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Diacetonitrile[*N*,*N*′-bis(3,4,5-trimethoxybenzylidene)ethylenediamine]copper(I) perchlorate

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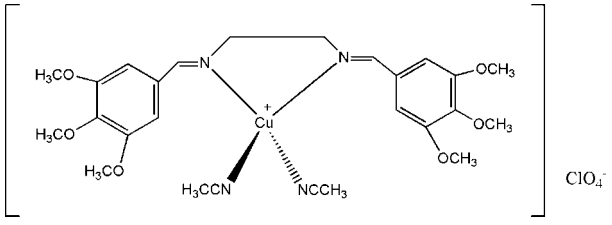
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.007 Å; R factor = 0.050; wR factor = 0.140; data-to-parameter ratio = 14.0.

In the title compound, $[Cu(C_2H_3N)_2(C_{22}H_{28}N_2O_6)]ClO_4$, the Cu atom is coordinated by two N atoms from one bidentate Schiff base ligand and two N atoms from two acetonitrile groups. The Cu atom adopts a tetrahedral geometry. The Cu—N(ligand) distances are 2.076 (3) and 2.089 (3) Å, and the Cu—N(acetonitrile) distances are 1.964 (4) and 1.975 (4) Å.

Related literature

For related literature, see: Amirnasr *et al.* (2006); Chowdhury *et al.* (2000); Dakin *et al.* (2000); Khalaji *et al.* (2007).



Experimental

Crystal data

$[Cu(C_2H_3N)_2(C_{22}H_{28}N_2O_6)]ClO_4$
M_r = 661.56
Triclinic, $P\overline{1}$
a = 9.869 (2) Å
b = 11.903 (3) Å
c = 14.904 (3) Å
α = 80.537 (4)°
β = 71.677 (4)°
γ = 68.285 (4)°
V = 1541.9 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.85 mm^{-1}
T = 294 (2) K
0.24 × 0.22 × 0.18 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.821, T_{max} = 0.862
8034 measured reflections
5414 independent reflections
3408 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.141
S = 1.01
5414 reflections
387 parameters
34 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2614).

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supporting information

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S1. Comment

Copper(I) complexes have long been used in organic synthesis as catalyst (Dakin *et al.*, 2000), and the design of supramolecular arrays (Amirnasr *et al.*, 2006).

The coordination of the Cu atom is nearly tetrahedral (Fig. 1), with four N atoms, two from two acetonitrile groups and the other two from one bidentate Schiff base ligand (3,4,5-MeO-ba)$_2$en, forming the CuN4 chromophore. Although a tetrahedral geometry is to be expected for a four-coordinated Cu(I) complexes, the geometry about the Cu(I) in this structure is distorted by the bite angle of the chelating ligand. The N(1)—Cu(1)—N(2) angle is 84.97 (13) and N(3)—Cu(1)—N(4) angle is 103.04 (16)° in this structure being smaller than the tetrahedral values, however, other angles are larger than the tetrahedral values, which posses approximate C2 local symmetry. The Cu—N bond lengths [Cu(1)—N(3), 1.964 (4); Cu(1)—N(4), 1.975 (4); Cu(1)—N(2), 2.076 (3) and Cu(1)—N(1) 2.089 (3) Å] agree well with the same distances in other tetrahedral copper(I) complexes (Chowdhury *et al.*, 2000.; Dakin *et al.*, 2000). The N(1)=C(7) and N(2)=C(13) bond lengths of 1.274 (5) and 1.277 (5) Å, respectively, conform to the value for a double bond, while the C(11)—N(1) and C(12)—N(2) bond lengths of 1.475 (5) and 1.468 (5) Å, respectively, conform to the value for a single bond and are comparable to the corresponding values observed in other tetrahedral copper(I) complexes (Chowdhury *et al.*, 2000.; Dakin *et al.*, 2000). The ligand adopts a *Z*,*Z* configuration in this structure.

S2. Experimental

The *N*,*N*′-Bis(3,4,5-trimethoxybenzylidene)ethylenediamine (3,4,5-MeO-ba)$_2$en) ligand was prepared as reported elsewhere (Khalaji *et al.*, 2007). The reaction between [Cu(CH$_3$CN)$_4$]ClO$_4$ (0.326 mg, 0.1 mol) and the (3,4,5-MeO-ba)$_2$en ligand (0.416 g, 0.1 mol) in 10 ml CH$_3$CN at room temperature lead to the formation of the copper(I) complex.

S3. Refinement

All H atoms were positioned geometrically (C—H=0.93–0.97 Å), and refined as riding with U_{iso}(H)=1.2U_{eq}(carrier) or 1.5$_{eq}$(methyl groups). All O—O distances of the ClO_4^- anion have been restrained to 2.35 (1) Å, and the Cl—O distances to 1.44 (1) Å. The displacement parameters of these O atoms have been restrained to an isotropic behaviour with an effective standard deviation of 0.01.

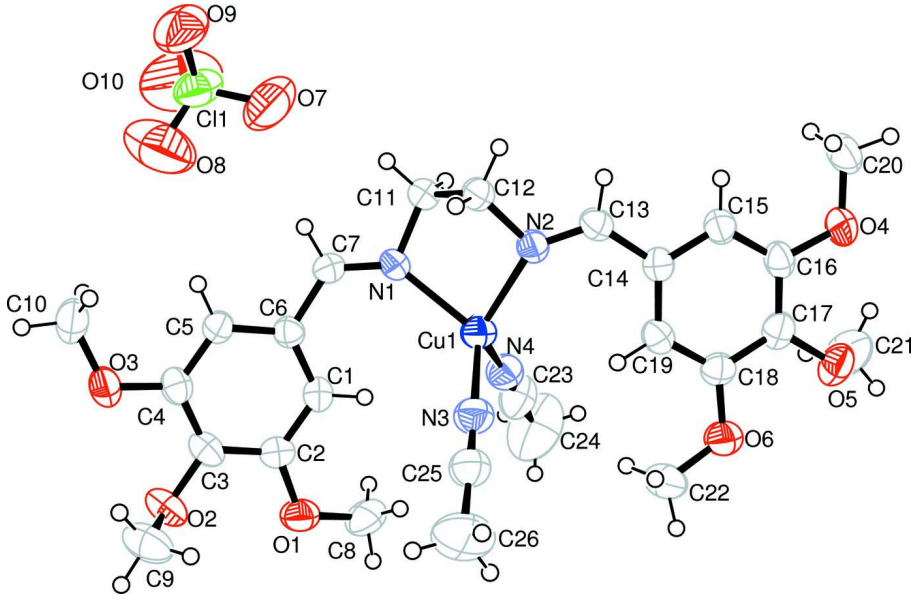

Figure 1

The molecular structure of the title compound. Displacement ellopsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

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Crystal data

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$\alpha = 80.537$ (4)°
$\beta = 71.677$ (4)°
$\gamma = 68.285$ (4)°
$V = 1541.9$ (6) Å^3
$Z = 2$
$F(000) = 688$
$D_x = 1.425$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2161 reflections
$\theta = 2.3$–22.6°
$\mu = 0.85$ mm^{-1}
$T = 294$ K
Block, blue
0.24 × 0.22 × 0.18 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.821$, $T_{max} = 0.862$
8034 measured reflections
5414 independent reflections
3408 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.4°$
$h = -11 \rightarrow 9$
$k = -14 \rightarrow 14$
$l = -17 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.141$
$S = 1.01$
5414 reflections
387 parameters
34 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

$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2 + 1.2218P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ 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	0.16626 (7)	0.63549 (5)	0.25396 (4)	0.0508 (2)
O1	0.3716 (4)	0.9169 (3)	0.3552 (2)	0.0588 (9)
O2	0.5608 (4)	0.8412 (3)	0.4633 (2)	0.0591 (9)
O3	0.7220 (4)	0.6058 (3)	0.4854 (2)	0.0602 (9)
O4	−0.3452 (4)	0.5705 (3)	0.0206 (2)	0.0612 (9)
O5	−0.4326 (3)	0.8102 (3)	0.0469 (2)	0.0612 (9)
O6	−0.3194 (4)	0.8895 (3)	0.1522 (2)	0.0575 (8)
N1	0.3752 (4)	0.5043 (3)	0.2585 (2)	0.0410 (8)
N2	0.1072 (4)	0.4906 (3)	0.2395 (2)	0.0419 (8)
N3	0.0368 (5)	0.7333 (4)	0.3633 (3)	0.0572 (10)
N4	0.1843 (5)	0.7587 (4)	0.1488 (3)	0.0563 (10)
C1	0.4243 (5)	0.7104 (4)	0.3181 (3)	0.0429 (10)
H1	0.3572	0.7356	0.2809	0.051*
C2	0.4436 (5)	0.7945 (4)	0.3627 (3)	0.0430 (10)
C3	0.5417 (5)	0.7562 (4)	0.4204 (3)	0.0454 (11)
C4	0.6249 (5)	0.6343 (4)	0.4300 (3)	0.0445 (11)
C5	0.6075 (5)	0.5508 (4)	0.3837 (3)	0.0413 (10)
H5	0.6643	0.4692	0.3890	0.050*
C6	0.5055 (4)	0.5889 (4)	0.3293 (3)	0.0390 (10)
C7	0.4868 (5)	0.4930 (4)	0.2891 (3)	0.0414 (10)
H7	0.5627	0.4175	0.2856	0.050*
C8	0.2938 (6)	0.9615 (4)	0.2841 (4)	0.0693 (15)
H8A	0.3606	0.9302	0.2245	0.104*
H8B	0.2611	1.0483	0.2792	0.104*
H8C	0.2070	0.9359	0.3006	0.104*
C9	0.4800 (7)	0.8526 (5)	0.5606 (3)	0.0781 (17)
H9A	0.3737	0.8725	0.5678	0.117*
H9B	0.4954	0.9156	0.5847	0.117*
H9C	0.5162	0.7774	0.5952	0.117*
C10	0.8171 (5)	0.4835 (5)	0.4891 (4)	0.0629 (14)

H10A	0.7560	0.4330	0.5154	0.094*
H10B	0.8822	0.4742	0.5280	0.094*
H10C	0.8778	0.4601	0.4263	0.094*
C11	0.3764 (5)	0.3933 (4)	0.2262 (3)	0.0454 (11)
H11A	0.4520	0.3231	0.2462	0.054*
H11B	0.4017	0.3972	0.1576	0.054*
C12	0.2208 (5)	0.3823 (4)	0.2684 (3)	0.0484 (11)
H12A	0.2186	0.3107	0.2466	0.058*
H12B	0.1979	0.3744	0.3368	0.058*
C13	0.0175 (5)	0.4718 (4)	0.2024 (3)	0.0438 (10)
H13	0.0289	0.3915	0.1986	0.053*
C14	−0.1009 (5)	0.5636 (4)	0.1656 (3)	0.0415 (10)
C15	−0.1659 (5)	0.5225 (4)	0.1129 (3)	0.0463 (11)
H15	−0.1354	0.4401	0.1048	0.056*
C16	−0.2752 (5)	0.6037 (4)	0.0728 (3)	0.0459 (11)
C17	−0.3221 (5)	0.7267 (4)	0.0850 (3)	0.0472 (11)
C18	−0.2617 (5)	0.7676 (4)	0.1413 (3)	0.0439 (10)
C19	−0.1508 (5)	0.6868 (4)	0.1807 (3)	0.0437 (10)
H19	−0.1096	0.7144	0.2172	0.052*
C20	−0.3010 (6)	0.4441 (5)	0.0093 (4)	0.0627 (14)
H20A	−0.1954	0.4137	−0.0245	0.094*
H20B	−0.3603	0.4312	−0.0255	0.094*
H20C	−0.3174	0.4024	0.0705	0.094*
C21	−0.3830 (7)	0.8362 (5)	−0.0515 (4)	0.0844 (18)
H21A	−0.2835	0.8417	−0.0672	0.127*
H21B	−0.4521	0.9118	−0.0688	0.127*
H21C	−0.3797	0.7728	−0.0854	0.127*
C22	−0.2715 (6)	0.9347 (4)	0.2153 (4)	0.0640 (14)
H22A	−0.2970	0.8969	0.2774	0.096*
H22B	−0.3215	1.0207	0.2179	0.096*
H22C	−0.1636	0.9168	0.1932	0.096*
C23	0.1908 (6)	0.8331 (5)	0.0939 (4)	0.0683 (15)
C24	0.1990 (9)	0.9299 (7)	0.0201 (6)	0.140 (3)
H24A	0.1483	0.9267	−0.0244	0.211*
H24B	0.3034	0.9196	−0.0121	0.211*
H24C	0.1507	1.0069	0.0484	0.211*
C25	−0.0322 (6)	0.7962 (5)	0.4216 (4)	0.0623 (13)
C26	−0.1195 (9)	0.8770 (7)	0.4981 (5)	0.122 (3)
H26A	−0.0530	0.8831	0.5308	0.183*
H26B	−0.1941	0.8458	0.5415	0.183*
H26C	−0.1694	0.9558	0.4728	0.183*
Cl1	0.90012 (16)	0.16995 (12)	0.24864 (12)	0.0791 (5)
O7	0.7647 (5)	0.2159 (4)	0.2193 (4)	0.1252 (17)
O8	0.8825 (8)	0.2455 (5)	0.3203 (4)	0.171 (2)
O9	0.9177 (5)	0.0509 (3)	0.2878 (4)	0.1263 (18)
O10	1.0251 (6)	0.1770 (5)	0.1751 (4)	0.181 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0576 (4)	0.0406 (3)	0.0556 (4)	−0.0112 (3)	−0.0229 (3)	−0.0059 (3)
O1	0.073 (2)	0.0404 (18)	0.062 (2)	−0.0110 (16)	−0.0250 (18)	−0.0062 (15)
O2	0.086 (2)	0.061 (2)	0.0467 (19)	−0.0406 (18)	−0.0180 (18)	−0.0074 (16)
O3	0.070 (2)	0.061 (2)	0.065 (2)	−0.0230 (18)	−0.0396 (19)	−0.0019 (17)
O4	0.060 (2)	0.067 (2)	0.069 (2)	−0.0138 (17)	−0.0355 (18)	−0.0186 (17)
O5	0.0487 (19)	0.072 (2)	0.053 (2)	−0.0032 (17)	−0.0211 (17)	−0.0051 (17)
O6	0.064 (2)	0.0464 (19)	0.062 (2)	−0.0118 (16)	−0.0244 (18)	−0.0060 (16)
N1	0.046 (2)	0.041 (2)	0.041 (2)	−0.0138 (16)	−0.0177 (17)	−0.0072 (16)
N2	0.046 (2)	0.040 (2)	0.045 (2)	−0.0157 (17)	−0.0179 (18)	−0.0002 (16)
N3	0.062 (3)	0.053 (2)	0.054 (3)	−0.012 (2)	−0.017 (2)	−0.009 (2)
N4	0.062 (3)	0.051 (2)	0.057 (3)	−0.019 (2)	−0.021 (2)	−0.001 (2)
C1	0.041 (2)	0.047 (3)	0.043 (3)	−0.016 (2)	−0.017 (2)	0.000 (2)
C2	0.044 (2)	0.039 (2)	0.043 (3)	−0.014 (2)	−0.007 (2)	−0.0030 (19)
C3	0.059 (3)	0.050 (3)	0.035 (2)	−0.030 (2)	−0.011 (2)	−0.002 (2)
C4	0.048 (3)	0.053 (3)	0.039 (2)	−0.024 (2)	−0.015 (2)	0.003 (2)
C5	0.040 (2)	0.039 (2)	0.046 (3)	−0.0119 (19)	−0.017 (2)	−0.0001 (19)
C6	0.037 (2)	0.043 (2)	0.036 (2)	−0.0124 (19)	−0.009 (2)	−0.0067 (19)
C7	0.040 (2)	0.037 (2)	0.045 (3)	−0.0072 (19)	−0.013 (2)	−0.0063 (19)
C8	0.078 (4)	0.043 (3)	0.079 (4)	−0.005 (3)	−0.034 (3)	0.005 (3)
C9	0.112 (5)	0.076 (4)	0.052 (3)	−0.038 (4)	−0.016 (3)	−0.018 (3)
C10	0.050 (3)	0.081 (4)	0.057 (3)	−0.013 (3)	−0.024 (3)	−0.005 (3)
C11	0.047 (3)	0.041 (2)	0.051 (3)	−0.010 (2)	−0.020 (2)	−0.010 (2)
C12	0.059 (3)	0.038 (2)	0.056 (3)	−0.014 (2)	−0.031 (2)	0.001 (2)
C13	0.047 (3)	0.041 (2)	0.049 (3)	−0.020 (2)	−0.015 (2)	−0.003 (2)
C14	0.039 (2)	0.046 (3)	0.042 (2)	−0.016 (2)	−0.012 (2)	−0.002 (2)
C15	0.042 (3)	0.051 (3)	0.050 (3)	−0.016 (2)	−0.014 (2)	−0.008 (2)
C16	0.040 (3)	0.062 (3)	0.039 (2)	−0.018 (2)	−0.011 (2)	−0.012 (2)
C17	0.040 (3)	0.059 (3)	0.038 (2)	−0.011 (2)	−0.010 (2)	−0.006 (2)
C18	0.042 (3)	0.046 (3)	0.040 (2)	−0.013 (2)	−0.006 (2)	−0.007 (2)
C19	0.046 (3)	0.050 (3)	0.040 (2)	−0.020 (2)	−0.011 (2)	−0.006 (2)
C20	0.066 (3)	0.073 (4)	0.063 (3)	−0.028 (3)	−0.026 (3)	−0.017 (3)
C21	0.091 (4)	0.086 (4)	0.054 (4)	−0.005 (3)	−0.024 (3)	0.006 (3)
C22	0.079 (4)	0.051 (3)	0.067 (3)	−0.023 (3)	−0.020 (3)	−0.011 (3)
C23	0.058 (3)	0.074 (4)	0.072 (4)	−0.026 (3)	−0.020 (3)	0.013 (3)
C24	0.127 (7)	0.140 (7)	0.138 (7)	−0.061 (6)	−0.040 (6)	0.082 (6)
C25	0.064 (3)	0.059 (3)	0.061 (3)	−0.015 (3)	−0.018 (3)	−0.008 (3)
C26	0.122 (6)	0.130 (6)	0.088 (5)	−0.010 (5)	−0.003 (4)	−0.061 (5)
Cl1	0.0556 (8)	0.0482 (8)	0.1228 (13)	−0.0165 (6)	−0.0139 (9)	0.0000 (8)
O7	0.096 (3)	0.092 (3)	0.170 (5)	−0.005 (3)	−0.056 (3)	0.015 (3)
O8	0.241 (6)	0.128 (4)	0.180 (5)	−0.090 (4)	−0.064 (5)	−0.029 (4)
O9	0.115 (4)	0.062 (3)	0.216 (5)	−0.036 (3)	−0.077 (4)	0.029 (3)
O10	0.120 (4)	0.152 (5)	0.209 (6)	−0.055 (4)	0.053 (4)	−0.015 (4)

Geometric parameters (Å, º)

Cu1—N3	1.964 (4)	C10—H10B	0.9600
Cu1—N4	1.975 (4)	C10—H10C	0.9600
Cu1—N2	2.076 (3)	C11—C12	1.511 (6)
Cu1—N1	2.089 (3)	C11—H11A	0.9700
O1—C2	1.367 (5)	C11—H11B	0.9700
O1—C8	1.422 (5)	C12—H12A	0.9700
O2—C3	1.377 (5)	C12—H12B	0.9700
O2—C9	1.420 (6)	C13—C14	1.456 (6)
O3—C4	1.372 (5)	C13—H13	0.9300
O3—C10	1.414 (6)	C14—C15	1.394 (6)
O4—C16	1.372 (5)	C14—C19	1.395 (6)
O4—C20	1.425 (5)	C15—C16	1.378 (6)
O5—C17	1.379 (5)	C15—H15	0.9300
O5—C21	1.413 (6)	C16—C17	1.386 (6)
O6—C18	1.366 (5)	C17—C18	1.400 (6)
O6—C22	1.426 (5)	C18—C19	1.382 (6)
N1—C7	1.274 (5)	C19—H19	0.9300
N1—C11	1.475 (5)	C20—H20A	0.9600
N2—C13	1.277 (5)	C20—H20B	0.9600
N2—C12	1.468 (5)	C20—H20C	0.9600
N3—C25	1.115 (6)	C21—H21A	0.9600
N4—C23	1.108 (6)	C21—H21B	0.9600
C1—C6	1.382 (6)	C21—H21C	0.9600
C1—C2	1.385 (6)	C22—H22A	0.9600
C1—H1	0.9300	C22—H22B	0.9600
C2—C3	1.398 (6)	C22—H22C	0.9600
C3—C4	1.387 (6)	C23—C24	1.463 (8)
C4—C5	1.385 (6)	C24—H24A	0.9600
C5—C6	1.390 (5)	C24—H24B	0.9600
C5—H5	0.9300	C24—H24C	0.9600
C6—C7	1.465 (5)	C25—C26	1.449 (8)
C7—H7	0.9300	C26—H26A	0.9600
C8—H8A	0.9600	C26—H26B	0.9600
C8—H8B	0.9600	C26—H26C	0.9600
C8—H8C	0.9600	Cl1—O10	1.387 (4)
C9—H9A	0.9600	Cl1—O9	1.410 (4)
C9—H9B	0.9600	Cl1—O7	1.422 (4)
C9—H9C	0.9600	Cl1—O8	1.436 (4)
C10—H10A	0.9600		

N3—Cu1—N4	103.04 (16)	N2—C12—C11	109.3 (3)
N3—Cu1—N2	115.70 (15)	N2—C12—H12A	109.8
N4—Cu1—N2	120.15 (14)	C11—C12—H12A	109.8
N3—Cu1—N1	120.65 (14)	N2—C12—H12B	109.8
N4—Cu1—N1	112.89 (15)	C11—C12—H12B	109.8
N2—Cu1—N1	84.97 (13)	H12A—C12—H12B	108.3

C2—O1—C8	117.0 (3)	N2—C13—C14	126.6 (4)
C3—O2—C9	114.4 (4)	N2—C13—H13	116.7
C4—O3—C10	116.4 (3)	C14—C13—H13	116.7
C16—O4—C20	116.7 (4)	C15—C14—C19	119.9 (4)
C17—O5—C21	114.5 (4)	C15—C14—C13	116.3 (4)
C18—O6—C22	117.5 (4)	C19—C14—C13	123.8 (4)
C7—N1—C11	115.9 (3)	C16—C15—C14	120.1 (4)
C7—N1—Cu1	137.8 (3)	C16—C15—H15	119.9
C11—N1—Cu1	105.8 (2)	C14—C15—H15	119.9
C13—N2—C12	116.2 (3)	O4—C16—C15	123.6 (4)
C13—N2—Cu1	137.6 (3)	O4—C16—C17	115.9 (4)
C12—N2—Cu1	105.3 (2)	C15—C16—C17	120.4 (4)
C25—N3—Cu1	174.3 (4)	O5—C17—C16	121.9 (4)
C23—N4—Cu1	175.7 (4)	O5—C17—C18	118.5 (4)
C6—C1—C2	119.5 (4)	C16—C17—C18	119.5 (4)
C6—C1—H1	120.2	O6—C18—C19	124.5 (4)
C2—C1—H1	120.2	O6—C18—C17	115.2 (4)
O1—C2—C1	124.6 (4)	C19—C18—C17	120.3 (4)
O1—C2—C3	115.3 (4)	C18—C19—C14	119.7 (4)
C1—C2—C3	120.1 (4)	C18—C19—H19	120.2
O2—C3—C4	120.6 (4)	C14—C19—H19	120.2
O2—C3—C2	119.3 (4)	O4—C20—H20A	109.5
C4—C3—C2	120.0 (4)	O4—C20—H20B	109.5
O3—C4—C5	124.6 (4)	H20A—C20—H20B	109.5
O3—C4—C3	115.8 (4)	O4—C20—H20C	109.5
C5—C4—C3	119.6 (4)	H20A—C20—H20C	109.5
C4—C5—C6	120.2 (4)	H20B—C20—H20C	109.5
C4—C5—H5	119.9	O5—C21—H21A	109.5
C6—C5—H5	119.9	O5—C21—H21B	109.5
C1—C6—C5	120.5 (4)	H21A—C21—H21B	109.5
C1—C6—C7	123.4 (4)	O5—C21—H21C	109.5
C5—C6—C7	116.0 (4)	H21A—C21—H21C	109.5
N1—C7—C6	125.5 (4)	H21B—C21—H21C	109.5
N1—C7—H7	117.2	O6—C22—H22A	109.5
C6—C7—H7	117.2	O6—C22—H22B	109.5
O1—C8—H8A	109.5	H22A—C22—H22B	109.5
O1—C8—H8B	109.5	O6—C22—H22C	109.5
H8A—C8—H8B	109.5	H22A—C22—H22C	109.5
O1—C8—H8C	109.5	H22B—C22—H22C	109.5
H8A—C8—H8C	109.5	N4—C23—C24	178.9 (7)
H8B—C8—H8C	109.5	C23—C24—H24A	109.5
O2—C9—H9A	109.5	C23—C24—H24B	109.5
O2—C9—H9B	109.5	H24A—C24—H24B	109.5
H9A—C9—H9B	109.5	C23—C24—H24C	109.5
O2—C9—H9C	109.5	H24A—C24—H24C	109.5
H9A—C9—H9C	109.5	H24B—C24—H24C	109.5
H9B—C9—H9C	109.5	N3—C25—C26	178.9 (6)
O3—C10—H10A	109.5	C25—C26—H26A	109.5

O3—C10—H10B	109.5	C25—C26—H26B	109.5
H10A—C10—H10B	109.5	H26A—C26—H26B	109.5
O3—C10—H10C	109.5	C25—C26—H26C	109.5
H10A—C10—H10C	109.5	H26A—C26—H26C	109.5
H10B—C10—H10C	109.5	H26B—C26—H26C	109.5
N1—C11—C12	108.6 (3)	O10—Cl1—O9	112.7 (3)
N1—C11—H11A	110.0	O10—Cl1—O7	111.7 (4)
C12—C11—H11A	110.0	O9—Cl1—O7	108.6 (3)
N1—C11—H11B	110.0	O10—Cl1—O8	106.8 (4)
C12—C11—H11B	110.0	O9—Cl1—O8	109.3 (3)
H11A—C11—H11B	108.4	O7—Cl1—O8	107.5 (3)

N3—Cu1—N1—C7	−40.7 (5)	C4—C5—C6—C7	−175.5 (4)
N4—Cu1—N1—C7	81.7 (5)	C11—N1—C7—C6	−176.6 (4)
N2—Cu1—N1—C7	−157.7 (4)	Cu1—N1—C7—C6	−6.1 (7)
N3—Cu1—N1—C11	130.4 (3)	C1—C6—C7—N1	−16.5 (7)
N4—Cu1—N1—C11	−107.2 (3)	C5—C6—C7—N1	161.2 (4)
N2—Cu1—N1—C11	13.5 (3)	C7—N1—C11—C12	133.0 (4)
N3—Cu1—N2—C13	86.2 (5)	Cu1—N1—C11—C12	−40.4 (4)
N4—Cu1—N2—C13	−38.5 (5)	C13—N2—C12—C11	128.1 (4)
N1—Cu1—N2—C13	−152.1 (5)	Cu1—N2—C12—C11	−43.2 (4)
N3—Cu1—N2—C12	−105.5 (3)	N1—C11—C12—N2	58.1 (4)
N4—Cu1—N2—C12	129.8 (3)	C12—N2—C13—C14	−177.9 (4)
N1—Cu1—N2—C12	16.2 (3)	Cu1—N2—C13—C14	−10.5 (7)
N4—Cu1—N3—C25	−27 (4)	N2—C13—C14—C15	168.6 (4)
N2—Cu1—N3—C25	−160 (4)	N2—C13—C14—C19	−11.8 (7)
N1—Cu1—N3—C25	100 (4)	C19—C14—C15—C16	2.5 (6)
N3—Cu1—N4—C23	13 (6)	C13—C14—C15—C16	−177.9 (4)
N2—Cu1—N4—C23	143 (6)	C20—O4—C16—C15	0.7 (6)
N1—Cu1—N4—C23	−119 (6)	C20—O4—C16—C17	−178.5 (4)
C8—O1—C2—C1	−11.7 (6)	C14—C15—C16—O4	−179.6 (4)
C8—O1—C2—C3	168.5 (4)	C14—C15—C16—C17	−0.4 (7)
C6—C1—C2—O1	178.7 (4)	C21—O5—C17—C16	−76.3 (6)
C6—C1—C2—C3	−1.6 (6)	C21—O5—C17—C18	106.9 (5)
C9—O2—C3—C4	−81.4 (5)	O4—C16—C17—O5	0.1 (6)
C9—O2—C3—C2	102.2 (5)	C15—C16—C17—O5	−179.1 (4)
O1—C2—C3—O2	−1.0 (6)	O4—C16—C17—C18	176.9 (4)
C1—C2—C3—O2	179.2 (4)	C15—C16—C17—C18	−2.4 (7)
O1—C2—C3—C4	−177.5 (4)	C22—O6—C18—C19	−5.9 (6)
C1—C2—C3—C4	2.8 (6)	C22—O6—C18—C17	174.7 (4)
C10—O3—C4—C5	4.6 (6)	O5—C17—C18—O6	−0.6 (6)
C10—O3—C4—C3	−174.6 (4)	C16—C17—C18—O6	−177.4 (4)
O2—C3—C4—O3	1.4 (6)	O5—C17—C18—C19	180.0 (4)
C2—C3—C4—O3	177.8 (4)	C16—C17—C18—C19	3.2 (6)
O2—C3—C4—C5	−177.9 (4)	O6—C18—C19—C14	179.5 (4)
C2—C3—C4—C5	−1.4 (6)	C17—C18—C19—C14	−1.1 (6)
O3—C4—C5—C6	179.8 (4)	C15—C14—C19—C18	−1.7 (6)
C3—C4—C5—C6	−1.1 (6)	C13—C14—C19—C18	178.7 (4)

C2—C1—C6—C5	−0.9 (6)	Cu1—N4—C23—C24	−151 (34)
C2—C1—C6—C7	176.6 (4)	Cu1—N3—C25—C26	−87 (36)
C4—C5—C6—C1	2.3 (6)		