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(μ_2-Bicarbonato-κ^2O,O')[μ_2-1,4,8,11,14,18,23,27-octaaza-6,16,25(1,3)-tribenzenabicyclo[9.9.9]nonacosaphane]dicopper(II) triperchlorate acetonitrile solvate

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Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.006 Å
R factor = 0.052
wR factor = 0.137
Data-to-parameter ratio = 13.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title complex, $[Cu_2(CHO_3)(C_{36}H_{54}N_8)](ClO_4)_3\cdot C_2H_3N$, at 180 K, the triamino caps of the dicopper(II) cryptate are approximately eclipsed and the benzene rings are arranged so as to form three arms of a twisted triskelion motif. The coordination geometry of one Cu atom is trigonal–bipyramidal, while the second resembles more closely a square pyramid. The latter arrangement accommodates a perchlorate anion coordinated loosely to Cu to give a very distorted octahedral geometry. The cryptate complexes adopt an approximately hexagonal close-packed (hcp) arrangement.

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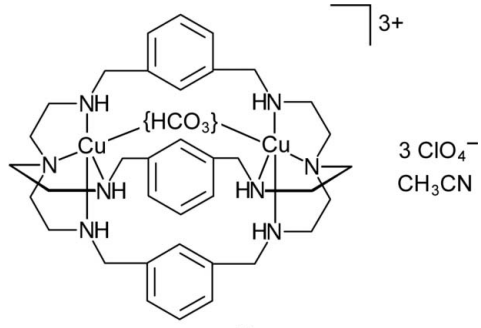
Comment

The title complex, $[C_{37}H_{55}Cu_2N_8O_3]^{3+}(ClO_4^-)_3\cdot C_2H_3N$, (I), contains a dicopper(II) complex of the *meta*-xylyl-linked cryptand $C_{36}H_{54}N_8$ (denoted hereinafter as *L*), in which the metal centres are bridged by a bicarbonate anion, HCO_3^- (Fig. 1). The intracomplex Cu1···Cu2 separation is 6.0853 (11) Å. In projection along the Cu···Cu axis (Fig. 2), the triamino caps at each end of the cryptate appear close to eclipsed, and the benzene rings adopt an arrangement that resembles three arms of a twisted triskelion motif. The C—OH bond of the bridging bicarbonate anion projects into a gap between two of the arms.



(I)

The environments of atoms Cu1 and Cu2 differ significantly (Table 1). For Cu1, the coordination geometry is trigonal–bipyramidal, with Cu1 lying 0.231 (2) Å (towards the centre of the complex) from the equatorial plane defined by atoms N2, N3 and N4. Atoms N1 and O2 lie in the axial coordination sites. For Cu2, the coordination geometry resembles more closely a square pyramid, with Cu2 lying 0.283 (2) Å from the basal plane defined by atoms N5, N6, N7 and O3. Atom N8 lies in the apical coordination site. The distortion towards square-pyramidal geometry for Cu2 reflects a 'flattening' of this end of the cryptand away from the open side to which the bicarbonate C—OH bond projects. This accommodates a perchlo-

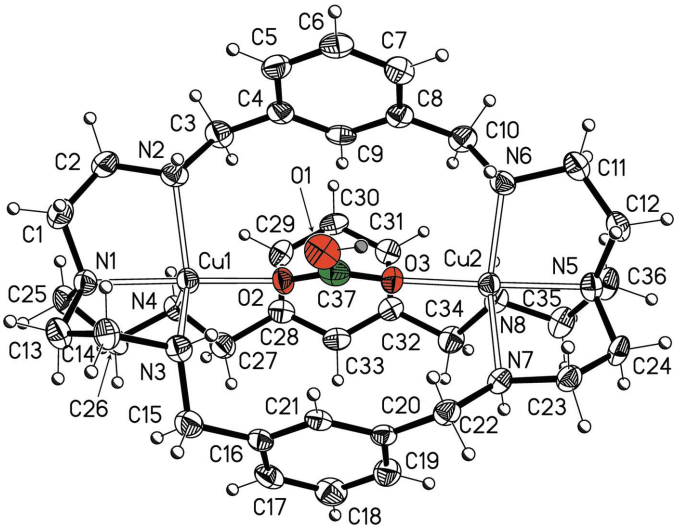


Figure 1
The cryptate unit in (I), showing displacement ellipsoids at the 50% probability level. H atoms are shown as spheres of arbitrary radii. The bicarbonate anion is highlighted in colour.

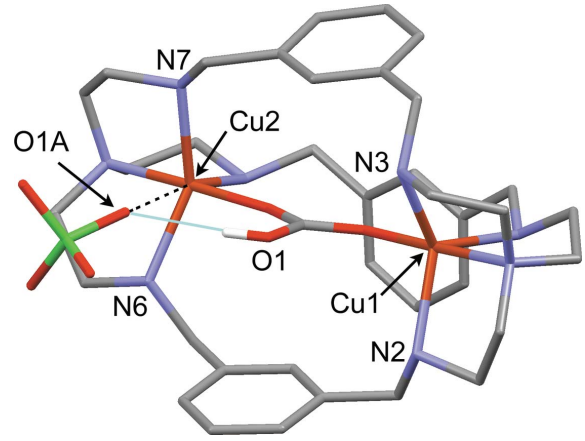


Figure 3
Detail of (I), showing a perchlorate anion approaching atom Cu2, giving rise to a distorted octahedral arrangement. The same O atom (O1*A*) also accepts a hydrogen bond from the bicarbonate anion. To accommodate the perchlorate anion, the cryptate is 'flattened' at the Cu2 end, reflected most clearly in the N6—Cu2—C7 and N2—Cu1—N3 angles (Table 1). H atoms bound to C and N atoms have been omitted.

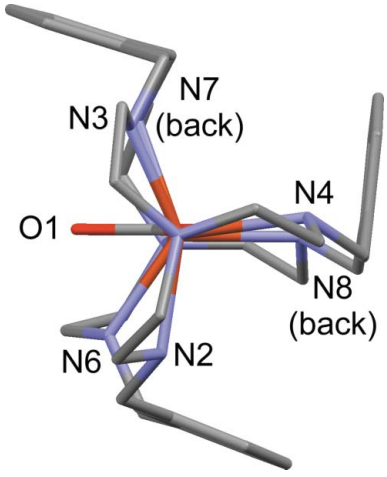


Figure 2
A projection of the cryptate in (I) along the Cu1···Cu2 vector, showing the triamino caps in an approximately eclipsed orientation, and the benzene rings forming three arms of a triskelion-like motif. The C37—O1 bond of the bicarbonate bridge projects between two of the arms. H atoms have been omitted.

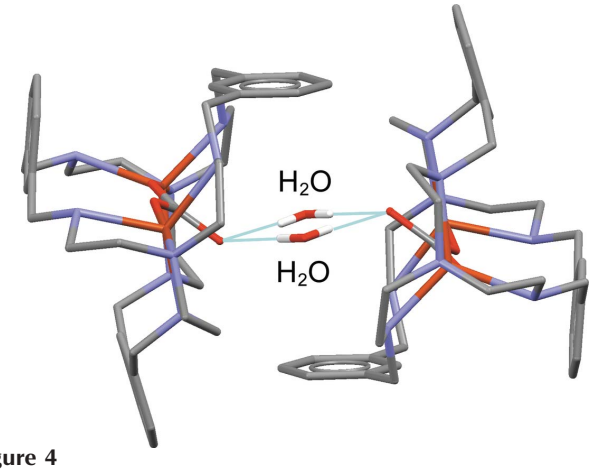


Figure 4
The hydrogen-bonded dimeric units in the carbonate-bridged cryptate $[Cu_2L(CO_3)](ClO_4^-)_2{\cdot}2H_2O$ (Dussart *et al.*, 2002), illustrating the unusual arrangement of the benzene rings that facilitates edge-to-face interactions between cryptates. H atoms bound to C and N atoms have been omitted.

rate anion, which approaches Cu2 [Cu2—O1*A* 3.035 (3) Å], suggesting a very distorted octahedral geometry (Fig. 3). Atom O1*A* also accepts a hydrogen bond from the OH group of the bicarbonate anion [O1···O1*A* 2.935 (5) Å, H1···O1*A* 2.10 Å and O1—H1···O1*A* 173.8°].

We and others have previously described several comparable dicopper(II) cryptates, with various diatomic and polyatomic anionic bridges. The conformation of *L* is observed to be dependent on the nature of the bridging group. In the cyanide-bridged complex $[Cu_2L(CN)](ClO_4^-)_3$, the cryptate adopts regular C_{3h} point symmetry, with a Cu···Cu separation of 5.081 (2) Å (Bond *et al.*, 2005). With polyatomic bridging groups, such as methyl carbonate (Dussart *et al.*, 2002), imidazole (Pierre *et al.*, 1995; Harding *et al.*, 1995), cyanate and azide (Harding *et al.*, 1996), the Cu···Cu separation is much greater (and variable, ranging from *ca* 5.66 to 6.24 Å) and the threefold symmetry about the Cu···Cu axis is lost. In each case, the benzene rings of the cryptand adopt the triskelion arrangement observed in (I) (Fig. 2). Each of these cryptates is also flattened at one end in the manner of (I), accommodating a perchlorate anion that approaches one Cu atom. In the carbonate-bridged complex, $[Cu_2L(CO_3)](ClO_4^-)_2{\cdot}2H_2O$ (Dussart *et al.*, 2002), the cryptand adopts a less regular arrangement (Fig. 4) in which one of the benzene rings is rotated *ca* 90° with respect to the arrangement observed in the other cases. This appears to be driven by the formation of hydrogen-bonded dimeric units *via* water molecules that bridge the carboxylate anions in neighbouring cryptates; the arrangement of the benzene rings facilitates edge-to-face interactions between cryptates. Flattening of the cryptate is not observed in this case.

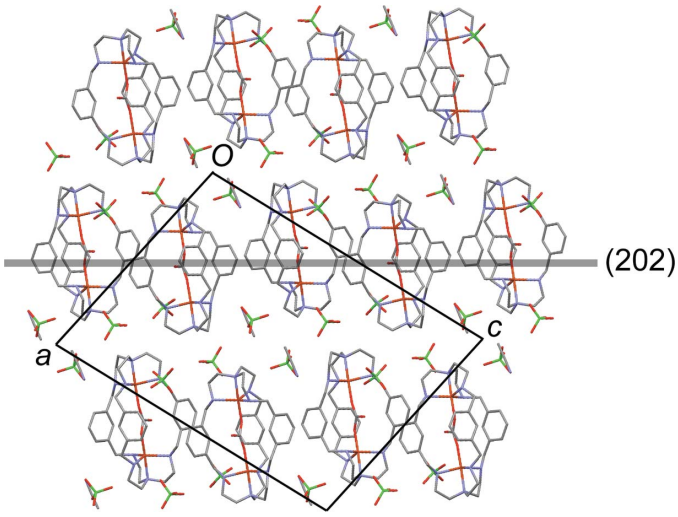


Figure 5
A projection of (I) along the *b* direction, showing layers of cryptates lying in the (202) planes, with their Cu···Cu vectors approximately perpendicular to these planes. The perchlorate anions and acetonitrile solvent molecules lie between the layers. H atoms have been omitted.

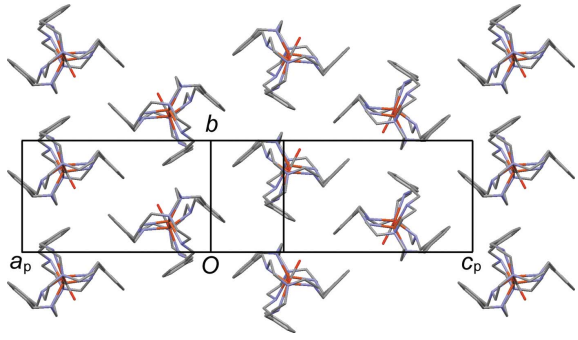


Figure 6
A projection on to a single layer in (202), showing face-to-face and edge-to-face arrangements between benzene rings in adjacent cryptands of (I). If the cryptands are considered to be cylindrically symmetric, the arrangement approximates hexagonal close-packed. H atoms have been omitted.

In the crystal structure of (I), the cryptate complexes lie in layers in the (202) planes (Fig. 5), with the Cu···Cu vectors lying approximately perpendicular to the layer planes. Projection on to a single layer (Fig. 6) highlights a combination of offset face-to-face and edge-to-face interactions between the benzene rings. If the cryptands are considered to be cylindrically symmetric, the layers are essentially close-packed in two dimensions. These layers stack in an *ABAB* manner (Fig. 5), so that the overall packing arrangement approximates hexagonal close-packed (hcp). The perchlorate anions and acetonitrile molecules are situated between the cryptand layers.

Experimental

A solution of $Cu(ClO_4)_2·6H_2O$ (178 mg, 0.48 mmol) dissolved in MeOH (5 ml) was added dropwise to the cryptand ligand, $C_{36}H_{54}N_8$ (121 mg, 0.2 mmol), dissolved in methanol (5 ml). The dark blue–green solution became turbid immediately, and a blue-green powder was filtered off after 2 h. Slow recrystallization from acetonitrile over several days yielded green laths of the acetonitrile solvate of (I). The acetonitrile solvent in the crystal structure is not retained over the period required for CHN analysis, which agrees with an unsolvated complex. Spectroscopic analysis: IR (Nujol, ν, cm^{-1}): 3436 (*s*), 2877 (*w*), 1635 (*ms*), 1450 (*m*), 1400 (*sh*), 1121 (*vs*), 801, 757, 702 (*w*), 627 (*ms*). CHN analysis {%, values in parentheses calculated for $[C_{37}H_{55}Cu_2N_8O_3](ClO_4)_3$}: C 40.74 (40.96), H 5.00 (5.11), N 9.97 (10.32). It is notable that, when the recrystallization system incorporates methanol, the product of recrystallation is the methyl carbonate-bridged dicopper(II) cryptate, rather than the bicarbonate-bridged complex (Dussart *et al.*, 2002).

Crystal data

$[Cu_2(CHO_3)(C_{36}H_{54}N_8)](ClO_4)_3·C_2H_3N$
M_r = 1126.37
Monoclinic, $P2_1/n$
a = 19.690 (4) Å
b = 8.862 (2) Å
c = 26.828 (5) Å
β = 100.721 (2)°
V = 4599.6 (16) Å^3
Z = 4
D_x = 1.627 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2245 reflections
θ = 4.8–24.0°
μ = 1.18 mm^{-1}
T = 180 (2) K
Lath, green
0.24 × 0.10 × 0.02 mm

Data collection

Bruker–Nonius X8APEX-II CCD area-detector diffractometer
Thin–slice ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.319, T_{max} = 0.977
16940 measured reflections
8362 independent reflections
5186 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 25.5°
$h = -23 \rightarrow 23$
$k = -10 \rightarrow 6$
$l = -32 \rightarrow 26$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.137
S = 0.99
8362 reflections
613 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0686P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O2	1.938 (3)	Cu2—N6	2.070 (3)
Cu1—N1	2.054 (3)	Cu2—N7	2.084 (3)
Cu1—N3	2.097 (4)	Cu2—N8	2.256 (4)
Cu1—N2	2.153 (3)	C37—O3	1.241 (5)
Cu1—N4	2.167 (4)	C37—O2	1.257 (5)
Cu2—O3	1.957 (3)	C37—O1	1.370 (6)
Cu2—N5	2.054 (3)		
O2—Cu1—N1	177.34 (14)	O3—Cu2—N5	178.32 (14)
O2—Cu1—N3	96.54 (13)	O3—Cu2—N6	94.51 (13)
N1—Cu1—N3	84.59 (14)	N5—Cu2—N6	84.18 (14)
O2—Cu1—N2	97.41 (12)	O3—Cu2—N7	97.17 (12)
N1—Cu1—N2	83.86 (13)	N5—Cu2—N7	84.50 (13)
N3—Cu1—N2	125.14 (14)	N6—Cu2—N7	145.49 (14)
O2—Cu1—N4	94.56 (12)	O3—Cu2—N8	96.71 (13)
N1—Cu1—N4	82.82 (13)	N5—Cu2—N8	82.65 (13)
N3—Cu1—N4	124.02 (14)	N6—Cu2—N8	105.63 (14)
N2—Cu1—N4	107.32 (14)	N7—Cu2—N8	105.08 (13)

H atoms bound to C atoms were positioned geometrically and allowed to ride during subsequent refinement, with C—H = 0.95 Å for the benzene rings and C—H = 0.99 Å for the methylene groups. In all cases, $U_{iso}(H) = 1.2U_{eq}(C)$. All H atoms bound to N atoms could be distinguished in a difference Fourier map, but were included in

calculated positions and allowed to ride, with N—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(N)$. The calculated positions were in good agreement with those indicated by the difference Fourier map. The H atom of the bicarbonate bridge could not be distinguished, but the C37—O1 bond length, together with the requirement for charge balance, confirms the presence of the OH group. The H atom was placed in a calculated position in the plane of the HCO_3^- group, so as to form the best hydrogen bond (AFIX 83 in *SHELXL97*). It was subsequently allowed to ride, with $U_{iso}(H) = 1.2U_{eq}(O)$.

Data collection: *APEX2* (Bruker–Nonius, 2004); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

JN thanks the Department of Chemistry at the University of Southern Denmark for hospitality and the Velux Foundation for funding during her stay in Odense. ADB and CJM are grateful to the Danish Natural Science Research Council (SNF) and Carlsbergfondet (Denmark) for provision of the X-ray equipment. JN also acknowledges the assistance of a Leverhulme Emeritus Fellowship during the preparation of this manuscript.

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supporting information

Acta Cryst. (2005). E**61**, m1379–m1382 [https://doi.org/10.1107/S1600536805018581]

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$F(000) = 2336$
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$\theta_{max} = 25.5°$, $\theta_{min} = 4.7°$
$h = -23\rightarrow23$
$k = -10\rightarrow6$
$l = -32\rightarrow26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.137$
$S = 0.99$
8362 reflections
613 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0686P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.73$ e Å^{-3}
$\Delta\rho_{min} = -0.54$ 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.
Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)
12.4504 (0.0203) *x* - 1.9579 (0.0106) *y* + 16.4173 (0.0275) *z* = 3.6818 (0.0064)
* 0.0000 (0.0000) N2 * 0.0000 (0.0000) N3 * 0.0000 (0.0000) N4 0.2306 (0.0019) Cu1
Rms deviation of fitted atoms = 0.0000
5.8803 (0.0256) *x* + 8.3060 (0.0047) *y* - 6.2322 (0.0352) *z* = 3.8216 (0.0144)
Angle to previous plane (with approximate e.s.d.) = 81.27 (0.10)
* -0.3190 (0.0020) N5 * 0.2995 (0.0019) N6 * 0.2895 (0.0018) N7 * -0.2700 (0.0017) O3 - 0.2827 (0.0018) Cu2
Rms deviation of fitted atoms = 0.2950

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	0.29017 (2)	0.27965 (6)	0.051599 (19)	0.02501 (16)
Cu2	0.53303 (2)	0.21943 (6)	0.227530 (18)	0.02325 (15)
N1	0.20900 (17)	0.3265 (4)	−0.00633 (13)	0.0272 (9)
N2	0.34657 (17)	0.2473 (4)	−0.00907 (13)	0.0275 (9)
H2C	0.3696	0.3371	−0.0126	0.033*
N3	0.26675 (17)	0.4895 (4)	0.08035 (13)	0.0259 (8)
H3C	0.3085	0.5388	0.0915	0.031*
N4	0.23184 (16)	0.0751 (4)	0.05740 (13)	0.0283 (9)
H4A	0.2442	0.0056	0.0347	0.034*
N5	0.61463 (17)	0.2021 (4)	0.28730 (13)	0.0268 (9)
N6	0.60866 (16)	0.2030 (4)	0.18355 (13)	0.0263 (8)
H6B	0.6098	0.2972	0.1685	0.032*
N7	0.48957 (17)	0.3559 (4)	0.27654 (12)	0.0226 (8)
H7B	0.4694	0.2925	0.2973	0.027*
N8	0.51275 (17)	−0.0192 (4)	0.25014 (13)	0.0265 (8)
H8A	0.5334	−0.0828	0.2298	0.032*
C1	0.2380 (2)	0.3465 (6)	−0.05358 (16)	0.0362 (12)
H1A	0.2583	0.4486	−0.0540	0.043*
H1B	0.2007	0.3364	−0.0837	0.043*
C2	0.2929 (2)	0.2288 (6)	−0.05545 (16)	0.0374 (12)
H2A	0.2726	0.1264	−0.0565	0.045*
H2B	0.3134	0.2429	−0.0861	0.045*
C3	0.3985 (2)	0.1236 (5)	−0.00546 (17)	0.0328 (11)
H3A	0.4011	0.0876	−0.0400	0.039*
H3B	0.3835	0.0380	0.0136	0.039*
C4	0.4695 (2)	0.1750 (5)	0.02077 (16)	0.0275 (11)
C5	0.5043 (2)	0.2841 (6)	−0.00168 (17)	0.0334 (11)
H5A	0.4838	0.3255	−0.0336	0.040*
C6	0.5688 (2)	0.3327 (6)	0.02246 (17)	0.0344 (12)

H6A	0.5922	0.4084	0.0071	0.041*
C7	0.5995 (2)	0.2722 (5)	0.06878 (17)	0.0308 (11)
H7A	0.6438	0.3061	0.0851	0.037*
C8	0.5652 (2)	0.1616 (5)	0.09137 (16)	0.0266 (10)
C9	0.5004 (2)	0.1141 (5)	0.06697 (16)	0.0261 (10)
H9A	0.4768	0.0385	0.0822	0.031*
C10	0.5988 (2)	0.0921 (5)	0.14057 (16)	0.0314 (11)
H10A	0.6443	0.0507	0.1370	0.038*
H10B	0.5699	0.0073	0.1486	0.038*
C11	0.6783 (2)	0.1848 (6)	0.21720 (17)	0.0359 (12)
H11A	0.7143	0.2332	0.2013	0.043*
H11B	0.6897	0.0763	0.2220	0.043*
C12	0.6762 (2)	0.2578 (6)	0.26778 (17)	0.0335 (12)
H12A	0.7189	0.2329	0.2922	0.040*
H12B	0.6737	0.3689	0.2638	0.040*
C13	0.1759 (2)	0.4706 (5)	0.00599 (18)	0.0337 (11)
H13A	0.1530	0.5210	−0.0256	0.040*
H13B	0.1406	0.4493	0.0269	0.040*
C14	0.2311 (2)	0.5706 (5)	0.03451 (16)	0.0321 (11)
H14A	0.2647	0.5973	0.0127	0.039*
H14B	0.2103	0.6650	0.0445	0.039*
C15	0.2266 (2)	0.4991 (6)	0.12225 (16)	0.0334 (11)
H15A	0.1821	0.4457	0.1118	0.040*
H15B	0.2162	0.6063	0.1280	0.040*
C16	0.2641 (2)	0.4323 (5)	0.17125 (16)	0.0269 (10)
C17	0.2316 (2)	0.3299 (6)	0.19773 (18)	0.0332 (11)
H17A	0.1857	0.2981	0.1844	0.040*
C18	0.2657 (2)	0.2739 (6)	0.24361 (19)	0.0378 (12)
H18A	0.2429	0.2042	0.2618	0.045*
C19	0.3327 (2)	0.3181 (5)	0.26334 (17)	0.0337 (12)
H19A	0.3555	0.2785	0.2950	0.040*
C20	0.3667 (2)	0.4195 (5)	0.23735 (15)	0.0240 (10)
C21	0.33109 (19)	0.4778 (5)	0.19178 (15)	0.0237 (10)
H21A	0.3531	0.5507	0.1742	0.028*
C22	0.4382 (2)	0.4756 (5)	0.25745 (16)	0.0269 (10)
H22A	0.4548	0.5319	0.2302	0.032*
H22B	0.4362	0.5473	0.2854	0.032*
C23	0.5515 (2)	0.4247 (5)	0.30857 (15)	0.0270 (10)
H23A	0.5377	0.4821	0.3368	0.032*
H23B	0.5740	0.4952	0.2881	0.032*
C24	0.6008 (2)	0.3013 (5)	0.32936 (16)	0.0285 (11)
H24A	0.6447	0.3459	0.3473	0.034*
H24B	0.5809	0.2405	0.3541	0.034*
C25	0.1586 (2)	0.1994 (5)	−0.01240 (17)	0.0318 (11)
H25A	0.1702	0.1261	−0.0373	0.038*
H25B	0.1115	0.2384	−0.0253	0.038*
C26	0.1602 (2)	0.1227 (5)	0.03730 (17)	0.0338 (11)
H26A	0.1441	0.1927	0.0614	0.041*

H26B	0.1293	0.0337	0.0327	0.041*
C27	0.2364 (2)	−0.0020 (6)	0.10667 (17)	0.0342 (11)
H27A	0.2009	−0.0822	0.1033	0.041*
H27B	0.2263	0.0715	0.1321	0.041*
C28	0.3067 (2)	−0.0713 (5)	0.12545 (16)	0.0266 (10)
C29	0.3397 (2)	−0.1557 (5)	0.09385 (17)	0.0301 (11)
H29A	0.3176	−0.1732	0.0597	0.036*
C30	0.4050 (2)	−0.2151 (5)	0.11157 (16)	0.0295 (10)
H30A	0.4277	−0.2724	0.0896	0.035*
C31	0.4366 (2)	−0.1903 (5)	0.16129 (16)	0.0288 (11)
H31A	0.4809	−0.2327	0.1735	0.035*
C32	0.4052 (2)	−0.1050 (5)	0.19334 (16)	0.0253 (10)
C33	0.3398 (2)	−0.0469 (5)	0.17505 (16)	0.0280 (10)
H33A	0.3172	0.0108	0.1970	0.034*
C34	0.4406 (2)	−0.0725 (6)	0.24700 (16)	0.0336 (11)
H34A	0.4140	0.0054	0.2616	0.040*
H34B	0.4409	−0.1653	0.2676	0.040*
C35	0.5536 (2)	−0.0310 (5)	0.30222 (16)	0.0324 (11)
H35A	0.5597	−0.1384	0.3122	0.039*
H35B	0.5290	0.0203	0.3264	0.039*
C36	0.6228 (2)	0.0412 (5)	0.30366 (17)	0.0330 (11)
H36A	0.6500	0.0358	0.3386	0.040*
H36B	0.6483	−0.0144	0.2810	0.040*
C37	0.4188 (2)	0.2857 (6)	0.13148 (18)	0.0345 (11)
O1	0.43582 (16)	0.4221 (4)	0.11308 (12)	0.0421 (9)
H1	0.4725	0.4542	0.1311	0.051*
O2	0.36435 (14)	0.2276 (3)	0.10716 (10)	0.0265 (7)
O3	0.45657 (14)	0.2315 (4)	0.16947 (11)	0.0354 (8)
Cl1	0.61258 (6)	0.62957 (13)	0.17221 (4)	0.0338 (3)
O1A	0.56061 (16)	0.5227 (4)	0.18270 (13)	0.0437 (9)
O1B	0.58808 (19)	0.6973 (4)	0.12405 (13)	0.0569 (11)
O1C	0.6221 (2)	0.7443 (4)	0.21059 (15)	0.0614 (11)
O1D	0.67583 (16)	0.5502 (4)	0.17237 (15)	0.0548 (10)
Cl2	0.79585 (6)	0.17227 (15)	0.09276 (5)	0.0429 (3)
O2A	0.8661 (2)	0.1466 (9)	0.1035 (3)	0.158 (3)
O2B	0.7664 (2)	0.0698 (5)	0.12314 (15)	0.0713 (12)
O2C	0.7673 (3)	0.1472 (5)	0.04070 (15)	0.0830 (14)
O2D	0.7788 (3)	0.3188 (5)	0.1048 (2)	0.118 (2)
Cl3	0.45995 (6)	0.21127 (16)	0.41217 (4)	0.0390 (3)
O3A	0.43582 (19)	0.1711 (5)	0.36017 (13)	0.0659 (12)
O3B	0.4050 (2)	0.2112 (7)	0.43867 (15)	0.0942 (18)
O3C	0.5109 (2)	0.1071 (5)	0.43351 (17)	0.0931 (17)
O3D	0.4919 (2)	0.3542 (5)	0.41699 (18)	0.0860 (14)
N1S	0.0634 (2)	0.2256 (6)	0.13863 (18)	0.0577 (13)
C1S	0.0288 (2)	0.2294 (6)	0.1001 (2)	0.0420 (13)
C2S	−0.0136 (3)	0.2325 (7)	0.0497 (2)	0.0579 (17)
H2S1	0.0022	0.3137	0.0298	0.087*
H2S2	−0.0620	0.2501	0.0523	0.087*

H2S3	−0.0097	0.1355	0.0329	0.087*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0223 (3)	0.0258 (3)	0.0253 (3)	0.0021 (2)	0.0002 (2)	−0.0031 (2)
Cu2	0.0232 (3)	0.0232 (3)	0.0224 (3)	0.0022 (2)	0.0018 (2)	−0.0004 (2)
N1	0.0254 (19)	0.030 (2)	0.0245 (19)	0.0030 (16)	0.0009 (15)	−0.0033 (17)
N2	0.0280 (19)	0.026 (2)	0.029 (2)	−0.0006 (16)	0.0080 (16)	−0.0078 (17)
N3	0.0274 (19)	0.021 (2)	0.029 (2)	0.0012 (16)	0.0042 (15)	−0.0029 (17)
N4	0.0245 (18)	0.027 (2)	0.032 (2)	0.0020 (16)	0.0038 (15)	0.0024 (18)
N5	0.0253 (18)	0.025 (2)	0.0274 (19)	0.0013 (16)	−0.0016 (15)	0.0007 (17)
N6	0.0235 (18)	0.026 (2)	0.029 (2)	0.0046 (16)	0.0064 (15)	0.0004 (17)
N7	0.0289 (18)	0.018 (2)	0.0205 (18)	−0.0007 (15)	0.0035 (14)	0.0028 (16)
N8	0.034 (2)	0.019 (2)	0.025 (2)	−0.0005 (16)	0.0026 (16)	−0.0001 (16)
C1	0.036 (3)	0.046 (3)	0.026 (2)	−0.003 (2)	0.001 (2)	0.002 (2)
C2	0.034 (3)	0.055 (4)	0.024 (2)	−0.002 (2)	0.005 (2)	−0.005 (2)
C3	0.033 (2)	0.028 (3)	0.037 (3)	0.005 (2)	0.006 (2)	−0.011 (2)
C4	0.027 (2)	0.028 (3)	0.029 (2)	0.0036 (19)	0.0078 (19)	−0.013 (2)
C5	0.037 (3)	0.038 (3)	0.027 (2)	0.005 (2)	0.012 (2)	−0.001 (2)
C6	0.037 (3)	0.034 (3)	0.036 (3)	−0.006 (2)	0.017 (2)	0.002 (2)
C7	0.029 (2)	0.027 (3)	0.037 (3)	−0.004 (2)	0.008 (2)	−0.007 (2)
C8	0.032 (2)	0.021 (3)	0.028 (2)	0.005 (2)	0.0086 (19)	−0.007 (2)
C9	0.031 (2)	0.019 (3)	0.033 (3)	0.0033 (19)	0.017 (2)	−0.005 (2)
C10	0.038 (3)	0.025 (3)	0.031 (3)	0.009 (2)	0.008 (2)	−0.003 (2)
C11	0.024 (2)	0.045 (4)	0.037 (3)	0.005 (2)	0.003 (2)	0.003 (2)
C12	0.021 (2)	0.042 (3)	0.036 (3)	−0.001 (2)	−0.0003 (19)	0.001 (2)
C13	0.028 (2)	0.032 (3)	0.038 (3)	0.006 (2)	0.000 (2)	0.000 (2)
C14	0.032 (2)	0.030 (3)	0.033 (3)	0.007 (2)	0.003 (2)	0.006 (2)
C15	0.030 (2)	0.035 (3)	0.035 (3)	0.004 (2)	0.005 (2)	−0.006 (2)
C16	0.025 (2)	0.028 (3)	0.028 (2)	0.0081 (19)	0.0058 (18)	−0.006 (2)
C17	0.021 (2)	0.037 (3)	0.043 (3)	−0.001 (2)	0.011 (2)	−0.004 (2)
C18	0.037 (3)	0.039 (3)	0.041 (3)	−0.003 (2)	0.017 (2)	0.008 (2)
C19	0.037 (3)	0.036 (3)	0.028 (2)	0.005 (2)	0.006 (2)	0.005 (2)
C20	0.026 (2)	0.024 (3)	0.024 (2)	0.0045 (18)	0.0078 (18)	−0.004 (2)
C21	0.023 (2)	0.023 (3)	0.028 (2)	0.0014 (18)	0.0103 (18)	−0.004 (2)
C22	0.032 (2)	0.023 (3)	0.025 (2)	0.0040 (19)	0.0051 (19)	−0.003 (2)
C23	0.031 (2)	0.026 (3)	0.023 (2)	0.0011 (19)	0.0029 (18)	−0.005 (2)
C24	0.034 (2)	0.028 (3)	0.020 (2)	0.000 (2)	−0.0046 (18)	−0.005 (2)
C25	0.023 (2)	0.034 (3)	0.036 (3)	−0.005 (2)	−0.0035 (19)	−0.010 (2)
C26	0.023 (2)	0.031 (3)	0.046 (3)	−0.002 (2)	0.004 (2)	−0.005 (2)
C27	0.029 (2)	0.037 (3)	0.036 (3)	0.001 (2)	0.007 (2)	0.002 (2)
C28	0.028 (2)	0.019 (3)	0.034 (3)	−0.0073 (19)	0.0098 (19)	−0.001 (2)
C29	0.037 (3)	0.025 (3)	0.027 (2)	−0.010 (2)	0.001 (2)	−0.001 (2)
C30	0.041 (3)	0.020 (3)	0.030 (2)	−0.002 (2)	0.015 (2)	−0.007 (2)
C31	0.033 (2)	0.020 (3)	0.034 (3)	0.0000 (19)	0.006 (2)	0.001 (2)
C32	0.031 (2)	0.018 (3)	0.028 (2)	−0.0065 (19)	0.0078 (19)	0.000 (2)
C33	0.032 (2)	0.023 (3)	0.032 (3)	−0.005 (2)	0.0135 (19)	0.000 (2)

C34	0.036 (3)	0.034 (3)	0.031 (3)	−0.006 (2)	0.007 (2)	0.003 (2)
C35	0.047 (3)	0.019 (3)	0.029 (3)	0.000 (2)	0.001 (2)	0.008 (2)
C36	0.042 (3)	0.022 (3)	0.030 (3)	0.007 (2)	−0.006 (2)	0.000 (2)
C37	0.038 (3)	0.027 (3)	0.041 (3)	0.007 (2)	0.013 (2)	0.000 (2)
O1	0.0435 (19)	0.031 (2)	0.052 (2)	−0.0041 (16)	0.0103 (16)	−0.0004 (17)
O2	0.0198 (14)	0.0296 (19)	0.0277 (16)	−0.0006 (13)	−0.0014 (12)	−0.0029 (14)
O3	0.0290 (16)	0.052 (2)	0.0232 (17)	0.0126 (15)	−0.0007 (13)	−0.0001 (16)
Cl1	0.0342 (6)	0.0262 (7)	0.0418 (7)	0.0002 (5)	0.0093 (5)	−0.0002 (6)
O1A	0.0425 (19)	0.031 (2)	0.062 (2)	0.0001 (15)	0.0214 (17)	0.0116 (18)
O1B	0.062 (2)	0.067 (3)	0.042 (2)	0.001 (2)	0.0093 (18)	0.023 (2)
O1C	0.069 (3)	0.047 (3)	0.064 (3)	0.002 (2)	0.000 (2)	−0.022 (2)
O1D	0.0333 (18)	0.048 (3)	0.083 (3)	0.0060 (17)	0.0085 (18)	−0.003 (2)
Cl2	0.0365 (7)	0.0338 (8)	0.0586 (8)	0.0039 (5)	0.0095 (6)	0.0065 (6)
O2A	0.039 (3)	0.251 (8)	0.190 (6)	0.044 (4)	0.040 (3)	0.124 (6)
O2B	0.085 (3)	0.079 (3)	0.056 (2)	−0.027 (2)	0.028 (2)	0.004 (2)
O2C	0.155 (4)	0.050 (3)	0.044 (2)	0.021 (3)	0.019 (3)	0.008 (2)
O2D	0.173 (5)	0.029 (3)	0.122 (4)	0.020 (3)	−0.052 (4)	−0.023 (3)
Cl3	0.0349 (6)	0.0486 (9)	0.0333 (6)	−0.0048 (6)	0.0057 (5)	0.0077 (6)
O3A	0.062 (2)	0.103 (4)	0.030 (2)	0.003 (2)	0.0010 (18)	0.009 (2)
O3B	0.053 (3)	0.181 (6)	0.055 (3)	−0.048 (3)	0.025 (2)	−0.026 (3)
O3C	0.104 (4)	0.065 (3)	0.086 (3)	0.024 (3)	−0.045 (3)	−0.006 (3)
O3D	0.104 (4)	0.046 (3)	0.111 (4)	−0.019 (3)	0.030 (3)	0.005 (3)
N1S	0.058 (3)	0.076 (4)	0.039 (3)	−0.009 (3)	0.009 (2)	0.000 (3)
C1S	0.036 (3)	0.051 (4)	0.044 (3)	−0.003 (2)	0.020 (2)	0.002 (3)
C2S	0.045 (3)	0.085 (5)	0.042 (3)	0.002 (3)	0.005 (3)	0.009 (3)

Geometric parameters (Å, º)

Cu1—O2	1.938 (3)	C15—H15B	0.990
Cu1—N1	2.054 (3)	C16—C17	1.381 (6)
Cu1—N3	2.097 (4)	C16—C21	1.391 (5)
Cu1—N2	2.153 (3)	C17—C18	1.380 (6)
Cu1—N4	2.167 (4)	C17—H17A	0.950
Cu2—O3	1.957 (3)	C18—C19	1.384 (6)
Cu2—N5	2.054 (3)	C18—H18A	0.950
Cu2—N6	2.070 (3)	C19—C20	1.385 (6)
Cu2—N7	2.084 (3)	C19—H19A	0.950
Cu2—N8	2.256 (4)	C20—C21	1.391 (5)
N1—C25	1.490 (5)	C20—C22	1.495 (5)
N1—C1	1.495 (5)	C21—H21A	0.950
N1—C13	1.498 (6)	C22—H22A	0.990
N2—C2	1.484 (5)	C22—H22B	0.990
N2—C3	1.490 (5)	C23—C24	1.500 (6)
N2—H2C	0.930	C23—H23A	0.990
N3—C14	1.483 (5)	C23—H23B	0.990
N3—C15	1.492 (5)	C24—H24A	0.990
N3—H3C	0.930	C24—H24B	0.990
N4—C26	1.475 (5)	C25—C26	1.492 (6)

N4—C27	1.475 (5)	C25—H25A	0.990
N4—H4A	0.930	C25—H25B	0.990
N5—C12	1.492 (5)	C26—H26A	0.990
N5—C36	1.492 (6)	C26—H26B	0.990
N5—C24	1.495 (5)	C27—C28	1.513 (6)
N6—C10	1.500 (5)	C27—H27A	0.990
N6—C11	1.504 (5)	C27—H27B	0.990
N6—H6B	0.930	C28—C29	1.380 (6)
N7—C23	1.485 (5)	C28—C33	1.385 (6)
N7—C22	1.489 (5)	C29—C30	1.388 (6)
N7—H7B	0.930	C29—H29A	0.950
N8—C35	1.481 (5)	C30—C31	1.381 (6)
N8—C34	1.484 (5)	C30—H30A	0.950
N8—H8A	0.930	C31—C32	1.376 (6)
C1—C2	1.510 (7)	C31—H31A	0.950
C1—H1A	0.990	C32—C33	1.389 (6)
C1—H1B	0.990	C32—C34	1.506 (6)
C2—H2A	0.990	C33—H33A	0.950
C2—H2B	0.990	C34—H34A	0.990
C3—C4	1.513 (6)	C34—H34B	0.990
C3—H3A	0.990	C35—C36	1.499 (6)
C3—H3B	0.990	C35—H35A	0.990
C4—C9	1.385 (6)	C35—H35B	0.990
C4—C5	1.386 (6)	C36—H36A	0.990
C5—C6	1.383 (6)	C36—H36B	0.990
C5—H5A	0.950	C37—O3	1.241 (5)
C6—C7	1.385 (6)	C37—O2	1.257 (5)
C6—H6A	0.950	C37—O1	1.370 (6)
C7—C8	1.392 (6)	O1—H1	0.840
C7—H7A	0.950	Cl1—O1B	1.425 (3)
C8—C9	1.386 (6)	Cl1—O1D	1.429 (3)
C8—C10	1.495 (6)	Cl1—O1C	1.434 (4)
C9—H9A	0.950	Cl1—O1A	1.459 (3)
C10—H10A	0.990	Cl2—O2A	1.378 (4)
C10—H10B	0.990	Cl2—O2D	1.394 (5)
C11—C12	1.511 (6)	Cl2—O2B	1.414 (4)
C11—H11A	0.990	Cl2—O2C	1.423 (4)
C11—H11B	0.990	Cl3—O3B	1.400 (4)
C12—H12A	0.990	Cl3—O3C	1.404 (4)
C12—H12B	0.990	Cl3—O3D	1.410 (4)
C13—C14	1.497 (6)	Cl3—O3A	1.433 (4)
C13—H13A	0.990	N1S—C1S	1.127 (6)
C13—H13B	0.990	C1S—C2S	1.452 (7)
C14—H14A	0.990	C2S—H2S1	0.980
C14—H14B	0.990	C2S—H2S2	0.980
C15—C16	1.504 (6)	C2S—H2S3	0.980
C15—H15A	0.990		

O2—Cu1—N1	177.34 (14)	N3—C14—H14B	109.9
O2—Cu1—N3	96.54 (13)	C13—C14—H14B	109.9
N1—Cu1—N3	84.59 (14)	H14A—C14—H14B	108.3
O2—Cu1—N2	97.41 (12)	N3—C15—C16	113.2 (3)
N1—Cu1—N2	83.86 (13)	N3—C15—H15A	108.9
N3—Cu1—N2	125.14 (14)	C16—C15—H15A	108.9
O2—Cu1—N4	94.56 (12)	N3—C15—H15B	108.9
N1—Cu1—N4	82.82 (13)	C16—C15—H15B	108.9
N3—Cu1—N4	124.02 (14)	H15A—C15—H15B	107.8
N2—Cu1—N4	107.32 (14)	C17—C16—C21	118.9 (4)
O3—Cu2—N5	178.32 (14)	C17—C16—C15	120.6 (4)
O3—Cu2—N6	94.51 (13)	C21—C16—C15	120.4 (4)
N5—Cu2—N6	84.18 (14)	C18—C17—C16	120.0 (4)
O3—Cu2—N7	97.17 (12)	C18—C17—H17A	120.0
N5—Cu2—N7	84.50 (13)	C16—C17—H17A	120.0
N6—Cu2—N7	145.49 (14)	C17—C18—C19	120.7 (4)
O3—Cu2—N8	96.71 (13)	C17—C18—H18A	119.6
N5—Cu2—N8	82.65 (13)	C19—C18—H18A	119.6
N6—Cu2—N8	105.63 (14)	C18—C19—C20	120.5 (4)
N7—Cu2—N8	105.08 (13)	C18—C19—H19A	119.8
C25—N1—C1	110.5 (3)	C20—C19—H19A	119.8
C25—N1—C13	111.1 (3)	C19—C20—C21	118.1 (4)
C1—N1—C13	109.6 (4)	C19—C20—C22	123.0 (4)
C25—N1—Cu1	109.8 (3)	C21—C20—C22	118.7 (4)
C1—N1—Cu1	107.4 (2)	C20—C21—C16	121.7 (4)
C13—N1—Cu1	108.3 (2)	C20—C21—H21A	119.1
C2—N2—C3	110.3 (3)	C16—C21—H21A	119.1
C2—N2—Cu1	105.2 (2)	N7—C22—C20	114.9 (4)
C3—N2—Cu1	119.6 (3)	N7—C22—H22A	108.5
C2—N2—H2C	107.1	C20—C22—H22A	108.5
C3—N2—H2C	107.1	N7—C22—H22B	108.5
Cu1—N2—H2C	107.1	C20—C22—H22B	108.5
C14—N3—C15	111.2 (3)	H22A—C22—H22B	107.5
C14—N3—Cu1	103.1 (3)	N7—C23—C24	108.7 (4)
C15—N3—Cu1	120.7 (3)	N7—C23—H23A	109.9
C14—N3—H3C	107.0	C24—C23—H23A	109.9
C15—N3—H3C	107.0	N7—C23—H23B	109.9
Cu1—N3—H3C	107.0	C24—C23—H23B	109.9
C26—N4—C27	110.8 (3)	H23A—C23—H23B	108.3
C26—N4—Cu1	102.6 (3)	N5—C24—C23	110.1 (3)
C27—N4—Cu1	120.4 (3)	N5—C24—H24A	109.6
C26—N4—H4A	107.4	C23—C24—H24A	109.6
C27—N4—H4A	107.4	N5—C24—H24B	109.6
Cu1—N4—H4A	107.4	C23—C24—H24B	109.6
C12—N5—C36	111.7 (3)	H24A—C24—H24B	108.1
C12—N5—C24	110.2 (3)	N1—C25—C26	110.1 (3)
C36—N5—C24	111.4 (3)	N1—C25—H25A	109.6
C12—N5—Cu2	105.7 (3)	C26—C25—H25A	109.6

C36—N5—Cu2	109.1 (3)	N1—C25—H25B	109.6
C24—N5—Cu2	108.7 (2)	C26—C25—H25B	109.6
C10—N6—C11	111.4 (3)	H25A—C25—H25B	108.2
C10—N6—Cu2	118.7 (3)	N4—C26—C25	108.5 (4)
C11—N6—Cu2	109.7 (3)	N4—C26—H26A	110.0
C10—N6—H6B	105.3	C25—C26—H26A	110.0
C11—N6—H6B	105.3	N4—C26—H26B	110.0
Cu2—N6—H6B	105.3	C25—C26—H26B	110.0
C23—N7—C22	109.8 (3)	H26A—C26—H26B	108.4
C23—N7—Cu2	102.4 (2)	N4—C27—C28	112.7 (3)
C22—N7—Cu2	121.9 (2)	N4—C27—H27A	109.0
C23—N7—H7B	107.3	C28—C27—H27A	109.0
C22—N7—H7B	107.3	N4—C27—H27B	109.0
Cu2—N7—H7B	107.3	C28—C27—H27B	109.0
C35—N8—C34	112.2 (3)	H27A—C27—H27B	107.8
C35—N8—Cu2	103.2 (2)	C29—C28—C33	119.0 (4)
C34—N8—Cu2	119.9 (3)	C29—C28—C27	121.4 (4)
C35—N8—H8A	107.0	C33—C28—C27	119.6 (4)
C34—N8—H8A	107.0	C28—C29—C30	120.4 (4)
Cu2—N8—H8A	107.0	C28—C29—H29A	119.8
N1—C1—C2	109.6 (4)	C30—C29—H29A	119.8
N1—C1—H1A	109.8	C31—C30—C29	119.6 (4)
C2—C1—H1A	109.8	C31—C30—H30A	120.2
N1—C1—H1B	109.8	C29—C30—H30A	120.2
C2—C1—H1B	109.8	C32—C31—C30	121.1 (4)
H1A—C1—H1B	108.2	C32—C31—H31A	119.5
N2—C2—C1	107.4 (4)	C30—C31—H31A	119.5
N2—C2—H2A	110.2	C31—C32—C33	118.6 (4)
C1—C2—H2A	110.2	C31—C32—C34	121.4 (4)
N2—C2—H2B	110.2	C33—C32—C34	120.1 (4)
C1—C2—H2B	110.2	C28—C33—C32	121.4 (4)
H2A—C2—H2B	108.5	C28—C33—H33A	119.3
N2—C3—C4	111.9 (4)	C32—C33—H33A	119.3
N2—C3—H3A	109.2	N8—C34—C32	112.5 (3)
C4—C3—H3A	109.2	N8—C34—H34A	109.1
N2—C3—H3B	109.2	C32—C34—H34A	109.1
C4—C3—H3B	109.2	N8—C34—H34B	109.1
H3A—C3—H3B	107.9	C32—C34—H34B	109.1
C9—C4—C5	119.4 (4)	H34A—C34—H34B	107.8
C9—C4—C3	120.9 (4)	N8—C35—C36	109.0 (4)
C5—C4—C3	119.7 (4)	N8—C35—H35A	109.9
C6—C5—C4	119.9 (4)	C36—C35—H35A	109.9
C6—C5—H5A	120.0	N8—C35—H35B	109.9
C4—C5—H5A	120.0	C36—C35—H35B	109.9
C5—C6—C7	120.6 (4)	H35A—C35—H35B	108.3
C5—C6—H6A	119.7	N5—C36—C35	110.7 (3)
C7—C6—H6A	119.7	N5—C36—H36A	109.5
C6—C7—C8	119.8 (4)	C35—C36—H36A	109.5

C6—C7—H7A	120.1	N5—C36—H36B	109.5
C8—C7—H7A	120.1	C35—C36—H36B	109.5
C9—C8—C7	119.1 (4)	H36A—C36—H36B	108.1
C9—C8—C10	120.6 (4)	O3—C37—O2	126.2 (5)
C7—C8—C10	120.2 (4)	O3—C37—O1	119.2 (4)
C4—C9—C8	121.2 (4)	O2—C37—O1	114.6 (4)
C4—C9—H9A	119.4	C37—O1—H1	109.5
C8—C9—H9A	119.4	C37—O2—Cu1	138.6 (3)
C8—C10—N6	112.5 (4)	C37—O3—Cu2	158.3 (3)
C8—C10—H10A	109.1	O1B—Cl1—O1D	110.9 (2)
N6—C10—H10A	109.1	O1B—Cl1—O1C	109.2 (2)
C8—C10—H10B	109.1	O1D—Cl1—O1C	110.4 (2)
N6—C10—H10B	109.1	O1B—Cl1—O1A	108.5 (2)
H10A—C10—H10B	107.8	O1D—Cl1—O1A	108.8 (2)
N6—C11—C12	108.6 (3)	O1C—Cl1—O1A	108.9 (2)
N6—C11—H11A	110.0	O2A—Cl2—O2D	112.4 (4)
C12—C11—H11A	110.0	O2A—Cl2—O2B	106.1 (3)
N6—C11—H11B	110.0	O2D—Cl2—O2B	108.8 (4)
C12—C11—H11B	110.0	O2A—Cl2—O2C	112.1 (4)
H11A—C11—H11B	108.3	O2D—Cl2—O2C	107.8 (3)
N5—C12—C11	109.5 (4)	O2B—Cl2—O2C	109.6 (3)
N5—C12—H12A	109.8	O3B—Cl3—O3C	110.7 (3)
C11—C12—H12A	109.8	O3B—Cl3—O3D	109.1 (3)
N5—C12—H12B	109.8	O3C—Cl3—O3D	106.3 (3)
C11—C12—H12B	109.8	O3B—Cl3—O3A	110.3 (2)
H12A—C12—H12B	108.2	O3C—Cl3—O3A	108.4 (3)
C14—C13—N1	108.3 (3)	O3D—Cl3—O3A	112.0 (3)
C14—C13—H13A	110.0	N1S—C1S—C2S	177.9 (6)
N1—C13—H13A	110.0	C1S—C2S—H2S1	109.5
C14—C13—H13B	110.0	C1S—C2S—H2S2	109.5
N1—C13—H13B	110.0	H2S1—C2S—H2S2	109.5
H13A—C13—H13B	108.4	C1S—C2S—H2S3	109.4
N3—C14—C13	108.8 (4)	H2S1—C2S—H2S3	109.5
N3—C14—H14A	109.9	H2S2—C2S—H2S3	109.5
C13—C14—H14A	109.9		

N3—Cu1—N1—C25	−126.3 (3)	C3—C4—C9—C8	−179.5 (4)
N2—Cu1—N1—C25	107.4 (3)	C7—C8—C9—C4	−0.1 (6)
N4—Cu1—N1—C25	−1.0 (3)	C10—C8—C9—C4	−178.4 (4)
N3—Cu1—N1—C1	113.5 (3)	C9—C8—C10—N6	−115.6 (4)
N2—Cu1—N1—C1	−12.7 (3)	C7—C8—C10—N6	66.2 (5)
N4—Cu1—N1—C1	−121.1 (3)	C11—N6—C10—C8	−138.0 (4)
N3—Cu1—N1—C13	−4.8 (3)	Cu2—N6—C10—C8	93.1 (4)
N2—Cu1—N1—C13	−131.1 (3)	C10—N6—C11—C12	−160.8 (4)
N4—Cu1—N1—C13	120.5 (3)	Cu2—N6—C11—C12	−27.3 (4)
O2—Cu1—N2—C2	160.4 (3)	C36—N5—C12—C11	70.8 (4)
N1—Cu1—N2—C2	−17.2 (3)	C24—N5—C12—C11	−164.9 (3)
N3—Cu1—N2—C2	−96.2 (3)	Cu2—N5—C12—C11	−47.7 (4)

N4—Cu1—N2—C2	63.3 (3)	N6—C11—C12—N5	50.3 (5)
O2—Cu1—N2—C3	35.9 (3)	C25—N1—C13—C14	153.9 (4)
N1—Cu1—N2—C3	−141.7 (3)	C1—N1—C13—C14	−83.7 (4)
N3—Cu1—N2—C3	139.3 (3)	Cu1—N1—C13—C14	33.2 (4)
N4—Cu1—N2—C3	−61.2 (3)	C15—N3—C14—C13	−81.3 (4)
O2—Cu1—N3—C14	158.4 (2)	Cu1—N3—C14—C13	49.5 (4)
N1—Cu1—N3—C14	−24.0 (3)	N1—C13—C14—N3	−57.0 (5)
N2—Cu1—N3—C14	54.5 (3)	C14—N3—C15—C16	−174.1 (4)
N4—Cu1—N3—C14	−101.6 (3)	Cu1—N3—C15—C16	65.0 (4)
O2—Cu1—N3—C15	−76.8 (3)	N3—C15—C16—C17	−130.3 (4)
N1—Cu1—N3—C15	100.8 (3)	N3—C15—C16—C21	52.7 (6)
N2—Cu1—N3—C15	179.4 (3)	C21—C16—C17—C18	−0.4 (7)
N4—Cu1—N3—C15	23.2 (3)	C15—C16—C17—C18	−177.5 (4)
O2—Cu1—N4—C26	152.7 (3)	C16—C17—C18—C19	−0.6 (7)
N1—Cu1—N4—C26	−26.8 (3)	C17—C18—C19—C20	0.0 (7)
N3—Cu1—N4—C26	51.6 (3)	C18—C19—C20—C21	1.5 (7)
N2—Cu1—N4—C26	−108.1 (3)	C18—C19—C20—C22	177.9 (4)
O2—Cu1—N4—C27	29.1 (3)	C19—C20—C21—C16	−2.6 (6)
N1—Cu1—N4—C27	−150.4 (3)	C22—C20—C21—C16	−179.1 (4)
N3—Cu1—N4—C27	−72.0 (3)	C17—C16—C21—C20	2.1 (6)
N2—Cu1—N4—C27	128.3 (3)	C15—C16—C21—C20	179.2 (4)
N6—Cu2—N5—C12	25.1 (3)	C23—N7—C22—C20	−163.5 (3)
N7—Cu2—N5—C12	−122.3 (3)	Cu2—N7—C22—C20	77.0 (4)
N8—Cu2—N5—C12	131.7 (3)	C19—C20—C22—N7	48.5 (6)
N6—Cu2—N5—C36	−95.1 (3)	C21—C20—C22—N7	−135.1 (4)
N7—Cu2—N5—C36	117.5 (3)	C22—N7—C23—C24	177.3 (3)
N8—Cu2—N5—C36	11.5 (3)	Cu2—N7—C23—C24	−51.9 (4)
N6—Cu2—N5—C24	143.3 (3)	C12—N5—C24—C23	91.4 (4)
N7—Cu2—N5—C24	−4.1 (3)	C36—N5—C24—C23	−144.1 (4)
N8—Cu2—N5—C24	−110.1 (3)	Cu2—N5—C24—C23	−23.9 (4)
O3—Cu2—N6—C10	−48.1 (3)	N7—C23—C24—N5	52.3 (5)
N5—Cu2—N6—C10	130.9 (3)	C1—N1—C25—C26	147.7 (4)
N7—Cu2—N6—C10	−157.7 (3)	C13—N1—C25—C26	−90.4 (4)
N8—Cu2—N6—C10	50.2 (3)	Cu1—N1—C25—C26	29.4 (4)
O3—Cu2—N6—C11	−177.7 (3)	C27—N4—C26—C25	−179.9 (4)
N5—Cu2—N6—C11	1.2 (3)	Cu1—N4—C26—C25	50.3 (4)
N7—Cu2—N6—C11	72.6 (4)	N1—C25—C26—N4	−55.4 (5)
N8—Cu2—N6—C11	−79.5 (3)	C26—N4—C27—C28	172.3 (4)
O3—Cu2—N7—C23	−149.8 (2)	Cu1—N4—C27—C28	−68.1 (4)
N5—Cu2—N7—C23	30.3 (2)	N4—C27—C28—C29	−46.3 (6)
N6—Cu2—N7—C23	−41.0 (4)	N4—C27—C28—C33	132.0 (4)
N8—Cu2—N7—C23	111.2 (2)	C33—C28—C29—C30	0.0 (6)
O3—Cu2—N7—C22	−26.9 (3)	C27—C28—C29—C30	178.4 (4)
N5—Cu2—N7—C22	153.3 (3)	C28—C29—C30—C31	0.5 (7)
N6—Cu2—N7—C22	82.0 (4)	C29—C30—C31—C32	−1.3 (7)
N8—Cu2—N7—C22	−125.8 (3)	C30—C31—C32—C33	1.5 (6)
O3—Cu2—N8—C35	−164.2 (3)	C30—C31—C32—C34	−177.6 (4)
N5—Cu2—N8—C35	17.3 (3)	C29—C28—C33—C32	0.2 (6)

N6—Cu2—N8—C35	99.2 (3)	C27—C28—C33—C32	−178.2 (4)
N7—Cu2—N8—C35	−64.9 (3)	C31—C32—C33—C28	−1.0 (6)
O3—Cu2—N8—C34	−38.7 (3)	C34—C32—C33—C28	178.1 (4)
N5—Cu2—N8—C34	142.9 (3)	C35—N8—C34—C32	−162.9 (4)
N6—Cu2—N8—C34	−135.3 (3)	Cu2—N8—C34—C32	75.9 (4)
N7—Cu2—N8—C34	60.6 (3)	C31—C32—C34—N8	48.1 (6)
C25—N1—C1—C2	−78.5 (4)	C33—C32—C34—N8	−131.0 (4)
C13—N1—C1—C2	158.7 (3)	C34—N8—C35—C36	−173.4 (4)
Cu1—N1—C1—C2	41.3 (4)	Cu2—N8—C35—C36	−43.0 (4)
C3—N2—C2—C1	173.7 (4)	C12—N5—C36—C35	−156.3 (4)
Cu1—N2—C2—C1	43.5 (4)	C24—N5—C36—C35	80.1 (4)
N1—C1—C2—N2	−58.3 (5)	Cu2—N5—C36—C35	−39.9 (4)
C2—N2—C3—C4	149.0 (4)	N8—C35—C36—N5	57.9 (5)
Cu1—N2—C3—C4	−89.0 (4)	O3—C37—O2—Cu1	174.2 (3)
N2—C3—C4—C9	114.9 (4)	O1—C37—O2—Cu1	−5.4 (7)
N2—C3—C4—C5	−65.3 (5)	N3—Cu1—O2—C37	−50.9 (4)
C9—C4—C5—C6	−1.0 (7)	N2—Cu1—O2—C37	75.9 (4)
C3—C4—C5—C6	179.2 (4)	N4—Cu1—O2—C37	−176.0 (4)
C4—C5—C6—C7	0.7 (7)	O2—C37—O3—Cu2	−175.6 (5)
C5—C6—C7—C8	−0.1 (7)	O1—C37—O3—Cu2	4.0 (11)
C6—C7—C8—C9	−0.2 (6)	N6—Cu2—O3—C37	−69.4 (8)
C6—C7—C8—C10	178.1 (4)	N7—Cu2—O3—C37	78.1 (8)
C5—C4—C9—C8	0.7 (6)	N8—Cu2—O3—C37	−175.7 (8)