

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

{ μ -6,6'-Dimethoxy-2,2'-[1,2-phenylenebis(nitrilomethylidene)]diphenolato}-methanolcopper(II)sodium(I)

Jiang Bian

South China Sea Institute of Oceanology, Chinese Academy of Sciences, Guangzhou 510301, People's Republic of China, and Institute of Microbiology, Chinese Academy of Sciences, Beijing 100101, People's Republic of China, and Graduate University of Chinese Academy of Sciences, Chinese Academy of Sciences, Beijing 100049, People's Republic of China

Correspondence e-mail: jiangbian2008@yahoo.cn

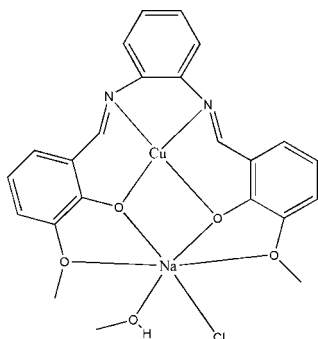
Received 8 March 2008; accepted 29 March 2008

Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.028; wR factor = 0.084; data-to-parameter ratio = 15.3.

In the title complex, $[\text{NaCu}(\text{C}_{22}\text{H}_{18}\text{N}_2\text{O}_4)\text{Cl}(\text{CH}_3\text{OH})]$, the Cu atom lies nearly in the plane defined by the N_2O_2 core of donor atoms, the out-of-plane distance being 0.001 (2) Å. The anion provides a planar cavity of four O atoms which accommodates a sodium cation. The coordination geometry around sodium is completed by the methanol O atom and a chloride ion. The four O atoms define a coordination plane containing the sodium cation [maximum displacement from the mean plane through the five atoms = 0.152 (3) Å for Na]. The crystal structure is stabilized by intermolecular C—H...Cl and O—H...Cl hydrogen bonds, which link the molecules into dimers. The crystal packing is further stabilized by weak π – π stacking interactions [centroid–centroid distances of 3.442 (4), 3.482 (3), 3.350 (2), 3.531 (4) 3.575 (2) and 3.604 (2) Å].

Related literature

For related literature, see: Molina *et al.* (1998); Lo *et al.* (2004, 2006).



Experimental

Crystal data

$[\text{NaCu}(\text{C}_{22}\text{H}_{18}\text{N}_2\text{O}_4)\text{Cl}(\text{CH}_3\text{O})]$
 $M_r = 528.41$
 Monoclinic, $P2_1/n$
 $a = 11.7986$ (2) Å
 $b = 7.9657$ (2) Å
 $c = 23.8291$ (3) Å
 $\beta = 93.283$ (2)°
 $V = 2235.88$ (7) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.16$ mm⁻¹
 $T = 295$ (2) K
 $0.22 \times 0.18 \times 0.12$ mm

Data collection

Bruker APEX CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2004)
 $T_{\min} = 0.785$, $T_{\max} = 0.874$
 20679 measured reflections
 4620 independent reflections
 3958 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.083$
 $S = 1.02$
 4620 reflections
 302 parameters
 1 restraint
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.39$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O5}-\text{H5A}\cdots\text{Cl1}^i$	0.86 (2)	2.34 (2)	3.193 (2)	172 (4)
$\text{C10}-\text{H10}\cdots\text{Cl1}^{ii}$	0.93	2.82	3.729 (2)	165

Symmetry codes: (i) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$; (ii) $-x + 1, -y, -z + 1$.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and local programs.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2383).

References

- Bruker (2001). SMART and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
 Lo, W. K., Wong, W. K., Guo, J. P., Wong, W. Y., Li, K. F. & Cheah, K. W. (2004). *Inorg. Chim. Acta*, **357**, 4510–4521.
 Lo, W. K., Wong, W. K., Wong, W. Y., Guo, J. P., Yeung, K. T., Cheng, Y. K., Yang, X. P. & Jones, R. A. (2006). *Inorg. Chem.* **45**, 9315–9325.
 Molina, R. H., Mederos, A., Dominguez, S., Gili, P., Perez, C. R., Castineiras, A., Solans, X., Lloret, F. & Real, J. A. (1998). *Inorg. Chem.* **37**, 5102–5108.
 Sheldrick, G. M. (2004). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

Acta Cryst. (2008). E64, m625 [doi:10.1107/S1600536808008453]

{ μ -6,6'-Dimethoxy-2,2'-[1,2-phenylenebis(nitrilomethyldiylidene)]diphenolato}methanolcopper(II)sodium(I)

J. Bian

Comment

It is known that phenylene bridged Schiff base ligand *N,N'*-1,2-Phenylene-bis(3-methoxysalicylideneiminato) as N- or O-donors exhibit excellent coordination capability to form supramolecular frameworks. Self-assembly by H-bonding, π - π stacking, and van der Waals interactions is also an important process in the formation of noncovalent supramolecular frameworks (Lo *et al.*, 2006; Molina *et al.*, 1998). The title compound, (I), was prepared by employing *N,N'*-1,2-Phenylene-bis(3-methoxysalicylideneiminato) as ligand. Here we present its crystal structure.

In the title complex, (I), the copper atoms lie nearly in the plane defined by the N_2O_2 core of donor atoms, the out-of-plane distances being 0.001 (2) Å. The anion provides a planar cavity of four oxygen atoms which accommodates a sodium cation. The coordination geometry around sodium is completed by the oxygen atom from methanol molecule and chloride ion. The four oxygen atoms [O1, O2, O3, O4] define a coordination plane containing the sodium cation (maximum displacement from the mean plane through the five atoms: 0.152 (3) Å for Na). The crystal structure is stabilized by intermolecular C—H \cdots Cl hydrogen bonds, which link the molecules into dimers. The packing is also stabilized by six intermolecular π - π stacking interactions, with relatively short distance Cg1 \cdots Cg4ⁱ 3.575 (2) Å, Cg1 \cdots Cg5ⁱⁱ 3.482 (3) Å, Cg2 \cdots Cg2ⁱ 3.604 (2) Å, Cg2 \cdots Cg4ⁱ 3.350 (2) Å, Cg3 \cdots Cg3ⁱⁱ 3.442 (4) Å, Cg3 \cdots Cg5ⁱⁱ 3.531 (4) Å, where Cg1, Cg2, Cg3, Cg4 and Cg5 are centroids of Cu1/N1/N2/C9/C14, Cu1/O2/N1/C6—C8, Cu1/O3/N2/C15/C16/C21, C2—C7 and C16—C21 rings, respectively [symmetry code: (i) 2 - x, 1 - y, -z, (ii) 1 - x, 1 - y, -z].

Experimental

The phenylene bridged Schiff base ligand *N,N'*-1,2-Phenylene-bis(3-methoxysalicylideneiminato) was prepared in excellent yield (92%) according to the literature method (Lo *et al.*, 2004) *via* the condensation of 1,2-diaminobenzene with *o*-vanillin and 5-(4'-methylphenyl)-3-methoxysalicylaldehyde, respectively, in a 2:1 mole ratio. The ¹H NMR spectrum of Schiff base ligand in CDCl₃ showed a singlet at δ 8.60 for the imino protons and a broad singlet at δ 13.23 for the hydroxyl protons, respectively.

To a solution of the *N,N'*-1,2-Phenylene-bis(3-methoxysalicylideneiminato) (0.38 g, 1 mmol) in methanol (10 ml), 0.134 g (1 mmol) CuCl₂, 0.06 g (1 mmol) NaCl powder was slowly added. After stirring for four hours, the solution was filtered to remove the precipitate and placed in a desiccator filled with methanol. Brown crystals were obtained about one week later. Elemental analysis [found (calculated)] for C₂₃H₂₂N₂O₅ClCuNa: C 52.20 (52.28), H 4.23 (4.20), N 5.20% (5.30%). IR /m C=N 1642 cm⁻¹.

Refinement

All H atoms were found on difference maps. The hydroxy proton atoms were refined freely, giving an O–H bond distance of 0.86 Å. The remaining atoms were placed in calculated positions, with C–H = 0.93 or 0.96 Å, and included in the final cycles of refinement using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C})$ (1.5 U_{eq} for methyl).

Figures

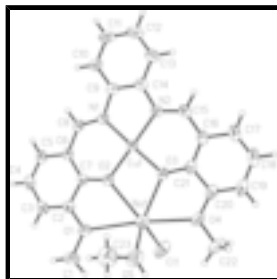


Fig. 1. View of the title compound (I), with displacement ellipsoids drawn at the 40% probability level.

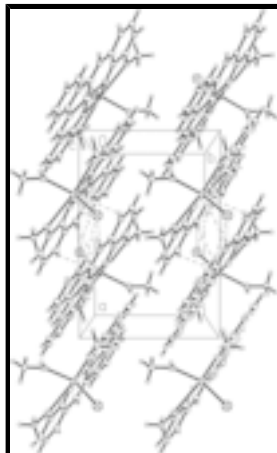


Fig. 2. Packing diagram of structure of (I), view along the *c* axis. Hydrogen bonds are shown as dashed lines.

{ μ -6,6'-Dimethoxy-2,2'-[1,2-phenylenebis(nitrilomethylidene)]diphenolato}methanolcopper(II)sodium(I)

Crystal data

[NaCu(C₂₂H₁₈N₂O₄)Cl(CH₄O)]

$M_r = 528.41$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 11.7986$ (2) Å

$b = 7.9657$ (2) Å

$c = 23.8291$ (3) Å

$\beta = 93.283$ (2)°

$V = 2235.88$ (7) Å³

$Z = 4$

$F_{000} = 1084$

$D_x = 1.570$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 3689 reflections

$\theta = 2.2$ – 26.6 °

$\mu = 1.16$ mm⁻¹

$T = 295$ (2) K

Block, brown

$0.22 \times 0.18 \times 0.12$ mm

Data collection

Bruker APEX CCD area-detector diffractometer	4620 independent reflections
Radiation source: fine-focus sealed tube	3958 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.018$
Detector resolution: 0 pixels mm^{-1}	$\theta_{\text{max}} = 26.5^\circ$
$T = 295(2)$ K	$\theta_{\text{min}} = 1.7^\circ$
φ and ω scans	$h = -14 \rightarrow 14$
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$k = -10 \rightarrow 10$
$T_{\text{min}} = 0.785$, $T_{\text{max}} = 0.874$	$l = -27 \rightarrow 29$
20679 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.028$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.083$	$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 1.0557P]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
4620 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
302 parameters	$\Delta\rho_{\text{max}} = 0.39 \text{ e } \text{\AA}^{-3}$
1 restraint	$\Delta\rho_{\text{min}} = -0.24 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.245877 (17)	0.00018 (3)	0.488480 (9)	0.03216 (8)
Na1	0.28232 (7)	-0.09373 (11)	0.62911 (3)	0.0476 (2)

supplementary materials

N1	0.32603 (13)	-0.03020 (18)	0.42070 (6)	0.0325 (3)
N2	0.14259 (12)	0.13666 (19)	0.44095 (6)	0.0343 (3)
O1	0.45834 (12)	-0.3066 (2)	0.61004 (6)	0.0500 (4)
O2	0.34391 (10)	-0.14186 (16)	0.53338 (5)	0.0364 (3)
O3	0.16904 (11)	0.04016 (17)	0.55486 (5)	0.0387 (3)
O4	0.10358 (13)	0.0706 (2)	0.65442 (6)	0.0577 (4)
O5	0.20263 (19)	-0.3239 (2)	0.67333 (9)	0.0760 (5)
C11	0.39839 (5)	0.09785 (10)	0.70798 (3)	0.0707 (2)
C1	0.5137 (2)	-0.4081 (4)	0.65277 (10)	0.0664 (7)
H1A	0.4732	-0.4008	0.6865	0.100*
H1B	0.5900	-0.3690	0.6602	0.100*
H1C	0.5150	-0.5227	0.6404	0.100*
C2	0.50487 (15)	-0.3024 (2)	0.55889 (8)	0.0358 (4)
C3	0.60488 (16)	-0.3766 (2)	0.54631 (9)	0.0410 (4)
H3	0.6460	-0.4385	0.5736	0.049*
C4	0.64579 (16)	-0.3597 (2)	0.49238 (9)	0.0427 (4)
H4	0.7142	-0.4096	0.4842	0.051*
C5	0.58578 (15)	-0.2708 (2)	0.45224 (9)	0.0382 (4)
H5	0.6142	-0.2593	0.4168	0.046*
C6	0.48040 (14)	-0.1950 (2)	0.46330 (8)	0.0324 (4)
C7	0.43811 (14)	-0.2087 (2)	0.51781 (7)	0.0308 (4)
C8	0.42240 (14)	-0.1073 (2)	0.41826 (7)	0.0334 (4)
H8	0.4566	-0.1051	0.3841	0.040*
C9	0.27193 (15)	0.0517 (2)	0.37354 (8)	0.0360 (4)
C10	0.30926 (19)	0.0474 (3)	0.31902 (9)	0.0488 (5)
H10	0.3754	-0.0099	0.3116	0.059*
C11	0.2474 (2)	0.1286 (3)	0.27618 (9)	0.0604 (6)
H11	0.2718	0.1248	0.2398	0.072*
C12	0.1496 (2)	0.2153 (3)	0.28688 (10)	0.0603 (6)
H12	0.1087	0.2693	0.2576	0.072*
C13	0.11237 (18)	0.2224 (3)	0.34051 (9)	0.0506 (5)
H13	0.0468	0.2818	0.3475	0.061*
C14	0.17298 (15)	0.1405 (2)	0.38442 (8)	0.0371 (4)
C15	0.05522 (15)	0.2153 (2)	0.45833 (8)	0.0395 (4)
H15	0.0102	0.2733	0.4315	0.047*
C16	0.02163 (15)	0.2213 (2)	0.51487 (9)	0.0391 (4)
C17	-0.07586 (17)	0.3182 (3)	0.52576 (11)	0.0521 (5)
H17	-0.1154	0.3727	0.4962	0.063*
C18	-0.11214 (19)	0.3325 (3)	0.57844 (11)	0.0603 (6)
H18	-0.1764	0.3958	0.5847	0.072*
C19	-0.05333 (18)	0.2524 (3)	0.62352 (10)	0.0545 (6)
H19	-0.0778	0.2646	0.6597	0.065*
C20	0.04028 (16)	0.1560 (3)	0.61461 (9)	0.0429 (4)
C21	0.08043 (14)	0.1367 (2)	0.55956 (8)	0.0356 (4)
C22	0.0796 (2)	0.0956 (4)	0.71220 (9)	0.0702 (7)
H22A	0.1302	0.0282	0.7358	0.105*
H22B	0.0026	0.0635	0.7177	0.105*
H22C	0.0899	0.2118	0.7218	0.105*
C23	0.2056 (3)	-0.4837 (4)	0.64857 (15)	0.0820 (9)

H23A	0.1700	-0.5636	0.6721	0.123*
H23B	0.2831	-0.5160	0.6444	0.123*
H23C	0.1658	-0.4807	0.6123	0.123*
H5A	0.172 (4)	-0.335 (6)	0.7048 (10)	0.161 (19)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.02835 (13)	0.03863 (14)	0.02980 (13)	0.00368 (8)	0.00441 (8)	0.00103 (8)
Na1	0.0472 (4)	0.0560 (5)	0.0399 (4)	-0.0035 (4)	0.0041 (3)	0.0006 (4)
N1	0.0334 (8)	0.0340 (8)	0.0302 (8)	-0.0024 (6)	0.0040 (6)	0.0005 (6)
N2	0.0304 (7)	0.0360 (8)	0.0364 (8)	-0.0001 (6)	0.0008 (6)	0.0012 (6)
O1	0.0527 (8)	0.0636 (9)	0.0337 (7)	0.0093 (7)	0.0017 (6)	0.0075 (7)
O2	0.0328 (6)	0.0442 (7)	0.0327 (6)	0.0075 (5)	0.0062 (5)	0.0032 (5)
O3	0.0327 (6)	0.0502 (7)	0.0337 (7)	0.0075 (6)	0.0069 (5)	-0.0006 (6)
O4	0.0513 (9)	0.0869 (12)	0.0361 (7)	0.0088 (8)	0.0126 (6)	-0.0058 (8)
O5	0.0989 (15)	0.0591 (11)	0.0731 (13)	-0.0056 (10)	0.0331 (11)	0.0029 (10)
Cl1	0.0488 (3)	0.1063 (5)	0.0580 (3)	-0.0131 (3)	0.0121 (3)	-0.0248 (4)
C1	0.0759 (17)	0.0821 (18)	0.0401 (12)	0.0095 (14)	-0.0066 (11)	0.0158 (12)
C2	0.0365 (9)	0.0344 (9)	0.0361 (9)	-0.0024 (7)	-0.0001 (7)	-0.0008 (7)
C3	0.0361 (9)	0.0351 (9)	0.0506 (11)	0.0030 (8)	-0.0073 (8)	0.0010 (8)
C4	0.0317 (9)	0.0386 (10)	0.0580 (12)	0.0041 (8)	0.0054 (8)	-0.0057 (9)
C5	0.0340 (9)	0.0352 (9)	0.0463 (11)	-0.0007 (7)	0.0104 (8)	-0.0040 (8)
C6	0.0309 (8)	0.0287 (8)	0.0381 (9)	-0.0024 (7)	0.0059 (7)	-0.0036 (7)
C7	0.0292 (8)	0.0284 (8)	0.0349 (9)	-0.0024 (7)	0.0015 (7)	-0.0024 (7)
C8	0.0343 (9)	0.0343 (9)	0.0323 (9)	-0.0037 (7)	0.0081 (7)	-0.0028 (7)
C9	0.0361 (9)	0.0382 (9)	0.0336 (9)	-0.0056 (8)	0.0000 (7)	0.0024 (8)
C10	0.0486 (12)	0.0625 (13)	0.0356 (10)	0.0021 (10)	0.0063 (9)	0.0027 (10)
C11	0.0619 (14)	0.0848 (17)	0.0345 (11)	-0.0027 (13)	0.0040 (10)	0.0124 (11)
C12	0.0591 (14)	0.0755 (16)	0.0450 (12)	0.0012 (12)	-0.0069 (10)	0.0210 (12)
C13	0.0440 (11)	0.0599 (13)	0.0472 (12)	0.0038 (10)	-0.0029 (9)	0.0123 (10)
C14	0.0352 (9)	0.0388 (10)	0.0372 (9)	-0.0050 (7)	-0.0001 (7)	0.0038 (8)
C15	0.0322 (9)	0.0384 (10)	0.0474 (11)	0.0013 (7)	-0.0018 (8)	0.0050 (8)
C16	0.0293 (9)	0.0369 (9)	0.0516 (11)	-0.0008 (7)	0.0056 (8)	-0.0034 (9)
C17	0.0375 (10)	0.0491 (12)	0.0702 (15)	0.0103 (9)	0.0072 (10)	0.0008 (11)
C18	0.0408 (11)	0.0566 (13)	0.0852 (18)	0.0111 (10)	0.0194 (12)	-0.0115 (13)
C19	0.0432 (11)	0.0598 (13)	0.0627 (14)	-0.0020 (10)	0.0216 (10)	-0.0168 (12)
C20	0.0348 (9)	0.0482 (11)	0.0466 (11)	-0.0054 (8)	0.0102 (8)	-0.0108 (9)
C21	0.0270 (8)	0.0378 (9)	0.0428 (10)	-0.0051 (7)	0.0074 (7)	-0.0071 (8)
C22	0.0670 (15)	0.108 (2)	0.0375 (12)	-0.0051 (15)	0.0183 (11)	-0.0125 (13)
C23	0.083 (2)	0.0695 (19)	0.093 (2)	-0.0177 (15)	0.0020 (18)	-0.0110 (15)

Geometric parameters (\AA , $^\circ$)

Cu1—O3	1.8947 (13)	C5—C6	1.420 (2)
Cu1—O2	1.9029 (12)	C5—H5	0.9300
Cu1—N1	1.9331 (15)	C6—C7	1.422 (2)
Cu1—N2	1.9472 (15)	C6—C8	1.423 (3)
Cu1—Na1	3.4363 (8)	C8—H8	0.9300

supplementary materials

Na1—O5	2.339 (2)	C9—C10	1.396 (3)
Na1—O3	2.4047 (15)	C9—C14	1.402 (3)
Na1—O2	2.4633 (14)	C10—C11	1.381 (3)
Na1—O4	2.5828 (17)	C10—H10	0.9300
Na1—Cl1	2.7279 (10)	C11—C12	1.380 (4)
Na1—O1	2.7392 (17)	C11—H11	0.9300
N1—C8	1.297 (2)	C12—C13	1.376 (3)
N1—C9	1.419 (2)	C12—H12	0.9300
N2—C15	1.295 (2)	C13—C14	1.395 (3)
N2—C14	1.414 (2)	C13—H13	0.9300
O1—C2	1.365 (2)	C15—C16	1.427 (3)
O1—C1	1.429 (3)	C15—H15	0.9300
O2—C7	1.305 (2)	C16—C21	1.409 (3)
O3—C21	1.308 (2)	C16—C17	1.421 (3)
O4—C20	1.356 (3)	C17—C18	1.354 (3)
O4—C22	1.435 (2)	C17—H17	0.9300
O5—C23	1.404 (3)	C18—C19	1.399 (4)
O5—H5A	0.86 (3)	C18—H18	0.9300
C1—H1A	0.9600	C19—C20	1.372 (3)
C1—H1B	0.9600	C19—H19	0.9300
C1—H1C	0.9600	C20—C21	1.428 (3)
C2—C3	1.368 (3)	C22—H22A	0.9600
C2—C7	1.431 (3)	C22—H22B	0.9600
C3—C4	1.405 (3)	C22—H22C	0.9600
C3—H3	0.9300	C23—H23A	0.9600
C4—C5	1.356 (3)	C23—H23B	0.9600
C4—H4	0.9300	C23—H23C	0.9600
O3—Cu1—O2	86.27 (5)	C5—C4—H4	119.9
O3—Cu1—N1	177.46 (6)	C3—C4—H4	119.9
O2—Cu1—N1	94.86 (6)	C4—C5—C6	121.22 (18)
O3—Cu1—N2	94.49 (6)	C4—C5—H5	119.4
O2—Cu1—N2	177.46 (6)	C6—C5—H5	119.4
N1—Cu1—N2	84.47 (6)	C5—C6—C7	119.57 (16)
O3—Cu1—Na1	42.40 (4)	C5—C6—C8	117.21 (16)
O2—Cu1—Na1	44.29 (4)	C7—C6—C8	123.23 (15)
N1—Cu1—Na1	138.39 (5)	O2—C7—C6	125.27 (16)
N2—Cu1—Na1	136.71 (5)	O2—C7—C2	117.55 (16)
O5—Na1—O3	117.28 (7)	C6—C7—C2	117.18 (15)
O5—Na1—O2	116.28 (7)	N1—C8—C6	125.73 (16)
O3—Na1—O2	64.46 (4)	N1—C8—H8	117.1
O5—Na1—O4	86.42 (7)	C6—C8—H8	117.1
O3—Na1—O4	61.32 (5)	C10—C9—C14	119.68 (18)
O2—Na1—O4	125.68 (5)	C10—C9—N1	125.01 (18)
O5—Na1—Cl1	109.09 (6)	C14—C9—N1	115.30 (16)
O3—Na1—Cl1	119.65 (5)	C11—C10—C9	119.6 (2)
O2—Na1—Cl1	124.19 (4)	C11—C10—H10	120.2
O4—Na1—Cl1	86.56 (5)	C9—C10—H10	120.2
O5—Na1—O1	85.27 (7)	C12—C11—C10	120.6 (2)
O3—Na1—O1	123.18 (5)	C12—C11—H11	119.7

O2—Na1—O1	58.89 (4)	C10—C11—H11	119.7
O4—Na1—O1	171.68 (6)	C13—C12—C11	120.4 (2)
C11—Na1—O1	96.03 (4)	C13—C12—H12	119.8
O5—Na1—Cu1	125.38 (6)	C11—C12—H12	119.8
O3—Na1—Cu1	32.09 (3)	C12—C13—C14	120.0 (2)
O2—Na1—Cu1	32.65 (3)	C12—C13—H13	120.0
O4—Na1—Cu1	93.39 (4)	C14—C13—H13	120.0
C11—Na1—Cu1	125.44 (3)	C13—C14—C9	119.59 (18)
O1—Na1—Cu1	91.53 (4)	C13—C14—N2	125.29 (18)
C8—N1—C9	122.57 (16)	C9—C14—N2	115.12 (16)
C8—N1—Cu1	124.68 (13)	N2—C15—C16	125.98 (18)
C9—N1—Cu1	112.62 (12)	N2—C15—H15	117.0
C15—N2—C14	122.97 (16)	C16—C15—H15	117.0
C15—N2—Cu1	124.58 (13)	C21—C16—C17	119.37 (19)
C14—N2—Cu1	112.45 (11)	C21—C16—C15	123.13 (16)
C2—O1—C1	117.35 (17)	C17—C16—C15	117.50 (19)
C2—O1—Na1	118.69 (11)	C18—C17—C16	121.1 (2)
C1—O1—Na1	123.52 (14)	C18—C17—H17	119.4
C7—O2—Cu1	125.64 (11)	C16—C17—H17	119.4
C7—O2—Na1	128.90 (11)	C17—C18—C19	120.3 (2)
Cu1—O2—Na1	103.06 (5)	C17—C18—H18	119.9
C21—O3—Cu1	126.40 (12)	C19—C18—H18	119.9
C21—O3—Na1	127.68 (12)	C20—C19—C18	120.3 (2)
Cu1—O3—Na1	105.50 (6)	C20—C19—H19	119.8
C20—O4—C22	118.06 (18)	C18—C19—H19	119.8
C20—O4—Na1	121.02 (11)	O4—C20—C19	126.06 (19)
C22—O4—Na1	120.19 (15)	O4—C20—C21	112.95 (16)
C23—O5—Na1	120.05 (18)	C19—C20—C21	121.0 (2)
C23—O5—H5A	107 (3)	O3—C21—C16	125.32 (17)
Na1—O5—H5A	133 (3)	O3—C21—C20	116.79 (17)
O1—C1—H1A	109.5	C16—C21—C20	117.89 (17)
O1—C1—H1B	109.5	O4—C22—H22A	109.5
H1A—C1—H1B	109.5	O4—C22—H22B	109.5
O1—C1—H1C	109.5	H22A—C22—H22B	109.5
H1A—C1—H1C	109.5	O4—C22—H22C	109.5
H1B—C1—H1C	109.5	H22A—C22—H22C	109.5
O1—C2—C3	125.50 (17)	H22B—C22—H22C	109.5
O1—C2—C7	112.95 (15)	O5—C23—H23A	109.5
C3—C2—C7	121.55 (17)	O5—C23—H23B	109.5
C2—C3—C4	120.32 (18)	H23A—C23—H23B	109.5
C2—C3—H3	119.8	O5—C23—H23C	109.5
C4—C3—H3	119.8	H23A—C23—H23C	109.5
C5—C4—C3	120.15 (17)	H23B—C23—H23C	109.5

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H5A \cdots C11 ⁱ	0.86 (2)	2.34 (2)	3.193 (2)	172 (4)
C10—H10 \cdots C11 ⁱⁱ	0.93	2.82	3.729 (2)	165

Symmetry codes: (i) $-x+1/2, y-1/2, -z+3/2$; (ii) $-x+1, -y, -z+1$.

Fig. 1

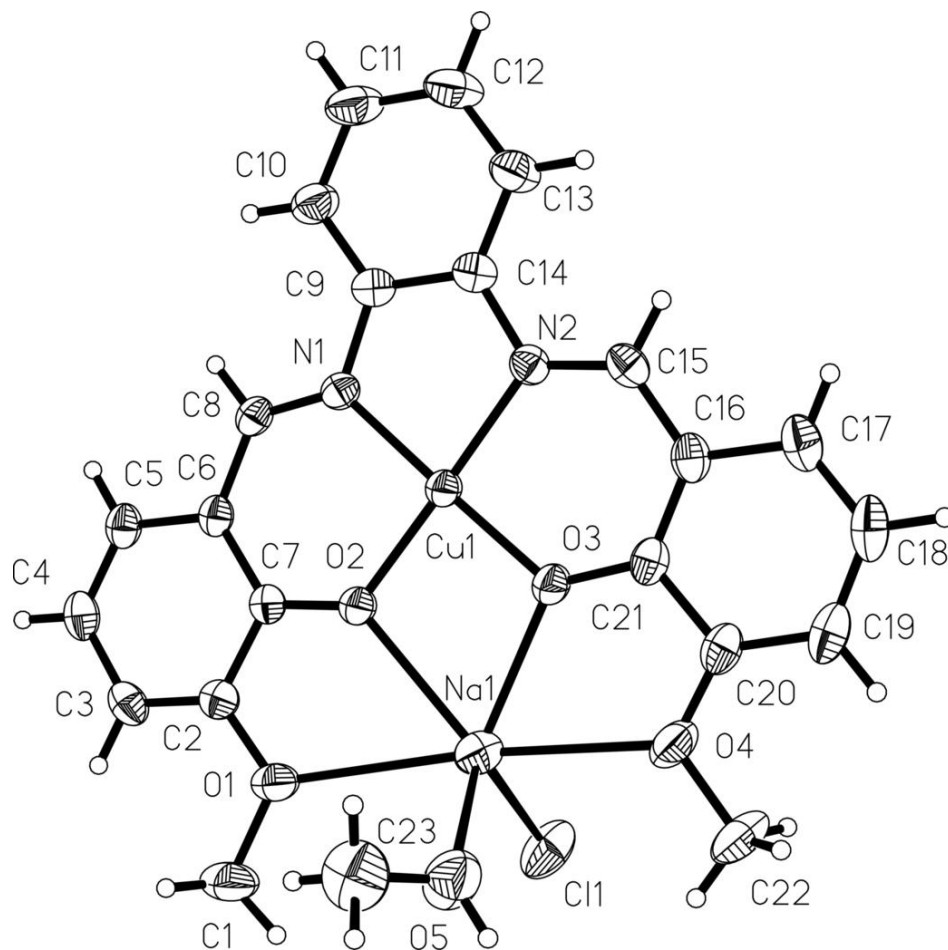


Fig. 2

