Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Bis{μ-2,4-di-*tert*-butyl-6-[3-(1*H*-imidazol-1-yl)propyliminomethyl]-phenolato}bis[acetatocopper(II)]

Onur Şahin,[a]* Orhan Büyükgüngör,[a] Mahmut Ulusoy[b] and Bekir Çetinkaya[b]

[a]Department of Physics, Ondokuz Mayıs University, TR-55139, Samsun, Turkey, and [b]Department of Chemistry, Ege University, TR-35100, Izmir, Turkey
Correspondence e-mail: onurs@omu.edu.tr

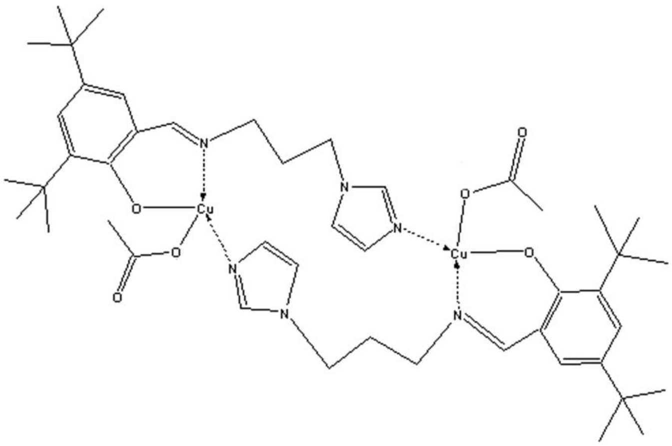
Received 30 October 2007; accepted 26 November 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.009 Å; disorder in main residue; R factor = 0.067; wR factor = 0.128; data-to-parameter ratio = 17.8.

In the centrosymmetric title compound, $[Cu_2(C_{21}H_{30}N_3O)_2(C_2H_3O_2)_2]$, each Cu atom has a distorted tetrahedral coordination geometry defined by N and O atoms in a chelate ring, N of an imidazole ring, and an acetate O atom. The uncoordinated acetate O atom is disordered over two sites with occupancies 0.7:0.3.

Related literature

For related literature, see: Djebbar *et al.* (1997); Hansen *et al.* (1996); Huang *et al.* (2002); Lacroix *et al.* (2004); Tas *et al.* (2004).



Experimental

Crystal data

$[Cu_2(C_{21}H_{30}N_3O)_2(C_2H_3O_2)_2]$
M_r = 926.13
Monoclinic, $P2_1/c$
a = 14.1745 (11) Å
b = 10.2898 (8) Å
c = 19.0850 (17) Å
β = 116.502 (6)°
V = 2491.1 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.90 mm^{-1}
T = 296 K
0.25 × 0.19 × 0.07 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.741, T_{max} = 0.914
34842 measured reflections
4905 independent reflections
2485 reflections with $I > 2\sigma(I)$
R_{int} = 0.167

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.128
S = 0.95
4905 reflections
275 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Selected bond lengths (Å).

N1—Cu1	1.957 (4)	O1—Cu1	1.910 (3)
N3—Cu1	1.989 (4)	O2—Cu1	1.966 (3)

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDSII diffractometer (purchased under grant No. F279 of the University Research Fund).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2164).

References

Djebbar, S. S., Benali, B. O. & Deloume, J. P. (1997). *Polyhedron*, **16**, 2175–2182.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Hansen, K. B., Leighton, J. L. & Jacobsen, E. N. (1996). *J. Am. Chem. Soc.* **118**, 10924–10925.
Huang, Y., Iwama, T. & Rawal, V. H. (2002). *Org. Lett.* **4**, 1163–1166.
Lacroix, P. G., Averseng, F., Malfant, I. & Nakatani, K. (2004). *Inorg. Chim. Acta*, **357**, 3825–3835.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Stoe & Cie (2002). *X-RED32* and *X-AREA*. Stoe & Cie, Darmstadt, Germany.
Tas, E., Aslanoglu, M., Guler, M. & Ulusoy, M. (2004). *J. Coord. Chem.* **57**, 583–589.

supporting information

Acta Cryst. (2008). E**64**, m51 [https://doi.org/10.1107/S1600536807063283]

Bis{*μ*-2,4-di-*tert*-butyl-6-[3-(1*H*-imidazol-1-yl)propyliminomethyl]phenolato}bis[acetatocopper(II)]

Onur Şahin, Orhan Büyükgüngör, Mahmut Ulusoy and Bekir Çetinkaya

S1. Comment

Considerable attention has been paid to the chemistry of metal complexes of Schiff bases containing nitrogen and other donors (Djebbar *et al.*, 1997). This may be attributed to their stability, biochemical and analytical uses, and potential applications in fields such as oxidation catalysis, electrochemical and molecular materials with non-linear optical properties, and therapeutic applications (Lacroix *et al.*, 2004). The use of the salen ligand framework in catalytic reactions has been receiving increasing interest due to the aforementioned advantage and its success in many newly discovered processes. Most notable is the asymmetric ring opening of epoxides by a Cr(salen)Cl catalyst which was developed by Jacobsen and co-workers in the mid-1990 s (Hansen *et al.*, 1996). A very important reaction in organic synthesis which involves the use of predominantly chromium-based salen complexes is the Diels-Alder reaction. Indeed, there is a report where these catalysts have been employed as part of a lengthy synthetic strategy to afford complex natural products (Huang *et al.*, 2002). In this study, we report the structural characterization of a dinuclear Cu(II) Schiff base complex, which was previously investigated by different techniques (Tas *et al.*, 2004). We envisaged that the free imidazole group of the proposed structure (I) should interact with aliphatic alkyl halides such as *n*-butyl bromide to give novel copper(II) complexes, leading to ionic liquids. However, all attempts under different and drastic conditions failed. This led us to reconsider the proposed structure (I). Therefore, for detailed information about the coordination mode of the ligands and for full characterization of the complex, a single-crystal X-ray determination has been carried out.

The centrosymmetric molecular structure, with the atomic labelling scheme, is presented in Fig.1. The copper atom is in a distorted tetrahedral coordination geometry defined by atoms N1 and O1 in a chelate ring, N3 of an imidazole ring, and an acetate atom O2. Atoms N1 and O1 are bonded to Cu1 to form a six-membered chelate ring (–C1—C2—C7—N1—Cu1—O1-). The dihedral angle between the phenyl ring and this chelate ring is 6.5 (4)°. The significant difference between Cu—*L* bond distances [Cu—O1 = 1.910 (3) Å, Cu—O2 = 1.966 (3) Å, Cu—N1 = 1.957 (4)Å and Cu—N3 = 1.989 (4) Å] has also been observed in other copper complexes. The longer Cu1···O3 distance and the larger Cu1—O2—C22 angle suggest there is no bonding interaction between atoms Cu1 and O3.

S2. Experimental

N-[1-(3-Aminopropyl)imidazole]-3,5-di-t-butylsalicylaldimine ligand and its copper(II) complex were synthesized according to the literature procedure (Tas *et al.*, 2004).

S3. Refinement

Atom O3 shows disorder and was modelled in two different positions as O3a and O3b with refined occupancy factors of 0.30 (4) and 0.70 (4). All H-atoms were refined using a riding model with C—H = 0.93Å [U_{iso}(H) = 1.2U_{eq}(parent atom)] for aromatic carbon, C—H = 0.97Å [U_{iso}(H) = 1.2U_{eq}(parent atom)] for methylene carbon and C—H = 0.96 Å [U_{iso}(H) =

$1.5U_{\mathrm{eq}}$(parent atom)] for methyl carbon atoms.

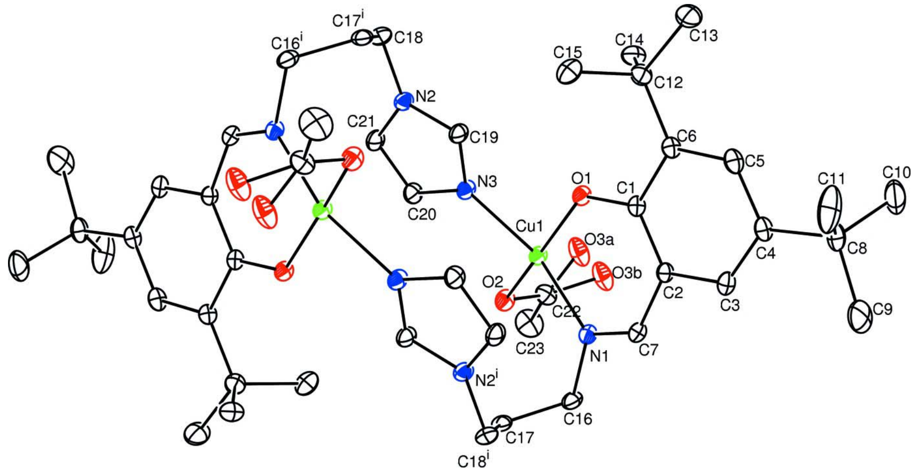


Figure 1

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) 1 - *x*, 1 - *y*, 1 - *z*.]

Bis{*μ*-2,4-di-*tert*-butyl-6-[3-(1*H*-imidazol-1- yl)propyliminomethyl]phenolato}bis[acetatocopper(II)]

Crystal data

$[Cu_2(C_{21}H_{30}N_3O)_2(C_2H_3O_2)_2]$
$M_r = 926.13$
Monoclinic, $P2_1/c$
Hall symbol: -P2ybc
$a = 14.1745\ (11)$ Å
$b = 10.2898\ (8)$ Å
$c = 19.0850\ (17)$ Å
$\beta = 116.502\ (6)°$
$V = 2491.1\ (4)$ Å^3
$Z = 2$

$F(000) = 980$
$D_x = 1.235$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 29181 reflections
$\theta = 1.6–27.9°$
$\mu = 0.90$ mm^{-1}
$T = 296$ K
Prism, black
0.25 × 0.19 × 0.07 mm

Data collection

STOE IPDSII
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration
(*X-RED32*; Stoe & Cie, 2002)
$T_{\min} = 0.741$, $T_{\max} = 0.914$

34842 measured reflections
4905 independent reflections
2485 reflections with $I > 2\sigma(I)$
$R_{\mathrm{int}} = 0.167$
$\theta_{\max} = 26.0°$, $\theta_{\min} = 2.2°$
$h = -17\rightarrow17$
$k = -12\rightarrow12$
$l = -23\rightarrow23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.128$
$S = 0.95$
4905 reflections
275 parameters
12 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

$w = 1/[\sigma^2(F_o^2) + (0.0447P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.6847 (4)	0.6496 (5)	0.4074 (3)	0.0479 (12)	
C2	0.6890 (4)	0.5548 (4)	0.3558 (3)	0.0478 (12)	
C3	0.7777 (4)	0.5428 (5)	0.3420 (3)	0.0573 (14)	
H3	0.7789	0.4768	0.3092	0.069*	
C4	0.8623 (4)	0.6239 (5)	0.3749 (3)	0.0570 (14)	
C5	0.8573 (4)	0.7181 (6)	0.4260 (3)	0.0635 (15)	
H5	0.9142	0.7745	0.4491	0.076*	
C6	0.7738 (4)	0.7346 (5)	0.4451 (3)	0.0531 (13)	
C7	0.6028 (4)	0.4685 (5)	0.3117 (3)	0.0556 (13)	
H7	0.6150	0.4070	0.2810	0.067*	
C8	0.9600 (5)	0.6182 (6)	0.3599 (4)	0.0752 (17)	
C9	0.9519 (6)	0.5078 (8)	0.3043 (6)	0.141 (4)	
H9A	0.9468	0.4264	0.3269	0.169*	
H9B	1.0136	0.5074	0.2955	0.169*	
H9C	0.8904	0.5200	0.2554	0.169*	
C10	0.9705 (7)	0.7427 (8)	0.3223 (5)	0.131 (3)	
H10A	1.0295	0.7362	0.3105	0.157*	
H10B	0.9814	0.8139	0.3576	0.157*	
H10C	0.9073	0.7573	0.2748	0.157*	
C11	1.0571 (5)	0.5926 (11)	0.4350 (5)	0.156 (4)	
H11A	1.0500	0.5106	0.4563	0.187*	
H11B	1.0656	0.6605	0.4719	0.187*	
H11C	1.1177	0.5902	0.4250	0.187*	
C12	0.7780 (4)	0.8338 (6)	0.5050 (3)	0.0671 (15)	
C13	0.8787 (5)	0.9195 (8)	0.5362 (4)	0.113 (3)	
H13A	0.8786	0.9778	0.5754	0.136*	
H13B	0.8796	0.9687	0.4938	0.136*	
H13C	0.9400	0.8650	0.5586	0.136*	
C14	0.6846 (5)	0.9279 (6)	0.4704 (3)	0.0811 (17)	
H14A	0.6199	0.8802	0.4537	0.097*	
H14B	0.6853	0.9722	0.4264	0.097*	
H14C	0.6900	0.9903	0.5094	0.097*	

C15	0.7796 (5)	0.7619 (7)	0.5764 (3)	0.0817 (18)	
H15A	0.7156	0.7132	0.5605	0.098*	
H15B	0.7854	0.8240	0.6157	0.098*	
H15C	0.8388	0.7039	0.5974	0.098*	
C16	0.4370 (4)	0.3671 (5)	0.2586 (3)	0.0649 (16)	
H16A	0.4696	0.3215	0.2306	0.078*	
H16B	0.3740	0.4095	0.2203	0.078*	
C17	0.4064 (5)	0.2697 (6)	0.3046 (3)	0.0698 (17)	
H17A	0.3537	0.2114	0.2679	0.084*	
H17B	0.3742	0.3162	0.3326	0.084*	
C18	0.5027 (5)	0.8115 (6)	0.6368 (4)	0.0771 (18)	
H18A	0.4521	0.8271	0.6571	0.092*	
H18B	0.5294	0.8949	0.6300	0.092*	
C19	0.4943 (4)	0.7166 (5)	0.5142 (3)	0.0657 (15)	
H19	0.5638	0.7362	0.5260	0.079*	
C20	0.3381 (4)	0.6471 (6)	0.4573 (3)	0.0665 (15)	
H20	0.2764	0.6086	0.4207	0.080*	
C21	0.3507 (5)	0.7013 (6)	0.5248 (4)	0.0705 (16)	
H21	0.3002	0.7066	0.5433	0.085*	
C22	0.2820 (5)	0.6256 (6)	0.2458 (4)	0.0721 (17)	
C23	0.1666 (5)	0.6146 (8)	0.1897 (4)	0.122 (3)	
H23A	0.1251	0.6322	0.2169	0.146*	
H23B	0.1518	0.5283	0.1683	0.146*	
H23C	0.1493	0.6763	0.1480	0.146*	
N1	0.5106 (3)	0.4662 (4)	0.3098 (2)	0.0543 (11)	
N2	0.4498 (4)	0.7462 (4)	0.5607 (3)	0.0620 (12)	
N3	0.4297 (3)	0.6572 (4)	0.4504 (2)	0.0596 (11)	
O1	0.6027 (2)	0.6631 (3)	0.42159 (19)	0.0557 (9)	
O2	0.3149 (3)	0.5524 (4)	0.3042 (2)	0.0705 (11)	
O3A	0.327 (3)	0.721 (4)	0.253 (2)	0.105 (5)	0.30 (4)
O3B	0.3390 (11)	0.6916 (16)	0.2238 (13)	0.105 (5)	0.70 (4)
Cu1	0.46586 (5)	0.58707 (6)	0.36829 (4)	0.0531 (2)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.035 (3)	0.061 (3)	0.044 (3)	0.006 (2)	0.014 (2)	0.010 (2)
C2	0.041 (3)	0.054 (3)	0.051 (3)	0.006 (2)	0.022 (2)	0.006 (2)
C3	0.056 (3)	0.065 (4)	0.060 (3)	0.020 (3)	0.033 (3)	0.019 (3)
C4	0.040 (3)	0.064 (4)	0.069 (3)	0.011 (2)	0.026 (3)	0.020 (3)
C5	0.035 (3)	0.081 (4)	0.068 (4)	−0.001 (3)	0.018 (3)	0.014 (3)
C6	0.037 (3)	0.064 (3)	0.052 (3)	0.001 (2)	0.014 (2)	0.007 (3)
C7	0.058 (3)	0.066 (4)	0.046 (3)	0.005 (3)	0.026 (3)	0.001 (2)
C8	0.056 (3)	0.093 (5)	0.092 (4)	0.007 (3)	0.047 (3)	0.020 (4)
C9	0.119 (7)	0.128 (7)	0.242 (11)	0.001 (5)	0.141 (8)	−0.009 (8)
C10	0.145 (7)	0.129 (7)	0.175 (8)	−0.003 (6)	0.121 (7)	0.028 (6)
C11	0.059 (4)	0.294 (13)	0.134 (6)	0.047 (7)	0.061 (5)	0.069 (8)
C12	0.052 (3)	0.077 (4)	0.067 (4)	−0.010 (3)	0.022 (3)	−0.005 (3)

C13	0.090 (5)	0.139 (7)	0.117 (5)	−0.054 (5)	0.052 (4)	−0.053 (5)
C14	0.089 (4)	0.066 (4)	0.087 (4)	−0.005 (4)	0.037 (4)	−0.014 (3)
C15	0.065 (4)	0.113 (5)	0.052 (3)	0.014 (4)	0.014 (3)	−0.002 (3)
C16	0.063 (4)	0.077 (4)	0.055 (3)	−0.008 (3)	0.026 (3)	−0.023 (3)
C17	0.071 (4)	0.075 (4)	0.073 (4)	−0.029 (3)	0.040 (3)	−0.039 (3)
C18	0.100 (5)	0.061 (4)	0.089 (4)	0.000 (3)	0.059 (4)	−0.024 (3)
C19	0.053 (3)	0.085 (4)	0.070 (4)	−0.011 (3)	0.036 (3)	−0.020 (3)
C20	0.046 (3)	0.085 (4)	0.072 (4)	−0.007 (3)	0.029 (3)	−0.006 (3)
C21	0.063 (4)	0.086 (4)	0.081 (4)	−0.002 (3)	0.049 (3)	−0.012 (3)
C22	0.054 (4)	0.067 (5)	0.092 (5)	0.001 (3)	0.029 (4)	0.002 (4)
C23	0.063 (4)	0.150 (8)	0.110 (5)	−0.001 (5)	0.001 (4)	0.012 (5)
N1	0.046 (2)	0.069 (3)	0.047 (2)	−0.002 (2)	0.020 (2)	−0.003 (2)
N2	0.063 (3)	0.064 (3)	0.070 (3)	−0.002 (2)	0.039 (3)	−0.014 (2)
N3	0.044 (3)	0.078 (3)	0.062 (3)	−0.002 (2)	0.028 (2)	−0.012 (2)
O1	0.0381 (19)	0.073 (2)	0.058 (2)	−0.0021 (16)	0.0235 (17)	−0.0077 (17)
O2	0.048 (2)	0.096 (3)	0.068 (2)	−0.004 (2)	0.0253 (19)	−0.007 (2)
O3A	0.079 (5)	0.092 (7)	0.162 (12)	0.008 (4)	0.070 (6)	0.041 (7)
O3B	0.079 (5)	0.092 (7)	0.162 (12)	0.008 (4)	0.070 (6)	0.041 (7)
Cu1	0.0392 (3)	0.0685 (4)	0.0521 (3)	−0.0025 (4)	0.0207 (2)	−0.0072 (4)

Geometric parameters (Å, º)

C1—O1	1.313 (5)	C14—H14C	0.960
C1—C2	1.407 (6)	C15—H15A	0.960
C1—C6	1.439 (7)	C15—H15B	0.960
C2—C3	1.399 (6)	C15—H15C	0.960
C2—C7	1.440 (7)	C16—N1	1.474 (6)
C3—C4	1.363 (7)	C16—C17	1.517 (7)
C3—H3	0.930	C16—H16A	0.970
C4—C5	1.400 (7)	C16—H16B	0.970
C4—C8	1.535 (7)	C17—C18^{i}	1.524 (8)
C5—C6	1.395 (7)	C17—H17A	0.970
C5—H5	0.930	C17—H17B	0.970
C6—C12	1.514 (7)	C18—N2	1.467 (7)
C7—N1	1.291 (6)	C18—C17^{i}	1.524 (8)
C7—H7	0.930	C18—H18A	0.970
C8—C11	1.503 (9)	C18—H18B	0.970
C8—C10	1.508 (9)	C19—N3	1.304 (6)
C8—C9	1.524 (10)	C19—N2	1.331 (6)
C9—H9A	0.960	C19—H19	0.930
C9—H9B	0.960	C20—C21	1.341 (7)
C9—H9C	0.960	C20—N3	1.366 (6)
C10—H10A	0.960	C20—H20	0.930
C10—H10B	0.960	C21—N2	1.341 (7)
C10—H10C	0.960	C21—H21	0.930
C11—H11A	0.960	C22—O3A	1.14 (4)
C11—H11B	0.960	C22—O2	1.249 (7)
C11—H11C	0.960	C22—O3B	1.263 (18)

C12—C14	1.532 (8)	C22—C23	1.509 (8)
C12—C15	1.541 (8)	C23—H23A	0.960
C12—C13	1.552 (8)	C23—H23B	0.960
C13—H13A	0.960	C23—H23C	0.960
C13—H13B	0.960	N1—Cu1	1.957 (4)
C13—H13C	0.960	N3—Cu1	1.989 (4)
C14—H14A	0.960	O1—Cu1	1.910 (3)
C14—H14B	0.960	O2—Cu1	1.966 (3)

O1—C1—C2	122.5 (4)	H14B—C14—H14C	109.5
O1—C1—C6	119.5 (4)	C12—C15—H15A	109.5
C2—C1—C6	118.0 (4)	C12—C15—H15B	109.5
C3—C2—C1	121.1 (5)	H15A—C15—H15B	109.5
C3—C2—C7	115.8 (5)	C12—C15—H15C	109.5
C1—C2—C7	123.1 (4)	H15A—C15—H15C	109.5
C4—C3—C2	122.7 (5)	H15B—C15—H15C	109.5
C4—C3—H3	118.7	N1—C16—C17	112.0 (4)
C2—C3—H3	118.7	N1—C16—H16A	109.2
C3—C4—C5	115.9 (5)	C17—C16—H16A	109.2
C3—C4—C8	125.0 (5)	N1—C16—H16B	109.2
C5—C4—C8	119.2 (5)	C17—C16—H16B	109.2
C6—C5—C4	125.4 (5)	H16A—C16—H16B	107.9
C6—C5—H5	117.3	C16—C17—C18^{i}	114.9 (5)
C4—C5—H5	117.3	C16—C17—H17A	108.5
C5—C6—C1	116.9 (5)	C18^{i}—C17—H17A	108.5
C5—C6—C12	121.8 (5)	C16—C17—H17B	108.5
C1—C6—C12	121.2 (4)	C18^{i}—C17—H17B	108.5
N1—C7—C2	127.8 (5)	H17A—C17—H17B	107.5
N1—C7—H7	116.1	N2—C18—C17^{i}	111.5 (4)
C2—C7—H7	116.1	N2—C18—H18A	109.3
C11—C8—C10	111.1 (7)	C17^{i}—C18—H18A	109.3
C11—C8—C9	106.6 (6)	N2—C18—H18B	109.3
C10—C8—C9	107.1 (6)	C17^{i}—C18—H18B	109.3
C11—C8—C4	110.3 (5)	H18A—C18—H18B	108.0
C10—C8—C4	110.2 (5)	N3—C19—N2	112.7 (5)
C9—C8—C4	111.4 (5)	N3—C19—H19	123.7
C8—C9—H9A	109.5	N2—C19—H19	123.7
C8—C9—H9B	109.5	C21—C20—N3	109.7 (5)
H9A—C9—H9B	109.5	C21—C20—H20	125.2
C8—C9—H9C	109.5	N3—C20—H20	125.2
H9A—C9—H9C	109.5	C20—C21—N2	107.1 (5)
H9B—C9—H9C	109.5	C20—C21—H21	126.5
C8—C10—H10A	109.5	N2—C21—H21	126.5
C8—C10—H10B	109.5	O3A—C22—O2	116 (2)
H10A—C10—H10B	109.5	O2—C22—O3B	125.6 (8)
C8—C10—H10C	109.5	O3A—C22—C23	121.2 (19)
H10A—C10—H10C	109.5	O2—C22—C23	116.3 (6)
H10B—C10—H10C	109.5	O3B—C22—C23	117.1 (9)

C8—C11—H11A	109.5	C22—C23—H23A	109.5
C8—C11—H11B	109.5	C22—C23—H23B	109.5
H11A—C11—H11B	109.5	H23A—C23—H23B	109.5
C8—C11—H11C	109.5	C22—C23—H23C	109.5
H11A—C11—H11C	109.5	H23A—C23—H23C	109.5
H11B—C11—H11C	109.5	H23B—C23—H23C	109.5
C6—C12—C14	111.4 (4)	C7—N1—C16	116.1 (4)
C6—C12—C15	108.9 (5)	C7—N1—Cu1	123.6 (3)
C14—C12—C15	110.7 (5)	C16—N1—Cu1	120.2 (3)
C6—C12—C13	113.1 (5)	C19—N2—C21	106.3 (5)
C14—C12—C13	106.0 (5)	C19—N2—C18	125.4 (5)
C15—C12—C13	106.6 (5)	C21—N2—C18	128.3 (5)
C12—C13—H13A	109.5	C19—N3—C20	104.3 (4)
C12—C13—H13B	109.5	C19—N3—Cu1	125.8 (4)
H13A—C13—H13B	109.5	C20—N3—Cu1	129.7 (4)
C12—C13—H13C	109.5	C1—O1—Cu1	128.9 (3)
H13A—C13—H13C	109.5	C22—O2—Cu1	108.4 (4)
H13B—C13—H13C	109.5	O1—Cu1—N1	93.07 (15)
C12—C14—H14A	109.5	O1—Cu1—O2	165.98 (17)
C12—C14—H14B	109.5	N1—Cu1—O2	93.98 (16)
H14A—C14—H14B	109.5	O1—Cu1—N3	89.40 (16)
C12—C14—H14C	109.5	N1—Cu1—N3	160.63 (17)
H14A—C14—H14C	109.5	O2—Cu1—N3	87.95 (16)

O1—C1—C2—C3	−179.9 (4)	C17—C16—N1—Cu1	−64.3 (5)
C6—C1—C2—C3	0.5 (6)	N3—C19—N2—C21	0.8 (7)
O1—C1—C2—C7	2.7 (7)	N3—C19—N2—C18	179.1 (5)
C6—C1—C2—C7	−176.9 (4)	C20—C21—N2—C19	−0.7 (7)
C1—C2—C3—C4	−2.5 (7)	C20—C21—N2—C18	−178.9 (5)
C7—C2—C3—C4	175.1 (4)	C17^{i}—C18—N2—C19	−62.9 (7)
C2—C3—C4—C5	2.3 (7)	C17^{i}—C18—N2—C21	115.0 (6)
C2—C3—C4—C8	−177.9 (5)	N2—C19—N3—C20	−0.7 (6)
C3—C4—C5—C6	−0.1 (7)	N2—C19—N3—Cu1	−176.3 (4)
C8—C4—C5—C6	−179.9 (5)	C21—C20—N3—C19	0.2 (6)
C4—C5—C6—C1	−1.8 (7)	C21—C20—N3—Cu1	175.6 (4)
C4—C5—C6—C12	176.1 (5)	C2—C1—O1—Cu1	−11.4 (6)
O1—C1—C6—C5	−178.2 (4)	C6—C1—O1—Cu1	168.3 (3)
C2—C1—C6—C5	1.5 (6)	O3A—C22—O2—Cu1	−26 (2)
O1—C1—C6—C12	4.0 (7)	O3B—C22—O2—Cu1	12.5 (16)
C2—C1—C6—C12	−176.4 (4)	C23—C22—O2—Cu1	−179.2 (5)
C3—C2—C7—N1	−174.9 (5)	C1—O1—Cu1—N1	11.6 (4)
C1—C2—C7—N1	2.6 (8)	C1—O1—Cu1—O2	−108.6 (7)
C3—C4—C8—C11	−119.3 (7)	C1—O1—Cu1—N3	172.3 (4)
C5—C4—C8—C11	60.5 (7)	C7—N1—Cu1—O1	−6.0 (4)
C3—C4—C8—C10	117.7 (6)	C16—N1—Cu1—O1	175.3 (4)
C5—C4—C8—C10	−62.5 (7)	C7—N1—Cu1—O2	161.9 (4)
C3—C4—C8—C9	−1.1 (8)	C16—N1—Cu1—O2	−16.9 (4)
C5—C4—C8—C9	178.7 (6)	C7—N1—Cu1—N3	−103.0 (6)

C5—C6—C12—C14	123.9 (5)	C16—N1—Cu1—N3	78.3 (6)
C1—C6—C12—C14	−58.3 (7)	C22—O2—Cu1—O1	33.7 (8)
C5—C6—C12—C15	−113.7 (5)	C22—O2—Cu1—N1	−86.3 (4)
C1—C6—C12—C15	64.1 (6)	C22—O2—Cu1—N3	113.0 (4)
C5—C6—C12—C13	4.6 (8)	C19—N3—Cu1—O1	−6.0 (5)
C1—C6—C12—C13	−177.6 (5)	C20—N3—Cu1—O1	179.6 (5)
N1—C16—C17—C18^{i}	−63.0 (6)	C19—N3—Cu1—N1	91.6 (7)
N3—C20—C21—N2	0.3 (7)	C20—N3—Cu1—N1	−82.9 (7)
C2—C7—N1—C16	179.6 (5)	C19—N3—Cu1—O2	−172.2 (5)
C2—C7—N1—Cu1	0.8 (7)	C20—N3—Cu1—O2	13.3 (5)
C17—C16—N1—C7	116.9 (5)		

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