Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Retraction of articles

This article reports the retraction of 39 articles published in *Acta Crystallographica Section E* between 2004 and 2009.

After thorough investigation (see Harrison *et al.*, 2010), 39 additional articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	Retracted by	DOI	Refcode
trans-Bis{1-[3-(cyclohexylamino)propyliminomethyl]-2-naphtholato}copper(II) dichloride dihydrate	Zhang (2004)	Journal	10.1107/S1600536804028296	BIPDUA
Bis(4-bromo-2-formylphenolato-κ^2O,O')copper(II)	Sun & Gao (2005)	Author	10.1107/S160053680500187X	FEYSUY
Bis(salicylaldehydo)zinc(II)	Xiong & Liu (2005)	Journal	10.1107/S1600536805010913	GAMDUU
Bis(4-bromo-2-formylphenolato-κ^2O,O')zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
Bis(2-formylphenolato-κ^2O,O')nickel(II)	Li & Chen (2006)	Journal	10.1107/S1600536806012931	IDAZAP
Bis(2-formylphenolato)cobalt(II)	Qiu (2006)	Journal	10.1107/S1600536806015704	GEJDUV
Bis(2-formylphenolato-κ^2O,O')manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraaqua(1,10-phenanthroline-κ^2N,N')copper(II) naphthalene-1,5-disulfonate dihydrate	Liu *et al.* (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraaqua(1,10-phenanthroline-κ^2N,N')nickel(II) naphthalene-1,5-disulfonate dihydrate	Liu & Fan (2006)	Author	10.1107/S1600536806035410	KERBEP
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratolutetium(III)copper(II)	Sui *et al.* (2006)	Journal	10.1107/S160053680604565X	HESPEP
Bis(2-formylphenolato-κ^2O,O')iron(II)	Yang *et al.* (2007)	Author	10.1107/S1600536807021721	PIFCAJ
2,6-Dimethoxybenzohydrazide	Qadeer *et al.* (2007*a*)	Journal	10.1107/S1600536807022593	PIFHES
2-(2,4-Dichlorophenylsulfanyl)acetohydrazide	Qadeer *et al.* (2007*b*)	Journal	10.1107/S1600536807022891	YIFSOW
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoeuropium(III)zinc(II)	Hu *et al.* (2007)	Author	10.1107/S1600536807031121	WIHKEE
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratocerium(III)zinc(II)	Sui, Zhang, Hu & Yin (2007)	Author	10.1107/S1600536807032564	WIHREL
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)zinc(II)	Chen *et al.* (2007)	Author	10.1107/S1600536807032540	WIHRIP
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)nickel(II)	Sui, Li *et al.* (2007)	Author	10.1107/S1600536807032618	UFACUA
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(methanol-1κO)-μ-nitrato-1:2κ^2O:O′-dinitrato-1κ^4O,O'-cerium(III)zinc(II)	Sui, Fang, Hu & Lin (2007)	Author	10.1107/S1600536807033314	UDUYIC
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratosamarium(III)nickel(II)	Sui, Zhang, Hu & Jiang (2007)	Author	10.1107/S1600536807037130	AFECEU
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratopraseodymium(III)zinc(II)	Sui, Fang & Yuan (2007)	Author	10.1107/S1600536807037488	AFICEY
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratolutetium(III)zinc(II)	Sui, Sui *et al.* (2007)	Author	10.1107/S1600536807037737	AFEFOH
catena-Poly[[chloridonickel(II)]-di-μ-chlorido-[chloridonickel(II)]-μ-4,4′-methylenebis(3,5-dimethylpyrazole)-κ^2N^2:$N^{2'}$]	Huang & Chen (2007)	Author	10.1107/S1600536807039384	VIJYOD
{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}zinc(II)	Liu *et al.* (2007*a*)	Author	10.1107/S1600536807040640	DIKYUS
trans-Bis(ethylenediamine-κ^2N,N')bis(nitrato-κO)zinc(II)	Liu, Zeng & Chen (2007)	Author	10.1107/S1600536807042390	XIKYEW
[N,N′-(o-Phenylene)bis(picolinamido)-κ^4N,N',N'',N''']cobalt(II)	Liu & Zeng (2007*a*)	Author	10.1107/S1600536807044571	XILFII
[N,N′-(o-Phenylene)dipicolinamide-κ^4N]nickel(II)	Liu & Zeng (2007*b*)	Author	10.1107/S1600536807048386	WINWEW
{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}manganese(II)	Liu *et al.* (2007*b*)	Author	10.1107/S1600536807052993	VIQPIV
N-(2-Amino-3-pyridyl)urea monohydrate	Li *et al.* (2007)	Author	10.1107/S1600536807047526	SIMFEA
N-(2-Fluorophenyl)carbamic acid monohydrate	Yang (2007)	Author	10.1107/S1600536807052464	WINMOW
Aqua(dimethylglyoxime-κ^2N,N')(3,5-dinitro-2-oxidobenzoato-κ^2O^1,O^2)-copper(II)	Liu & Wen (2007)	Author	10.1107/S1600536807054244	HIQCAM
μ-Acetato-tri-μ-ferrocenecarboxylatobis[(N,N-dimethylformamide)-copper(II)]	Liu, Lin *et al.* (2007)	Journal	10.1107/S1600536807059041	HIQQEE

 doi:10.1107/S1600536809054300

Table 1 (continued)

Title	Reference	Retracted by	DOI	Refcode
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoeuropium(III)zinc(II)	Hu *et al.* (2008)	Author	10.1107/S160053680706151X	MIRPAF
Bis(4-chloro-2-formylphenolato)nickel(II)	Li *et al.* (2008)	Author	10.1107/S1600536807056309	RISTET
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoterbium(III)zinc(II)	Chen *et al.* (2008)	Author	10.1107/S1600536808006958	QIXHIP
Bis(2-ethoxy-6-formylphenolato-κ^2O^1,O^6)nickel(II)	Han (2008)	Journal	10.1107/S160053680800809X	QIXLIT
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoholmium(III)zinc(II)	Xiao, Sui *et al.* (2008)	Author	10.1107/S1600536808013743	BIZTUA
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoholmium(III)nickel(II)	Xiao, Fu *et al.* (2008)	Author	10.1107/S1600536808013755	BIZVAI
Hydrogen-bonding patterns in the cocrystal terephthalic acid–4,4′-bipyridine (2/1)	Wang *et al.* (2009)	Journal	10.1107/S160053680903236X	DUCZEH
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(ethanol-1κO)-μ-nitrato-1:2κ^2O:O′-dinitrato-1κ^4O,O′-samarium(III)zinc(II)	Huang *et al.* (2009)	Journal	10.1107/S1600536809033558	YUCWAV

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Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

trans-Bis{1-[3-(cyclohexylamino)propylimino-methyl]-2-naphtholato}copper(II) dichloride dihydrate

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Received 25 October 2004
Accepted 3 November 2004
Online 13 November 2004

Key indicators

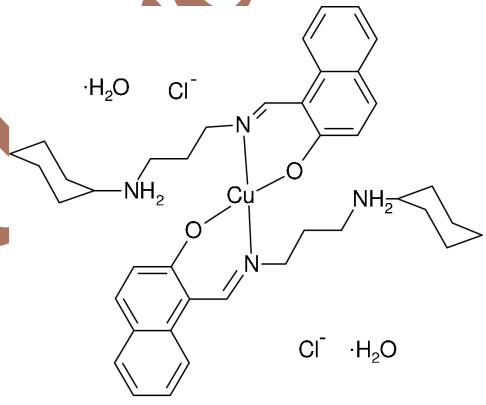
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.005 Å
R factor = 0.053
wR factor = 0.150
Data-to-parameter ratio = 17.1

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

In the title centrosymmetric mononuclear copper(II) compound, $[Cu(C_{20}H_{26}N_2O)_2]Cl_2\cdot 2H_2O$, the Cu^{II} atom is coordinated by two N atoms and two O atoms from two Schiff base ligands. The coordination geometry is slightly distorted square planar. In the crystal structure, the ions and molecules are linked together by intermolecular O—H···Cl and N—H···Cl hydrogen bonds.

Comment

Copper compounds containing Schiff base ligands have been of great interest for many years (Chang *et al.*, 1998). These compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Bhatia *et al.*, 1981). As an extension of our work on the structural characterization of Schiff base copper compounds, a new mononuclear copper(II) complex, (I), is reported here.



(I)

The structure of (I) (Fig. 1) consists of a mononuclear $[Cu(C_{20}H_{26}N_2O)_2]^{2+}$ cation, two uncoordinated chloride anions and two uncoordinated water molecules. The Cu atom, on an inversion center, is in a slightly distorted square-planar geometry and is four-coordinated by two N atoms and two O atoms from two Schiff base ligands. The two *trans* angles at the copper(II) center are exactly 180°, by virtue of the crystallographic symmetry (Table 1), and the other angles are close to 90°, *viz*. 88.20 (9) and 91.80 (9)°, indicating a slight deviation from perfect square-planar geometry. The Cu1—O1 bond length [1.832 (2) Å] is comparable to that observed in another Schiff base complex [1.888 (4) Å; You *et al.*, 2004]. The Cu1—N1 bond length [1.913 (2) Å] is slightly shorter than the value [2.002 (4) Å] observed in the same previously reported

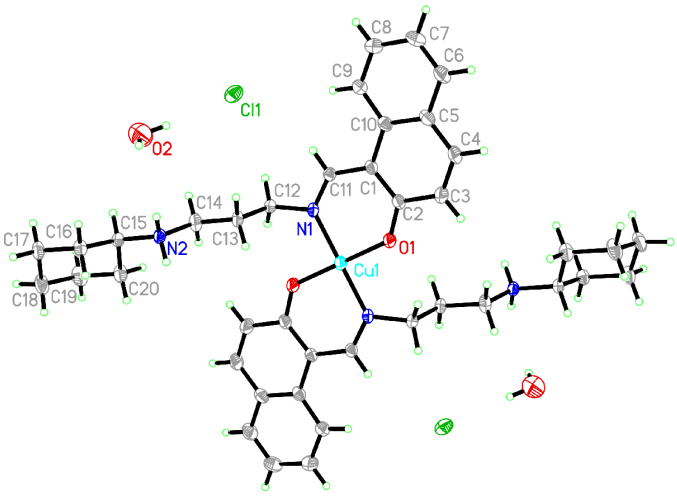


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme for the asymmetric unit. The other half of the complex is generated by the symmetry code $(2-x, 2-y, 1-z)$.

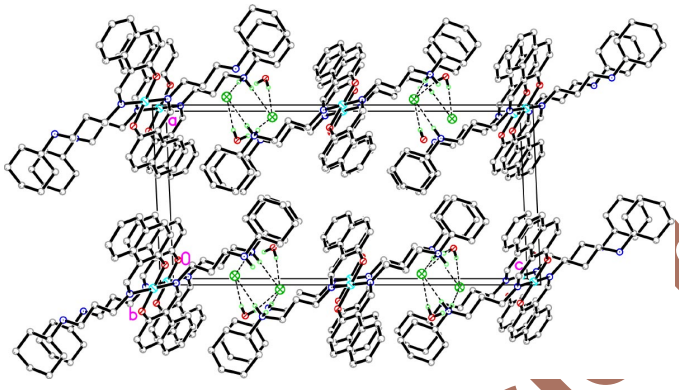


Figure 2
The crystal packing of (I), viewed along the *b* axis. Hydrogen bonds are shown as dashed lines. H atoms have been omitted.

complex. All other bond lengths are in normal ranges (Allen *et al.*, 1987). As expected, the cyclohexyl groups in the complex adopt chair conformations to minimize steric effects.

In the crystal structure of (I), the uncoordinated water molecules, chloride anions, and the amine N atoms of the Schiff base ligands contribute to the formation of hydrogen bonds (Fig. 2 and Table 2).

Experimental

N-Cyclohexyl-1,3-diaminopropane (0.2 mmol, 31.2 mg) and 2-hydroxy-1-naphthaldehyde (0.2 mmol, 17.2 mg) were dissolved in ethanol (10 ml). The mixture was stirred for 10 min to obtain a clear yellow solution. To this solution was added an aqueous solution (5 ml) of $CuCl_2{\cdot}2H_2O$ (0.1 mmol, 17.1 mg) with stirring. The mixture was stirred at room temperature for 1 h and then filtered. After allowing the brown filtrate to stand in air for 8 d, blue block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

Crystal data

$[Cu(C_{20}H_{26}N_2O)_2]Cl_2{\cdot}2H_2O$
$M_r = 791.33$
Monoclinic, $P2_1/c$
$a = 11.224$ (3) Å
$b = 7.432$ (2) Å
$c = 23.673$ (6) Å
$\beta = 92.578$ (5)°
$V = 1972.7$ (9) Å^3
$Z = 2$
$D_x = 1.332$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1827 reflections
$\theta = 1.9$–25.0°
$\mu = 0.73$ mm^{-1}
$T = 273$ (2) K
Block, blue
0.22 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.855$, $T_{max} = 0.898$
11158 measured reflections
4076 independent reflections
3269 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 26.5°$
$h = -10 \rightarrow 14$
$k = -9 \rightarrow 8$
$l = -29 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.150$
$S = 1.05$
4076 reflections
238 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0818P)^2 + 0.9065P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.832 (2)	Cu1—N1	1.913 (2)
O1—Cu1—O1^{i}	180	O1^{i}—Cu1—N1	88.20 (9)
O1—Cu1—N1	91.80 (9)	N1—Cu1—N1^{i}	180

Symmetry code: (i) $2-x, 2-y, 1-z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2D···Cl1^{ii}	0.86 (4)	2.49 (3)	3.340 (5)	172 (3)
O2—H2C···Cl1	0.86 (3)	2.36 (2)	3.201 (4)	168 (4)
N2—H2B···Cl1^{iii}	0.90	2.25	3.140 (3)	172
N2—H2A···Cl1^{ii}	0.90	2.34	3.229 (3)	170

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

The H atoms of the water molecules were located in a difference Fourier map and refined isotropically, with the O—H and H···H distances restrained to 0.84 (1) and 1.37 (2) Å, respectively. All other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and N—H distances of 0.90 Å, and with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The author thanks Xianyang Teachers College for a research grant.

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