.6
N10—Cu2—N9	81.80 (12)	C11—C12—C13	120.1 (4)
O3—Cu2—N8	82.37 (11)	C11—C12—H12	119.9
N10—Cu2—N8	157.06 (12)	C13—C12—H12	119.9
N9—Cu2—N8	102.95 (12)	N5—C13—C12	122.2 (4)
O3—Cu2—Cl2	98.08 (9)	N5—C13—H13	118.9
N10—Cu2—Cl2	104.13 (9)	C12—C13—H13	118.9
N9—Cu2—Cl2	93.58 (9)	C15—C14—C7	121.8 (4)
N8—Cu2—Cl2	98.01 (9)	C15—C14—H14	119.1
C2—N1—N2	102.5 (3)	C7—C14—H14	119.1
C3—N2—N1	110.4 (3)	C14—C15—C10	120.8 (4)
C3—N2—H2	124.8	C14—C15—H15	119.6
N1—N2—H2	124.8	C10—C15—H15	119.6
C3—N3—C2	102.9 (3)	O4—C16—O3	125.3 (3)
C3—N3—Cu1	148.2 (3)	O4—C16—C17	121.5 (3)
C2—N3—Cu1	107.7 (2)	O3—C16—C17	113.2 (3)
C4—N4—C8	117.4 (3)	N6—C17—N8	113.8 (3)
C4—N4—Cu1	129.7 (3)	N6—C17—C16	128.4 (3)
C8—N4—Cu1	112.8 (2)	N8—C17—C16	117.8 (3)
C13—N5—C9	118.3 (3)	N7—C18—N8	109.3 (3)
C13—N5—Cu1	129.2 (3)	N7—C18—H18	125.4
C9—N5—Cu1	112.3 (2)	N8—C18—H18	125.4
C17—N6—N7	102.6 (3)	N9—C19—C20	122.5 (4)
C18—N7—N6	111.1 (3)	N9—C19—H19	118.8
C18—N7—H7	124.5	C20—C19—H19	118.8
N6—N7—H7	124.5	C21—C20—C19	119.7 (4)
C18—N8—C17	103.3 (3)	C21—C20—H20	120.1
C18—N8—Cu2	147.2 (3)	C19—C20—H20	120.1
C17—N8—Cu2	108.4 (2)	C20—C21—C22	119.1 (4)
C19—N9—C23	118.3 (3)	C20—C21—H21	120.5
C19—N9—Cu2	129.9 (3)	C22—C21—H21	120.5
C23—N9—Cu2	111.6 (2)	C23—C22—C21	117.2 (4)
C28—N10—C24	118.5 (3)	C23—C22—C29	118.7 (4)
C28—N10—Cu2	129.0 (3)	C21—C22—C29	124.0 (4)
C24—N10—Cu2	112.4 (2)	N9—C23—C22	123.2 (3)
C1—O1—Cu1	117.9 (2)	N9—C23—C24	117.1 (3)
C16—O3—Cu2	117.8 (2)	C22—C23—C24	119.8 (3)
O2—C1—O1	125.4 (4)	N10—C24—C25	122.7 (3)
O2—C1—C2	121.1 (3)	N10—C24—C23	116.5 (3)
O1—C1—C2	113.4 (3)	C25—C24—C23	120.8 (3)
N1—C2—N3	114.1 (3)	C24—C25—C26	117.4 (4)
N1—C2—C1	128.0 (3)	C24—C25—C30	118.0 (4)
N3—C2—C1	118.0 (3)	C26—C25—C30	124.6 (4)
N2—C3—N3	110.2 (3)	C27—C26—C25	119.8 (4)
N2—C3—H3	124.9	C27—C26—H26	120.1
N3—C3—H3	124.9	C25—C26—H26	120.1
N4—C4—C5	122.7 (4)	C26—C27—C28	119.2 (4)
N4—C4—H4	118.6	C26—C27—H27	120.4

C5—C4—H4	118.6	C28—C27—H27	120.4
C6—C5—C4	120.4 (4)	N10—C28—C27	122.5 (4)
C6—C5—H5	119.8	N10—C28—H28	118.8
C4—C5—H5	119.8	C27—C28—H28	118.8
C5—C6—C7	118.6 (4)	C30—C29—C22	121.3 (4)
C5—C6—H6	120.7	C30—C29—H29	119.4
C7—C6—H6	120.7	C22—C29—H29	119.4
C8—C7—C6	117.1 (4)	C29—C30—C25	121.4 (4)
C8—C7—C14	118.9 (3)	C29—C30—H30	119.3
C6—C7—C14	124.0 (4)	C25—C30—H30	119.3

C2—N1—N2—C3	−0.7 (4)	C4—N4—C8—C9	177.8 (3)
O1—Cu1—N3—C3	−169.9 (5)	Cu1—N4—C8—C9	−4.7 (4)
N4—Cu1—N3—C3	22.6 (5)	C6—C7—C8—N4	0.4 (6)
N5—Cu1—N3—C3	118.3 (5)	C14—C7—C8—N4	178.8 (4)
Cl1—Cu1—N3—C3	−74.2 (5)	C6—C7—C8—C9	−178.4 (4)
O1—Cu1—N3—C2	−7.0 (2)	C14—C7—C8—C9	0.1 (5)
N4—Cu1—N3—C2	−174.4 (2)	C13—N5—C9—C10	0.4 (5)
N5—Cu1—N3—C2	−78.7 (3)	Cu1—N5—C9—C10	−176.7 (3)
Cl1—Cu1—N3—C2	88.8 (2)	C13—N5—C9—C8	−179.1 (3)
O1—Cu1—N4—C4	−132.5 (5)	Cu1—N5—C9—C8	3.9 (4)
N5—Cu1—N4—C4	−177.7 (3)	N4—C8—C9—N5	0.5 (5)
N3—Cu1—N4—C4	−24.2 (4)	C7—C8—C9—N5	179.3 (3)
Cl1—Cu1—N4—C4	78.1 (3)	N4—C8—C9—C10	−179.0 (3)
O1—Cu1—N4—C8	50.4 (6)	C7—C8—C9—C10	−0.2 (5)
N5—Cu1—N4—C8	5.2 (2)	N5—C9—C10—C11	0.0 (5)
N3—Cu1—N4—C8	158.7 (2)	C8—C9—C10—C11	179.5 (3)
Cl1—Cu1—N4—C8	−99.0 (2)	N5—C9—C10—C15	−179.5 (3)
O1—Cu1—N5—C13	7.7 (3)	C8—C9—C10—C15	0.0 (5)
N4—Cu1—N5—C13	178.4 (3)	C9—C10—C11—C12	−0.6 (5)
N3—Cu1—N5—C13	78.0 (4)	C15—C10—C11—C12	178.9 (3)
Cl1—Cu1—N5—C13	−89.3 (3)	C10—C11—C12—C13	0.8 (6)
O1—Cu1—N5—C9	−175.7 (2)	C9—N5—C13—C12	−0.2 (5)
N4—Cu1—N5—C9	−4.9 (2)	Cu1—N5—C13—C12	176.3 (3)
N3—Cu1—N5—C9	−105.4 (3)	C11—C12—C13—N5	−0.4 (6)
Cl1—Cu1—N5—C9	87.3 (2)	C8—C7—C14—C15	0.2 (6)
C17—N6—N7—C18	0.5 (4)	C6—C7—C14—C15	178.5 (4)
O3—Cu2—N8—C18	169.9 (5)	C7—C14—C15—C10	−0.4 (6)
N10—Cu2—N8—C18	−122.5 (5)	C9—C10—C15—C14	0.3 (6)
N9—Cu2—N8—C18	−22.8 (5)	C11—C10—C15—C14	−179.2 (4)
Cl2—Cu2—N8—C18	72.8 (5)	Cu2—O3—C16—O4	178.5 (3)
O3—Cu2—N8—C17	5.3 (2)	Cu2—O3—C16—C17	−1.4 (4)
N10—Cu2—N8—C17	72.9 (4)	N7—N6—C17—N8	−0.2 (4)
N9—Cu2—N8—C17	172.6 (2)	N7—N6—C17—C16	178.9 (4)
Cl2—Cu2—N8—C17	−91.8 (2)	C18—N8—C17—N6	−0.1 (4)
O3—Cu2—N9—C19	134.2 (5)	Cu2—N8—C17—N6	171.4 (3)
N10—Cu2—N9—C19	179.6 (3)	C18—N8—C17—C16	−179.3 (3)
N8—Cu2—N9—C19	22.4 (4)	Cu2—N8—C17—C16	−7.8 (4)

Cl2—Cu2—N9—C19	−76.6 (3)	O4—C16—C17—N6	7.6 (6)
O3—Cu2—N9—C23	−52.5 (6)	O3—C16—C17—N6	−172.5 (4)
N10—Cu2—N9—C23	−7.1 (2)	O4—C16—C17—N8	−173.4 (3)
N8—Cu2—N9—C23	−164.3 (2)	O3—C16—C17—N8	6.5 (5)
Cl2—Cu2—N9—C23	96.6 (2)	N6—N7—C18—N8	−0.6 (4)
O3—Cu2—N10—C28	−7.4 (3)	C17—N8—C18—N7	0.4 (4)
N9—Cu2—N10—C28	−177.8 (3)	Cu2—N8—C18—N7	−164.6 (4)
N8—Cu2—N10—C28	−73.9 (5)	C23—N9—C19—C20	−1.6 (6)
Cl2—Cu2—N10—C28	90.6 (3)	Cu2—N9—C19—C20	171.3 (3)
O3—Cu2—N10—C24	176.6 (2)	N9—C19—C20—C21	0.5 (6)
N9—Cu2—N10—C24	6.3 (2)	C19—C20—C21—C22	0.8 (6)
N8—Cu2—N10—C24	110.2 (3)	C20—C21—C22—C23	−1.0 (6)
Cl2—Cu2—N10—C24	−85.4 (2)	C20—C21—C22—C29	178.4 (4)
N4—Cu1—O1—C1	114.0 (5)	C19—N9—C23—C22	1.4 (5)
N5—Cu1—O1—C1	158.6 (3)	Cu2—N9—C23—C22	−172.7 (3)
N3—Cu1—O1—C1	3.5 (3)	C19—N9—C23—C24	−178.9 (3)
Cl1—Cu1—O1—C1	−96.7 (3)	Cu2—N9—C23—C24	7.0 (4)
N10—Cu2—O3—C16	−161.1 (3)	C21—C22—C23—N9	−0.1 (5)
N9—Cu2—O3—C16	−116.3 (5)	C29—C22—C23—N9	−179.5 (3)
N8—Cu2—O3—C16	−2.2 (3)	C21—C22—C23—C24	−179.8 (3)
Cl2—Cu2—O3—C16	94.9 (3)	C29—C22—C23—C24	0.7 (5)
Cu1—O1—C1—O2	−178.0 (3)	C28—N10—C24—C25	−0.8 (5)
Cu1—O1—C1—C2	0.8 (4)	Cu2—N10—C24—C25	175.7 (3)
N2—N1—C2—N3	0.3 (4)	C28—N10—C24—C23	179.2 (3)
N2—N1—C2—C1	180.0 (4)	Cu2—N10—C24—C23	−4.4 (4)
C3—N3—C2—N1	0.2 (4)	N9—C23—C24—N10	−1.8 (5)
Cu1—N3—C2—N1	−170.7 (3)	C22—C23—C24—N10	177.9 (3)
C3—N3—C2—C1	−179.5 (3)	N9—C23—C24—C25	178.2 (3)
Cu1—N3—C2—C1	9.6 (4)	C22—C23—C24—C25	−2.1 (5)
O2—C1—C2—N1	−8.4 (6)	N10—C24—C25—C26	0.5 (5)
O1—C1—C2—N1	172.8 (4)	C23—C24—C25—C26	−179.4 (3)
O2—C1—C2—N3	171.3 (4)	N10—C24—C25—C30	−178.0 (3)
O1—C1—C2—N3	−7.5 (5)	C23—C24—C25—C30	2.0 (5)
N1—N2—C3—N3	0.9 (4)	C24—C25—C26—C27	0.4 (6)
C2—N3—C3—N2	−0.6 (4)	C30—C25—C26—C27	178.8 (4)
Cu1—N3—C3—N2	162.7 (4)	C25—C26—C27—C28	−1.1 (6)
C8—N4—C4—C5	0.6 (6)	C24—N10—C28—C27	0.1 (6)
Cu1—N4—C4—C5	−176.4 (3)	Cu2—N10—C28—C27	−175.7 (3)
N4—C4—C5—C6	0.4 (6)	C26—C27—C28—N10	0.8 (6)
C4—C5—C6—C7	−1.0 (6)	C23—C22—C29—C30	0.7 (6)
C5—C6—C7—C8	0.6 (6)	C21—C22—C29—C30	−178.7 (4)
C5—C6—C7—C14	−177.7 (4)	C22—C29—C30—C25	−0.8 (6)
C4—N4—C8—C7	−1.0 (5)	C24—C25—C30—C29	−0.6 (6)
Cu1—N4—C8—C7	176.5 (3)	C26—C25—C30—C29	−179.0 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O4^{i}	0.86	1.99	2.835 (4)	166
N7—H7···O2^{ii}	0.86	1.94	2.797 (4)	172

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