Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(Salicylato)[tris(1-methyl-1*H*-benzimidazol-2-ylmethyl)amine]copper(II) perchlorate dimethylformamide disolvate

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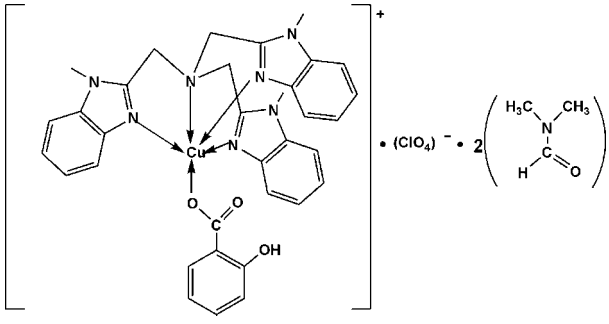
Received 17 October 2007; accepted 21 November 2007

Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.048; wR factor = 0.134; data-to-parameter ratio = 12.7.

In the title complex, $[Cu(C_7H_5O_3)(C_{27}H_{27}N_7)]ClO_4\cdot 2C_3H_7NO$, the Cu^{II} ion is five-coordinated by four N atoms from the tris(1-methyl-1*H*-benzimidazol-2-ylmethyl)amine ligand and an O atom of the monodentate salicylate ligand. The N_4O donor set defines a coordination geometry intermediate between square-pyramidal and trigonal–bipyramidal. The crystal structure is stabilized by O—H···O interactions. The atoms of the aromatic ring of the salicylate ligand are disordered over two sites of equal occupancy. In addition, one of the dimethylformamide solvent molecules is partially disordered over two positions, of approximately equal occupancy.

Related literature

For related literature, see: Addison *et al.* (1984); Allen *et al.* (1987); Spek (2003); Youngme *et al.* (2007).



Experimental

Crystal data

$[Cu(C_7H_5O_3)(C_{27}H_{27}N_7)]ClO_4\cdot 2C_3H_7NO$
M_r = 895.85
Triclinic, $P\overline{1}$
a = 12.3507 (4) Å
b = 12.6632 (5) Å
c = 14.4152 (4) Å
α = 85.721 (1)°
β = 70.886 (1)°
γ = 76.503 (1)°
V = 2071.40 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.66 mm^{-1}
T = 153 (2) K
0.54 × 0.52 × 0.39 mm

Data collection

Rigaku R-AXIS SPIDER diffractometer
Absorption correction: multi-scan (Higashi, 1995)
T_{min} = 0.718, T_{max} = 0.783
17142 measured reflections
7660 independent reflections
7110 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.134
S = 1.05
7660 reflections
603 parameters
24 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.88 e Å^{-3}
$\Delta\rho_{min}$ = −0.86 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3′—H3O'···O1	0.84 (6)	1.72 (6)	2.493 (6)	152 (5)
O3—H3O···O2	0.83 (7)	1.87 (6)	2.562 (7)	140 (4)

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge financial support from the Qing Lan Talent Engineering Funds of Lanzhou Jiaotong University and the Middle-Young Age Science Foundation of Gansu Province (grant No. 3YS061-A25-023).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2203).

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supporting information

Acta Cryst. (2008). E**64**, m19 [https://doi.org/10.1107/S1600536807061661]

(Salicylato)[tris(1-methyl-1*H*-benzimidazol-2-ylmethyl)amine]copper(II) perchlorate dimethylformamide disolvate

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S1. Comment

The asymmetric unit of the title complex, (Fig. 1), comprises a [Cu(Mentb)(salicylate)] cation, a perchlorate anion, and two dimethylformamide (DMF) molecules of crystallization, where Mentb = tris(*N*-methylbenzimidazol-2-ylmethyl)-amine. The Cu atom is five-coordinate within a N_4O ligand set. The Mentb ligand functions as a tetradentate N-donor, and an O atom of a monodentate salicylate anion completes the coordination environment. The coordination environment of the Cu^{II} centre has an intermediate coordination geometry as seen in the value of $\tau = 0.45$, *cf.* $\tau = 0$ for an ideal square pyramid and $\tau = 1$ for an ideal trigonal bipyramid (Addison *et al.*, 1984). The Cu···O2 distance of 2.960 (2) Å indicates that the O2 atom is non-coordinating. The distances and angles in Mentb and salicylate are as expected (Allen *et al.*, 1987). O—H···O Hydrogen-bonding interactions play an important role in the crystal packing (Table 1). The atoms of the aromatic ring of the salicylate ligand are disordered over two sites with equal occupancy and one of the lattice DMF molecules is partially disordered over two positions, of approximately equal occupancy.

S2. Experimental

To a stired solution of tris(*N*-methylbenzimidazol-2-ylmethyl)amine (0.0899 g, 0.2 mmol) in hot MeOH (10 ml) was added $Cu(ClO_4)_2(H_2O)_6$ (0.0741 g, 0.2 mmol), followed by a solution of Na(salicylate) (0.0320 g, 0.2 mmol) in MeOH (5 ml). A blue-green crystalline product formed rapidly. The precipitate was filtered off, washed with MeOH and absolute Et_2O, and dried *in vacuo*. The dried precipitate was dissolved in DMF to yield a blue-green solution that was allowed to evaporate at room temperature. Blue-green crystals suitable for X-ray diffraction studies were obtained after two weeks. Yield, 0.12 g (67%). Analysis found: C 53.63, H 5.18, N 14.07, Cu 7.09%. $C_{40}H_{46}ClCuN_9O_9$ requires: C 53.45, H 5.15, N 13.95, Cu 7.41%.

S3. Refinement

The aromatic ring of the salicylate ligand was disordered over two sites and from refinement, these were determined to be of equal occupancy. One of the lattice dimethylformamide molecules is partially disordered over two positions and from refinement, the major component was found to have an occupancy factor = 0.552 (15). All H atoms were geometrically positioned and refined using a riding-model approximation with C—H distances ranging from 0.95 to 0.99 Å and O—H = 0.83 (1) Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$ or $U_{iso}(H) = 0.52U_{eq}(O)$.

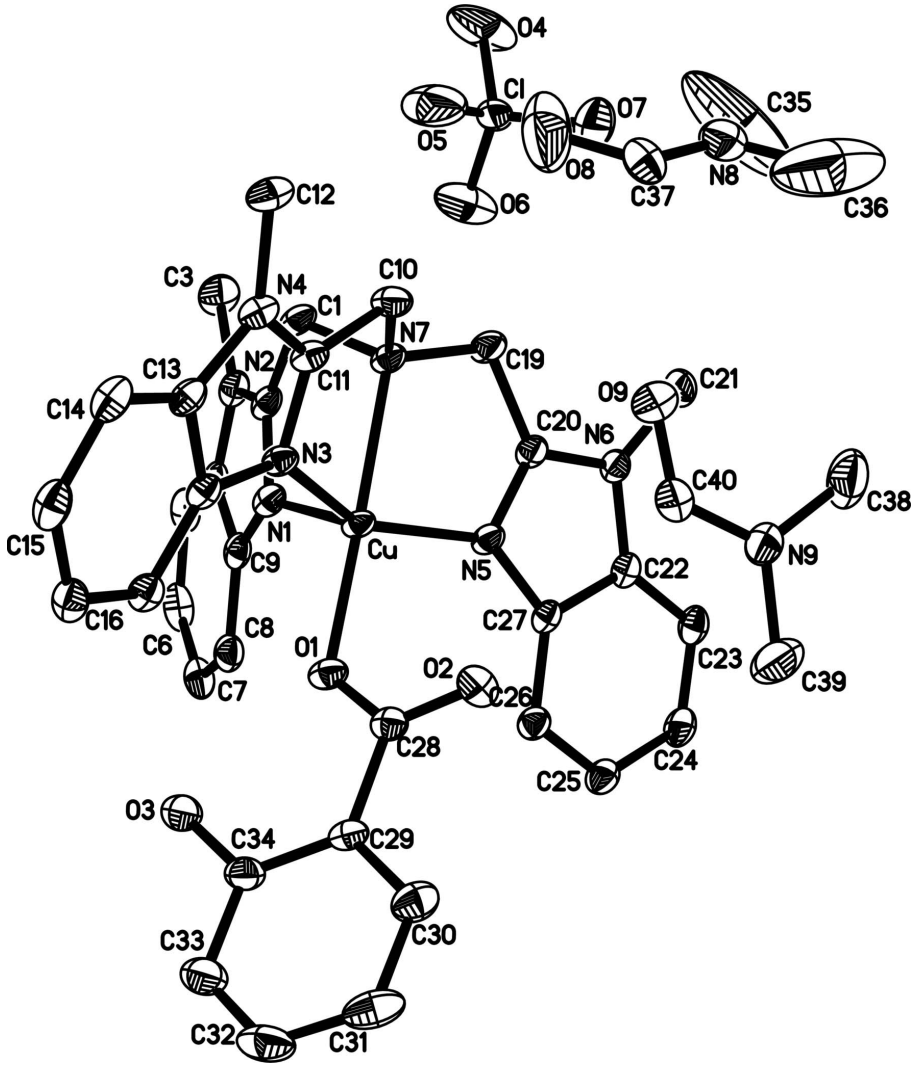

Figure 1

Molecular structure and atom numbering for the components of (I). Hydrogen atoms have been omitted for clarity and the displacement ellipsoids are shown at the 30% probability level. The salicylate anion is disordered over two positions of equal occupancy and one of the lattice dimethylformamide molecules is partially disordered over two positions, only one orientation of each is shown for reasons of clarity.

(Salicylato)[tris(1-methyl-1*H*-benzimidazol-2-ylmethyl)amine]copper(II) perchlorate dimethylformamide disolvate

Crystal data

$[Cu(C_7H_5O_3)(C_{27}H_{27}N_7)]ClO_4\cdot 2C_3H_7NO$
$M_r = 895.85$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 12.3507\ (4)$ Å
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$c = 14.4152\ (4)$ Å
$\alpha = 85.721\ (1)°$
$\beta = 70.886\ (1)°$
$\gamma = 76.503\ (1)°$
$V = 2071.40\ (12)$ Å^3
$Z = 2$
$F(000) = 934$
$D_x = 1.436$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 18119 reflections
$\theta = 3.2–27.5°$
$\mu = 0.66$ mm^{-1}

T = 153 K
Block, blue

0.54 × 0.52 × 0.39 mm

Data collection

Rigaku R-axis Spider diffractometer
Radiation source: Rotating Anode
Graphite monochromator
ω scans
Absorption correction: multi-scan (Higashi, 1995)
T_{min} = 0.718, T_{max} = 0.783

17142 measured reflections
7660 independent reflections
7110 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 25.5°, θ_{min} = 3.2°
h = −14→14
k = −15→15
l = −16→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.134
S = 1.05
7660 reflections
603 parameters
24 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0705P)^2 + 2.6589P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.88 e Å^{-3}
$\Delta\rho_{min}$ = −0.86 e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0075 (10)

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}	Occ. (<1)
Cu	0.23086 (3)	0.18111 (2)	0.28279 (2)	0.02632 (13)	
Cl	0.46206 (8)	0.24356 (7)	0.61206 (7)	0.0542 (2)	
O1	0.12367 (17)	0.19029 (15)	0.20785 (14)	0.0333 (4)	
O2	0.21747 (19)	0.30068 (18)	0.10096 (16)	0.0440 (5)	
O4	0.5081 (4)	0.2148 (5)	0.6893 (3)	0.136 (2)	
O5	0.5122 (4)	0.1574 (3)	0.5410 (5)	0.155 (3)	
O6	0.3371 (3)	0.2617 (3)	0.6404 (2)	0.0865 (11)	
O7	0.4971 (3)	0.3351 (3)	0.5646 (3)	0.0789 (9)	
O8	0.7130 (4)	0.1796 (3)	0.2226 (4)	0.1226 (17)	
O9	0.4655 (2)	0.3831 (2)	0.1943 (2)	0.0642 (7)	
N1	0.1330 (2)	0.12553 (17)	0.42437 (16)	0.0303 (5)	
N2	0.1388 (2)	0.08381 (18)	0.57588 (17)	0.0347 (5)	

N3	0.35227 (19)	0.05833 (17)	0.20799 (15)	0.0272 (5)
N4	0.54005 (19)	−0.03060 (18)	0.16286 (16)	0.0309 (5)
N5	0.1866 (2)	0.33208 (17)	0.33286 (16)	0.0305 (5)
N6	0.2204 (2)	0.45780 (17)	0.41241 (16)	0.0299 (5)
N7	0.3577 (2)	0.16453 (18)	0.35884 (17)	0.0317 (5)
N8	0.7165 (3)	0.3526 (3)	0.2367 (3)	0.0630 (9)
N9	0.3491 (3)	0.5382 (2)	0.1623 (2)	0.0463 (6)
C1	0.3300 (3)	0.0824 (2)	0.4377 (2)	0.0339 (6)
H1A	0.3651	0.0083	0.4100	0.041*
H1B	0.3636	0.0913	0.4895	0.041*
C2	0.2003 (3)	0.0973 (2)	0.48048 (19)	0.0310 (6)
C3	0.1859 (4)	0.0485 (3)	0.6570 (2)	0.0516 (9)
H3A	0.2275	−0.0280	0.6477	0.062*
H3B	0.1212	0.0568	0.7193	0.062*
H3C	0.2406	0.0929	0.6583	0.062*
C4	0.0213 (3)	0.1061 (2)	0.5821 (2)	0.0356 (6)
C5	−0.0806 (3)	0.1079 (2)	0.6602 (2)	0.0441 (7)
H5	−0.0786	0.0891	0.7248	0.053*
C6	−0.1852 (3)	0.1383 (3)	0.6399 (2)	0.0487 (8)
H6	−0.2569	0.1410	0.6919	0.058*
C7	−0.1888 (3)	0.1654 (2)	0.5443 (2)	0.0433 (7)
H7	−0.2626	0.1860	0.5332	0.052*
C8	−0.0868 (3)	0.1625 (2)	0.4663 (2)	0.0363 (6)
H8	−0.0889	0.1801	0.4016	0.044*
C9	0.0192 (3)	0.1327 (2)	0.48621 (19)	0.0307 (6)
C10	0.4740 (2)	0.1227 (2)	0.2862 (2)	0.0360 (6)
H10A	0.5298	0.0832	0.3196	0.043*
H10B	0.5058	0.1834	0.2484	0.043*
C11	0.4568 (2)	0.0481 (2)	0.21948 (19)	0.0294 (5)
C12	0.6630 (2)	−0.0650 (3)	0.1588 (2)	0.0382 (7)
H12A	0.6853	−0.0072	0.1852	0.046*
H12B	0.7128	−0.0799	0.0905	0.046*
H12C	0.6731	−0.1310	0.1980	0.046*
C13	0.4861 (2)	−0.0758 (2)	0.11005 (18)	0.0292 (5)
C14	0.5307 (3)	−0.1582 (2)	0.0407 (2)	0.0364 (6)
H14	0.6105	−0.1966	0.0225	0.044*
C15	0.4529 (3)	−0.1815 (2)	−0.0005 (2)	0.0390 (7)
H15	0.4801	−0.2368	−0.0491	0.047*
C16	0.3349 (3)	−0.1261 (2)	0.0271 (2)	0.0358 (6)
H16	0.2841	−0.1450	−0.0030	0.043*
C17	0.2903 (2)	−0.0445 (2)	0.09713 (19)	0.0305 (6)
H17	0.2100	−0.0075	0.1161	0.037*
C18	0.3680 (2)	−0.0191 (2)	0.13840 (18)	0.0265 (5)
C19	0.3507 (3)	0.2711 (2)	0.4003 (2)	0.0400 (7)
H19A	0.4259	0.2940	0.3699	0.048*
H19B	0.3365	0.2643	0.4719	0.048*
C20	0.2527 (3)	0.3542 (2)	0.38059 (19)	0.0301 (6)
C21	0.2778 (3)	0.5092 (2)	0.4650 (2)	0.0394 (7)

H21A	0.3125	0.4548	0.5053	0.047*	
H21B	0.2196	0.5671	0.5073	0.047*	
H21C	0.3396	0.5400	0.4176	0.047*	
C22	0.1228 (2)	0.5066 (2)	0.38473 (19)	0.0292 (5)	
C23	0.0509 (3)	0.6106 (2)	0.4013 (2)	0.0361 (6)	
H23	0.0662	0.6645	0.4348	0.043*	
C24	−0.0432 (3)	0.6311 (2)	0.3666 (2)	0.0388 (7)	
H24	−0.0944	0.7010	0.3767	0.047*	
C25	−0.0660 (3)	0.5522 (2)	0.3167 (2)	0.0362 (6)	
H25	−0.1324	0.5696	0.2944	0.043*	
C26	0.0066 (2)	0.4492 (2)	0.2993 (2)	0.0318 (6)	
H26	−0.0080	0.3960	0.2647	0.038*	
C27	0.1017 (2)	0.4270 (2)	0.33478 (18)	0.0273 (5)	
C28	0.1456 (2)	0.2419 (2)	0.12643 (18)	0.0308 (6)	
O3	0.1645 (6)	0.3536 (6)	−0.0564 (5)	0.0758 (18)	0.50
C29	0.0846 (10)	0.2304 (10)	0.0545 (6)	0.037 (4)*	0.50
C30	0.0955 (13)	0.2819 (11)	−0.0356 (8)	0.040 (4)*	0.50
C31	0.0378 (17)	0.2540 (18)	−0.0951 (13)	0.039 (3)	0.50
H31	0.0465	0.2886	−0.1571	0.047*	0.50
C32	−0.032 (2)	0.1780 (18)	−0.0685 (13)	0.043 (4)	0.50
H32	−0.0620	0.1558	−0.1149	0.051*	0.50
C33	−0.0584 (13)	0.1344 (16)	0.0255 (10)	0.034 (3)	0.50
H33	−0.1185	0.0953	0.0527	0.041*	0.50
C34	0.0142 (17)	0.1550 (15)	0.0749 (12)	0.058 (5)	0.50
H34	0.0158	0.1111	0.1310	0.069*	0.50
O3′	−0.0091 (4)	0.0935 (4)	0.1671 (3)	0.0461 (10)	0.50
C29′	0.0772 (7)	0.2233 (7)	0.0627 (5)	0.019 (3)*	0.50
C34′	0.0954 (15)	0.2843 (13)	−0.0231 (8)	0.049 (4)	0.50
H34′	0.1467	0.3325	−0.0336	0.058*	0.50
C33′	0.044 (2)	0.280 (2)	−0.0947 (15)	0.063 (5)	0.50
H33′	0.0543	0.3244	−0.1513	0.076*	0.50
C32′	−0.025 (2)	0.2027 (19)	−0.0751 (14)	0.057 (5)	0.50
H32′	−0.0674	0.1970	−0.1181	0.069*	0.50
C31′	−0.0328 (15)	0.1338 (18)	0.0054 (8)	0.045 (4)	0.50
H31′	−0.0651	0.0723	0.0072	0.054*	0.50
C30′	0.0039 (13)	0.1504 (10)	0.0836 (7)	0.022 (2)*	0.50
C35	0.6697 (8)	0.3959 (11)	0.3338 (4)	0.246 (8)	
H35A	0.6266	0.4712	0.3325	0.296*	
H35B	0.7340	0.3937	0.3601	0.296*	
H35C	0.6162	0.3525	0.3757	0.296*	
C36	0.7496 (7)	0.4342 (8)	0.1654 (6)	0.204 (6)	
H36A	0.8281	0.4425	0.1608	0.245*	
H36B	0.6929	0.5034	0.1853	0.245*	
H36C	0.7504	0.4124	0.1013	0.245*	
C37	0.7209 (7)	0.2688 (3)	0.1846 (4)	0.044 (3)	0.448 (15)
H37	0.7304	0.2779	0.1166	0.053*	0.448 (15)
C37′	0.7054 (10)	0.2553 (4)	0.2738 (6)	0.181 (12)	0.552 (15)
H37′	0.6912	0.2440	0.3423	0.217*	0.552 (15)

C38	0.3954 (5)	0.6093 (3)	0.2048 (4)	0.0790 (14)	
H38A	0.4637	0.5674	0.2218	0.095*	
H38B	0.3349	0.6430	0.2642	0.095*	
H38C	0.4191	0.6659	0.1574	0.095*	
C39	0.2527 (4)	0.5877 (4)	0.1252 (4)	0.0725 (12)	
H39A	0.2245	0.5307	0.1036	0.087*	
H39B	0.2801	0.6350	0.0696	0.087*	
H39C	0.1885	0.6307	0.1774	0.087*	
C40	0.3882 (3)	0.4317 (3)	0.1615 (3)	0.0477 (8)	
H40	0.3531	0.3893	0.1331	0.057*	
H3O′	0.026 (5)	0.117 (4)	0.199 (4)	0.024 (15)*	0.50
H3O	0.191 (6)	0.365 (6)	−0.013 (4)	0.040 (19)*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu	0.0330 (2)	0.02317 (18)	0.02454 (19)	0.00196 (13)	−0.01623 (14)	−0.00412 (12)
Cl	0.0642 (5)	0.0541 (5)	0.0705 (6)	−0.0295 (4)	−0.0514 (5)	0.0309 (4)
O1	0.0366 (10)	0.0345 (10)	0.0295 (10)	0.0003 (8)	−0.0167 (8)	−0.0024 (8)
O2	0.0433 (12)	0.0474 (12)	0.0464 (12)	−0.0162 (10)	−0.0163 (10)	−0.0021 (10)
O4	0.130 (3)	0.239 (5)	0.110 (3)	−0.122 (4)	−0.101 (3)	0.117 (3)
O5	0.133 (4)	0.066 (2)	0.317 (7)	0.039 (2)	−0.164 (5)	−0.075 (3)
O6	0.0596 (18)	0.153 (3)	0.0614 (18)	−0.045 (2)	−0.0287 (15)	0.025 (2)
O7	0.087 (2)	0.0645 (18)	0.088 (2)	−0.0302 (16)	−0.0294 (18)	0.0329 (16)
O8	0.084 (3)	0.074 (2)	0.182 (5)	−0.035 (2)	0.006 (3)	0.003 (3)
O9	0.0589 (16)	0.0487 (14)	0.093 (2)	−0.0068 (12)	−0.0405 (15)	0.0104 (14)
N1	0.0414 (13)	0.0237 (10)	0.0252 (11)	0.0002 (9)	−0.0141 (10)	−0.0045 (8)
N2	0.0560 (15)	0.0253 (11)	0.0275 (11)	−0.0089 (10)	−0.0197 (11)	0.0012 (9)
N3	0.0307 (11)	0.0278 (11)	0.0233 (10)	−0.0001 (9)	−0.0127 (9)	−0.0019 (8)
N4	0.0282 (11)	0.0333 (12)	0.0268 (11)	−0.0002 (9)	−0.0085 (9)	0.0032 (9)
N5	0.0416 (13)	0.0233 (11)	0.0301 (11)	−0.0006 (9)	−0.0201 (10)	−0.0021 (9)
N6	0.0423 (13)	0.0244 (11)	0.0268 (11)	−0.0076 (9)	−0.0156 (10)	−0.0012 (9)
N7	0.0403 (13)	0.0263 (11)	0.0323 (12)	0.0006 (9)	−0.0217 (10)	−0.0025 (9)
N8	0.062 (2)	0.0539 (19)	0.089 (3)	−0.0119 (15)	−0.0444 (19)	−0.0043 (17)
N9	0.0543 (16)	0.0393 (14)	0.0481 (16)	−0.0129 (12)	−0.0197 (13)	0.0074 (12)
C1	0.0459 (16)	0.0279 (13)	0.0297 (13)	0.0034 (11)	−0.0222 (12)	−0.0013 (11)
C2	0.0483 (16)	0.0199 (12)	0.0267 (13)	−0.0009 (11)	−0.0184 (12)	−0.0034 (10)
C3	0.078 (2)	0.055 (2)	0.0323 (16)	−0.0202 (18)	−0.0302 (17)	0.0130 (14)
C4	0.0589 (19)	0.0199 (12)	0.0307 (14)	−0.0118 (12)	−0.0154 (13)	−0.0022 (10)
C5	0.066 (2)	0.0352 (16)	0.0333 (15)	−0.0229 (15)	−0.0110 (15)	0.0009 (12)
C6	0.060 (2)	0.0383 (16)	0.0436 (18)	−0.0239 (15)	−0.0012 (16)	−0.0061 (13)
C7	0.0446 (17)	0.0330 (15)	0.0524 (19)	−0.0146 (13)	−0.0105 (15)	−0.0052 (13)
C8	0.0454 (16)	0.0245 (13)	0.0395 (15)	−0.0073 (12)	−0.0136 (13)	−0.0042 (11)
C9	0.0437 (15)	0.0186 (12)	0.0287 (13)	−0.0048 (10)	−0.0105 (12)	−0.0052 (10)
C10	0.0338 (14)	0.0403 (15)	0.0376 (15)	−0.0028 (12)	−0.0199 (12)	−0.0016 (12)
C11	0.0300 (13)	0.0311 (13)	0.0258 (12)	−0.0012 (10)	−0.0115 (11)	0.0016 (10)
C12	0.0273 (14)	0.0456 (17)	0.0350 (15)	0.0017 (12)	−0.0094 (12)	0.0066 (12)
C13	0.0331 (14)	0.0271 (13)	0.0220 (12)	−0.0020 (10)	−0.0059 (11)	0.0047 (10)

C14	0.0411 (16)	0.0294 (14)	0.0270 (13)	0.0014 (12)	−0.0021 (12)	0.0011 (11)
C15	0.0551 (18)	0.0273 (14)	0.0266 (13)	−0.0040 (13)	−0.0055 (13)	−0.0030 (11)
C16	0.0506 (17)	0.0307 (14)	0.0277 (13)	−0.0109 (12)	−0.0132 (12)	−0.0009 (11)
C17	0.0366 (14)	0.0294 (13)	0.0234 (12)	−0.0051 (11)	−0.0085 (11)	0.0008 (10)
C18	0.0325 (13)	0.0240 (12)	0.0193 (11)	−0.0012 (10)	−0.0070 (10)	0.0007 (9)
C19	0.0570 (19)	0.0273 (14)	0.0467 (17)	−0.0006 (13)	−0.0364 (15)	−0.0046 (12)
C20	0.0429 (15)	0.0247 (12)	0.0260 (13)	−0.0050 (11)	−0.0172 (12)	−0.0005 (10)
C21	0.0560 (19)	0.0321 (14)	0.0387 (16)	−0.0144 (13)	−0.0228 (14)	−0.0031 (12)
C22	0.0377 (14)	0.0236 (12)	0.0242 (12)	−0.0060 (10)	−0.0077 (11)	0.0005 (10)
C23	0.0467 (17)	0.0231 (13)	0.0360 (15)	−0.0058 (12)	−0.0102 (13)	−0.0041 (11)
C24	0.0409 (16)	0.0229 (13)	0.0460 (17)	0.0005 (11)	−0.0095 (13)	−0.0033 (12)
C25	0.0340 (14)	0.0298 (14)	0.0409 (16)	−0.0017 (11)	−0.0110 (12)	0.0018 (12)
C26	0.0358 (14)	0.0266 (13)	0.0326 (14)	−0.0028 (11)	−0.0128 (12)	−0.0019 (11)
C27	0.0343 (14)	0.0211 (12)	0.0241 (12)	−0.0026 (10)	−0.0085 (11)	0.0000 (9)
C28	0.0296 (13)	0.0290 (13)	0.0315 (14)	0.0018 (11)	−0.0109 (11)	−0.0070 (11)
O3	0.085 (4)	0.093 (5)	0.060 (4)	−0.039 (4)	−0.033 (3)	0.040 (3)
C31	0.050 (6)	0.042 (9)	0.033 (5)	−0.017 (5)	−0.021 (4)	0.010 (4)
C32	0.043 (6)	0.045 (9)	0.047 (6)	−0.011 (6)	−0.020 (4)	−0.008 (5)
C33	0.022 (6)	0.043 (5)	0.034 (5)	−0.003 (4)	−0.007 (5)	−0.004 (4)
C34	0.049 (8)	0.060 (7)	0.066 (7)	0.005 (4)	−0.034 (6)	0.000 (4)
O3′	0.046 (3)	0.053 (3)	0.048 (3)	−0.020 (2)	−0.022 (2)	0.012 (2)
C34′	0.059 (6)	0.065 (7)	0.022 (4)	−0.009 (3)	−0.020 (4)	0.016 (4)
C33′	0.091 (11)	0.062 (13)	0.044 (6)	−0.008 (7)	−0.041 (7)	0.012 (6)
C32′	0.085 (12)	0.051 (11)	0.051 (7)	0.011 (7)	−0.055 (8)	−0.015 (5)
C31′	0.029 (7)	0.058 (7)	0.045 (8)	−0.003 (5)	−0.009 (6)	−0.020 (6)
C35	0.223 (10)	0.52 (2)	0.068 (4)	−0.264 (14)	−0.006 (5)	−0.058 (8)
C36	0.091 (5)	0.354 (16)	0.136 (7)	−0.021 (7)	−0.039 (5)	0.118 (9)
C37	0.041 (4)	0.050 (5)	0.044 (4)	−0.016 (3)	−0.009 (3)	−0.009 (3)
C37′	0.084 (9)	0.099 (10)	0.39 (4)	0.017 (7)	−0.125 (16)	−0.079 (15)
C38	0.132 (4)	0.047 (2)	0.078 (3)	−0.034 (2)	−0.051 (3)	0.009 (2)
C39	0.071 (3)	0.070 (3)	0.076 (3)	−0.006 (2)	−0.034 (2)	0.025 (2)
C40	0.0492 (19)	0.0411 (17)	0.057 (2)	−0.0154 (15)	−0.0198 (16)	0.0012 (15)

Geometric parameters (Å, º)

Cu—O1	1.9441 (19)	C14—H14	0.9500
Cu—N3	1.983 (2)	C15—C16	1.400 (4)
Cu—N5	1.983 (2)	C15—H15	0.9500
Cu—N7	2.153 (2)	C16—C17	1.384 (4)
Cu—N1	2.165 (2)	C16—H16	0.9500
Cl—O7	1.386 (3)	C17—C18	1.387 (4)
Cl—O4	1.397 (3)	C17—H17	0.9500
Cl—O6	1.427 (3)	C19—C20	1.496 (4)
Cl—O5	1.435 (5)	C19—H19A	0.9900
O1—C28	1.280 (3)	C19—H19B	0.9900
O2—C28	1.237 (3)	C21—H21A	0.9800
O8—C37′	1.220 (3)	C21—H21B	0.9800
O8—C37	1.229 (3)	C21—H21C	0.9800

O9—C40	1.221 (4)	C22—C23	1.394 (4)
N1—C2	1.316 (4)	C22—C27	1.398 (4)
N1—C9	1.382 (4)	C23—C24	1.375 (4)
N2—C2	1.356 (4)	C23—H23	0.9500
N2—C4	1.386 (4)	C24—C25	1.402 (4)
N2—C3	1.467 (4)	C24—H24	0.9500
N3—C11	1.331 (3)	C25—C26	1.387 (4)
N3—C18	1.391 (3)	C25—H25	0.9500
N4—C11	1.345 (3)	C26—C27	1.392 (4)
N4—C13	1.387 (4)	C26—H26	0.9500
N4—C12	1.461 (3)	C28—C29	1.4997 (10)
N5—C20	1.313 (3)	C28—C29′	1.5001 (10)
N5—C27	1.393 (3)	O3—C30	1.3399 (10)
N6—C20	1.347 (3)	O3—H3O	0.828 (10)
N6—C22	1.388 (4)	C29—C30	1.3899 (10)
N6—C21	1.462 (3)	C29—C34	1.3899 (10)
N7—C10	1.477 (4)	C30—C31	1.3898 (10)
N7—C19	1.489 (3)	C31—C32	1.3899 (10)
N7—C1	1.492 (4)	C31—H31	0.9500
N8—C37′	1.325 (3)	C32—C33	1.3897 (10)
N8—C37	1.326 (3)	C32—H32	0.9500
N8—C35	1.425 (3)	C33—C34	1.3903 (10)
N8—C36	1.434 (3)	C33—H33	0.9500
N9—C40	1.321 (4)	C34—H34	0.9500
N9—C38	1.437 (5)	O3′—C30′	1.3398 (10)
N9—C39	1.455 (5)	O3′—H3O′	0.830 (10)
C1—C2	1.487 (4)	C29′—C30′	1.3896 (10)
C1—H1A	0.9900	C29′—C34′	1.3901 (10)
C1—H1B	0.9900	C34′—C33′	1.3899 (10)
C3—H3A	0.9800	C34′—H34′	0.9500
C3—H3B	0.9800	C33′—C32′	1.3899 (10)
C3—H3C	0.9800	C33′—H33′	0.9500
C4—C5	1.383 (4)	C32′—C31′	1.3898 (10)
C4—C9	1.406 (4)	C32′—H32′	0.9500
C5—C6	1.379 (5)	C31′—C30′	1.3903 (10)
C5—H5	0.9500	C31′—H31′	0.9500
C6—C7	1.408 (5)	C35—H35A	0.9800
C6—H6	0.9500	C35—H35B	0.9800
C7—C8	1.382 (4)	C35—H35C	0.9800
C7—H7	0.9500	C36—H36A	0.9800
C8—C9	1.392 (4)	C36—H36B	0.9800
C8—H8	0.9500	C36—H36C	0.9800
C10—C11	1.491 (4)	C37—H37	0.9500
C10—H10A	0.9900	C37′—H37′	0.9500
C10—H10B	0.9900	C38—H38A	0.9800
C12—H12A	0.9800	C38—H38B	0.9800
C12—H12B	0.9800	C38—H38C	0.9800
C12—H12C	0.9800	C39—H39A	0.9800

C13—C14	1.386 (4)	C39—H39B	0.9800
C13—C18	1.406 (4)	C39—H39C	0.9800
C14—C15	1.376 (5)	C40—H40	0.9500
O1—Cu—N3	96.36 (8)	C17—C18—N3	131.4 (2)
O1—Cu—N5	100.54 (8)	C17—C18—C13	120.5 (2)
N3—Cu—N5	149.64 (10)	N3—C18—C13	108.1 (2)
O1—Cu—N7	176.47 (8)	N7—C19—C20	109.5 (2)
N3—Cu—N7	80.21 (9)	N7—C19—H19A	109.8
N5—Cu—N7	82.24 (9)	C20—C19—H19A	109.8
O1—Cu—N1	102.12 (9)	N7—C19—H19B	109.8
N3—Cu—N1	110.14 (8)	C20—C19—H19B	109.8
N5—Cu—N1	90.79 (9)	H19A—C19—H19B	108.2
N7—Cu—N1	79.92 (9)	N5—C20—N6	113.0 (2)
O7—Cl—O4	110.4 (2)	N5—C20—C19	122.9 (2)
O7—Cl—O6	109.2 (2)	N6—C20—C19	124.0 (2)
O4—Cl—O6	114.4 (2)	N6—C21—H21A	109.5
O7—Cl—O5	106.2 (3)	N6—C21—H21B	109.5
O4—Cl—O5	107.9 (3)	H21A—C21—H21B	109.5
O6—Cl—O5	108.5 (2)	N6—C21—H21C	109.5
C28—O1—Cu	117.26 (16)	H21A—C21—H21C	109.5
C37′—O8—C37	60.9 (5)	H21B—C21—H21C	109.5
C2—N1—C9	105.7 (2)	N6—C22—C23	131.5 (3)
C2—N1—Cu	110.55 (19)	N6—C22—C27	106.2 (2)
C9—N1—Cu	141.28 (18)	C23—C22—C27	122.3 (3)
C2—N2—C4	106.6 (2)	C24—C23—C22	116.4 (3)
C2—N2—C3	127.4 (3)	C24—C23—H23	121.8
C4—N2—C3	125.9 (3)	C22—C23—H23	121.8
C11—N3—C18	105.9 (2)	C23—C24—C25	122.2 (3)
C11—N3—Cu	113.72 (17)	C23—C24—H24	118.9
C18—N3—Cu	140.14 (18)	C25—C24—H24	118.9
C11—N4—C13	106.8 (2)	C26—C25—C24	121.2 (3)
C11—N4—C12	127.3 (2)	C26—C25—H25	119.4
C13—N4—C12	126.0 (2)	C24—C25—H25	119.4
C20—N5—C27	106.0 (2)	C25—C26—C27	117.3 (3)
C20—N5—Cu	114.92 (18)	C25—C26—H26	121.4
C27—N5—Cu	139.03 (18)	C27—C26—H26	121.4
C20—N6—C22	106.6 (2)	C26—C27—N5	131.1 (2)
C20—N6—C21	126.7 (2)	C26—C27—C22	120.7 (2)
C22—N6—C21	126.7 (2)	N5—C27—C22	108.2 (2)
C10—N7—C19	111.9 (2)	O2—C28—O1	124.0 (2)
C10—N7—C1	109.9 (2)	O2—C28—C29	116.3 (4)
C19—N7—C1	111.5 (2)	O1—C28—C29	119.7 (4)
C10—N7—Cu	106.43 (16)	O2—C28—C29′	122.4 (4)
C19—N7—Cu	110.25 (16)	O1—C28—C29′	113.6 (3)
C1—N7—Cu	106.65 (17)	C29—C28—C29′	6.1 (6)
C37′—N8—C37	55.8 (5)	C30—O3—H3O	117 (5)
C37′—N8—C35	89.1 (7)	C30—C29—C34	114.2 (6)

C37—N8—C35	142.0 (6)	C30—C29—C28	127.5 (8)
C37′—N8—C36	159.2 (7)	C34—C29—C28	118.1 (8)
C37—N8—C36	104.8 (6)	O3—C30—C31	126.7 (10)
C35—N8—C36	111.5 (7)	O3—C30—C29	114.6 (9)
C40—N9—C38	121.4 (3)	C31—C30—C29	118.7 (10)
C40—N9—C39	121.2 (3)	C30—C31—C32	123.3 (19)
C38—N9—C39	117.3 (3)	C30—C31—H31	118.3
C2—C1—N7	109.2 (2)	C32—C31—H31	118.3
C2—C1—H1A	109.8	C33—C32—C31	120 (2)
N7—C1—H1A	109.8	C33—C32—H32	119.8
C2—C1—H1B	109.8	C31—C32—H32	119.8
N7—C1—H1B	109.8	C32—C33—C34	111.6 (17)
H1A—C1—H1B	108.3	C32—C33—H33	124.2
N1—C2—N2	113.1 (3)	C34—C33—H33	124.2
N1—C2—C1	120.4 (2)	C29—C34—C33	129.7 (12)
N2—C2—C1	126.5 (2)	C29—C34—H34	115.1
N2—C3—H3A	109.5	C33—C34—H34	115.1
N2—C3—H3B	109.5	C30′—O3′—H3O′	108 (4)
H3A—C3—H3B	109.5	C30′—C29′—C34′	121.5 (5)
N2—C3—H3C	109.5	C30′—C29′—C28	124.7 (6)
H3A—C3—H3C	109.5	C34′—C29′—C28	113.8 (7)
H3B—C3—H3C	109.5	C33′—C34′—C29′	124.5 (13)
C5—C4—N2	132.5 (3)	C33′—C34′—H34′	117.7
C5—C4—C9	121.9 (3)	C29′—C34′—H34′	117.7
N2—C4—C9	105.5 (3)	C34′—C33′—C32′	113.3 (19)
C6—C5—C4	116.9 (3)	C34′—C33′—H33′	123.3
C6—C5—H5	121.6	C32′—C33′—H33′	123.3
C4—C5—H5	121.6	C31′—C32′—C33′	121.9 (19)
C5—C6—C7	121.9 (3)	C31′—C32′—H32′	119.0
C5—C6—H6	119.1	C33′—C32′—H32′	119.1
C7—C6—H6	119.1	C32′—C31′—C30′	123.4 (15)
C8—C7—C6	121.1 (3)	C32′—C31′—H31′	118.3
C8—C7—H7	119.4	C30′—C31′—H31′	118.3
C6—C7—H7	119.4	O3′—C30′—C29′	118.5 (7)
C7—C8—C9	117.4 (3)	O3′—C30′—C31′	127.2 (9)
C7—C8—H8	121.3	C29′—C30′—C31′	113.5 (8)
C9—C8—H8	121.3	N8—C35—H35A	109.5
N1—C9—C8	130.1 (3)	N8—C35—H35B	109.5
N1—C9—C4	109.1 (3)	H35A—C35—H35B	109.5
C8—C9—C4	120.8 (3)	N8—C35—H35C	109.5
N7—C10—C11	107.0 (2)	H35A—C35—H35C	109.5
N7—C10—H10A	110.3	H35B—C35—H35C	109.5
C11—C10—H10A	110.3	N8—C36—H36A	109.5
N7—C10—H10B	110.3	N8—C36—H36B	109.5
C11—C10—H10B	110.3	H36A—C36—H36B	109.5
H10A—C10—H10B	108.6	N8—C36—H36C	109.5
N3—C11—N4	112.9 (2)	H36A—C36—H36C	109.5
N3—C11—C10	120.6 (2)	H36B—C36—H36C	109.5

N4—C11—C10	126.5 (2)	O8—C37—N8	121.2 (5)
N4—C12—H12A	109.5	O8—C37—H37	119.4
N4—C12—H12B	109.5	N8—C37—H37	119.4
H12A—C12—H12B	109.5	O8—C37′—N8	122.0 (6)
N4—C12—H12C	109.5	O8—C37′—H37′	119.0
H12A—C12—H12C	109.5	N8—C37′—H37′	119.0
H12B—C12—H12C	109.5	N9—C38—H38A	109.5
C14—C13—N4	131.1 (3)	N9—C38—H38B	109.5
C14—C13—C18	122.5 (3)	H38A—C38—H38B	109.5
N4—C13—C18	106.4 (2)	N9—C38—H38C	109.5
C15—C14—C13	116.3 (3)	H38A—C38—H38C	109.5
C15—C14—H14	121.8	H38B—C38—H38C	109.5
C13—C14—H14	121.8	N9—C39—H39A	109.5
C14—C15—C16	121.8 (3)	N9—C39—H39B	109.5
C14—C15—H15	119.1	H39A—C39—H39B	109.5
C16—C15—H15	119.1	N9—C39—H39C	109.5
C17—C16—C15	121.8 (3)	H39A—C39—H39C	109.5
C17—C16—H16	119.1	H39B—C39—H39C	109.5
C15—C16—H16	119.1	O9—C40—N9	125.6 (3)
C16—C17—C18	117.0 (3)	O9—C40—H40	117.2
C16—C17—H17	121.5	N9—C40—H40	117.2
C18—C17—H17	121.5		

N3—Cu—O1—C28	−81.64 (19)	C16—C17—C18—N3	178.8 (3)
N5—Cu—O1—C28	73.03 (19)	C16—C17—C18—C13	−0.7 (4)
N1—Cu—O1—C28	166.14 (18)	C11—N3—C18—C17	−179.1 (3)
O1—Cu—N1—C2	169.54 (17)	Cu—N3—C18—C17	−5.8 (5)
N3—Cu—N1—C2	68.04 (18)	C11—N3—C18—C13	0.4 (3)
N5—Cu—N1—C2	−89.50 (18)	Cu—N3—C18—C13	173.7 (2)
N7—Cu—N1—C2	−7.53 (17)	C14—C13—C18—C17	0.1 (4)
O1—Cu—N1—C9	−32.1 (3)	N4—C13—C18—C17	179.1 (2)
N3—Cu—N1—C9	−133.6 (3)	C14—C13—C18—N3	−179.5 (2)
N5—Cu—N1—C9	68.9 (3)	N4—C13—C18—N3	−0.5 (3)
N7—Cu—N1—C9	150.8 (3)	C10—N7—C19—C20	121.5 (3)
O1—Cu—N3—C11	161.35 (18)	C1—N7—C19—C20	−115.0 (3)
N5—Cu—N3—C11	37.7 (3)	Cu—N7—C19—C20	3.2 (3)
N7—Cu—N3—C11	−17.86 (18)	C27—N5—C20—N6	−1.5 (3)
N1—Cu—N3—C11	−93.24 (19)	Cu—N5—C20—N6	179.33 (18)
O1—Cu—N3—C18	−11.6 (3)	C27—N5—C20—C19	176.3 (3)
N5—Cu—N3—C18	−135.3 (3)	Cu—N5—C20—C19	−2.8 (4)
N7—Cu—N3—C18	169.2 (3)	C22—N6—C20—N5	1.5 (3)
N1—Cu—N3—C18	93.8 (3)	C21—N6—C20—N5	−178.0 (3)
O1—Cu—N5—C20	−174.3 (2)	C22—N6—C20—C19	−176.4 (3)
N3—Cu—N5—C20	−51.5 (3)	C21—N6—C20—C19	4.2 (4)
N7—Cu—N5—C20	3.5 (2)	N7—C19—C20—N5	−0.5 (4)
N1—Cu—N5—C20	83.3 (2)	N7—C19—C20—N6	177.1 (3)
O1—Cu—N5—C27	7.0 (3)	C20—N6—C22—C23	177.3 (3)
N3—Cu—N5—C27	129.7 (3)	C21—N6—C22—C23	−3.3 (5)

N7—Cu—N5—C27	−175.2 (3)	C20—N6—C22—C27	−0.8 (3)
N1—Cu—N5—C27	−95.5 (3)	C21—N6—C22—C27	178.7 (2)
N3—Cu—N7—C10	29.85 (17)	N6—C22—C23—C24	−177.2 (3)
N5—Cu—N7—C10	−125.28 (19)	C27—C22—C23—C24	0.5 (4)
N1—Cu—N7—C10	142.53 (18)	C22—C23—C24—C25	−0.3 (4)
N3—Cu—N7—C19	151.4 (2)	C23—C24—C25—C26	−0.5 (5)
N5—Cu—N7—C19	−3.7 (2)	C24—C25—C26—C27	1.0 (4)
N1—Cu—N7—C19	−95.9 (2)	C25—C26—C27—N5	177.2 (3)
N3—Cu—N7—C1	−87.44 (17)	C25—C26—C27—C22	−0.7 (4)
N5—Cu—N7—C1	117.43 (17)	C20—N5—C27—C26	−177.1 (3)
N1—Cu—N7—C1	25.23 (16)	Cu—N5—C27—C26	1.7 (5)
C10—N7—C1—C2	−153.0 (2)	C20—N5—C27—C22	1.0 (3)
C19—N7—C1—C2	82.3 (3)	Cu—N5—C27—C22	179.8 (2)
Cu—N7—C1—C2	−38.1 (2)	N6—C22—C27—C26	178.2 (2)
C9—N1—C2—N2	0.7 (3)	C23—C22—C27—C26	−0.1 (4)
Cu—N1—C2—N2	166.89 (17)	N6—C22—C27—N5	−0.1 (3)
C9—N1—C2—C1	−179.7 (2)	C23—C22—C27—N5	−178.4 (2)
Cu—N1—C2—C1	−13.6 (3)	Cu—O1—C28—O2	−12.6 (3)
C4—N2—C2—N1	−0.5 (3)	Cu—O1—C28—C29	165.8 (6)
C3—N2—C2—N1	177.3 (3)	Cu—O1—C28—C29′	166.4 (4)
C4—N2—C2—C1	−180.0 (2)	O2—C28—C29—C30	−3.1 (17)
C3—N2—C2—C1	−2.2 (4)	O1—C28—C29—C30	178.4 (13)
N7—C1—C2—N1	36.4 (3)	C29′—C28—C29—C30	173 (9)
N7—C1—C2—N2	−144.1 (2)	O2—C28—C29—C34	172.3 (14)
C2—N2—C4—C5	−178.4 (3)	O1—C28—C29—C34	−6.2 (17)
C3—N2—C4—C5	3.8 (5)	C29′—C28—C29—C34	−11 (8)
C2—N2—C4—C9	0.0 (3)	C34—C29—C30—O3	−179.2 (16)
C3—N2—C4—C9	−177.9 (3)	C28—C29—C30—O3	−4 (2)
N2—C4—C5—C6	177.5 (3)	C34—C29—C30—C31	0 (3)
C9—C4—C5—C6	−0.7 (4)	C28—C29—C30—C31	175.2 (15)
C4—C5—C6—C7	0.5 (4)	O3—C30—C31—C32	180 (2)
C5—C6—C7—C8	0.1 (5)	C29—C30—C31—C32	1 (3)
C6—C7—C8—C9	−0.6 (4)	C30—C31—C32—C33	7 (4)
C2—N1—C9—C8	178.0 (3)	C31—C32—C33—C34	−15 (3)
Cu—N1—C9—C8	19.0 (5)	C30—C29—C34—C33	−10 (3)
C2—N1—C9—C4	−0.7 (3)	C28—C29—C34—C33	174.4 (19)
Cu—N1—C9—C4	−159.7 (2)	C32—C33—C34—C29	17 (3)
C7—C8—C9—N1	−178.2 (3)	O2—C28—C29′—C30′	173.7 (10)
C7—C8—C9—C4	0.5 (4)	O1—C28—C29′—C30′	−5.3 (13)
C5—C4—C9—N1	179.1 (2)	C29—C28—C29′—C30′	170 (9)
N2—C4—C9—N1	0.5 (3)	O2—C28—C29′—C34′	−4.7 (13)
C5—C4—C9—C8	0.2 (4)	O1—C28—C29′—C34′	176.3 (10)
N2—C4—C9—C8	−178.4 (2)	C29—C28—C29′—C34′	−9 (8)
C19—N7—C10—C11	−155.3 (2)	C30′—C29′—C34′—C33′	0 (3)
C1—N7—C10—C11	80.4 (3)	C28—C29′—C34′—C33′	178.7 (19)
Cu—N7—C10—C11	−34.8 (2)	C29′—C34′—C33′—C32′	−3 (4)
C18—N3—C11—N4	−0.2 (3)	C34′—C33′—C32′—C31′	−4 (4)
Cu—N3—C11—N4	−175.55 (17)	C33′—C32′—C31′—C30′	15 (4)

C18—N3—C11—C10	177.2 (2)	C34′—C29′—C30′—O3′	179.5 (14)
Cu—N3—C11—C10	1.9 (3)	C28—C29′—C30′—O3′	1 (2)
C13—N4—C11—N3	0.0 (3)	C34′—C29′—C30′—C31′	9 (2)
C12—N4—C11—N3	−178.5 (2)	C28—C29′—C30′—C31′	−169.1 (13)
C13—N4—C11—C10	−177.3 (3)	C32′—C31′—C30′—O3′	174 (2)
C12—N4—C11—C10	4.3 (4)	C32′—C31′—C30′—C29′	−16 (3)
N7—C10—C11—N3	24.1 (3)	C37′—O8—C37—N8	1.9 (7)
N7—C10—C11—N4	−158.9 (2)	C37′—N8—C37—O8	−1.8 (7)
C11—N4—C13—C14	179.2 (3)	C35—N8—C37—O8	−27.8 (14)
C12—N4—C13—C14	−2.3 (4)	C36—N8—C37—O8	169.9 (7)
C11—N4—C13—C18	0.3 (3)	C37—O8—C37′—N8	−1.9 (7)
C12—N4—C13—C18	178.8 (2)	C37—N8—C37′—O8	1.9 (7)
N4—C13—C14—C15	−178.1 (3)	C35—N8—C37′—O8	166.2 (10)
C18—C13—C14—C15	0.7 (4)	C36—N8—C37′—O8	−21 (2)
C13—C14—C15—C16	−0.9 (4)	C38—N9—C40—O9	−0.9 (6)
C14—C15—C16—C17	0.3 (4)	C39—N9—C40—O9	−177.2 (4)
C15—C16—C17—C18	0.5 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3′—H3*O*′···O1	0.84 (6)	1.72 (6)	2.493 (6)	152 (5)
O3—H3*O*···O2	0.83 (7)	1.87 (6)	2.562 (7)	140 (4)