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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

References

Chen, Q. (2006). *Acta Cryst.* E**62**, m56–m57.
Chen, J.-R., Sui, Y., Luo, Q.-Y. & Jiang, R.-Q. (2007). *Acta Cryst.* E**63**, m2091–m2092.
Chen, J.-R., Sui, Y., Wen, J.-W. & Yin, L.-Y. (2008). *Acta Cryst.* E**64**, m562–m563.
Han, Z.-Q. (2008). *Acta Cryst.* E**64**, m592.
Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* E**66**, e1–e2.
Hu, R.-H., Sui, Y., Chen, L. & He, C.-M. (2008). *Acta Cryst.* E**64**, m8–m9.
Hu, R.-H., Sui, Y., Fang, X.-N. & Chen, H.-M. (2007). *Acta Cryst.* E**63**, m2039–m2040.
Huang, C.-F. & Chen, H.-L. (2007). *Acta Cryst.* E**63**, m2356–m2357.
Huang, Q., Sui, Y.-H. & Zhang, G.-X. (2009). *Acta Cryst.* E**65**, m1161–m1162.
Li, Y.-G. & Chen, H.-J. (2006). *Acta Cryst.* E**62**, m1038–m1039.
Li, N.-G., Tao, R.-M. & Fu, B.-F (2007). *Acta Cryst.* E**63**, o4228.
Li, Z., Zhang, X. & Pu, X. (2008). *Acta Cryst.* E**64**, m215.
Liu, J.-T. & Fan, S.-D. (2006). *Acta Cryst.* E**62**, m2507–m2508.
Liu, J.-T., Fan, S.-D. & Li, D.-Q. (2006). *Acta Cryst.* E**62**, m2165–m2166.
Liu, D., Lin, J., Xu, Y., Huang, C. & Li, X. (2007). *Acta Cryst.* E**63**, m3094.
Liu, Y.-Q. & Wen, H.-R. (2007). *Acta Cryst.* E**63**, m2928.
Liu, Y.-Q. & Zeng, X.-R. (2007*a*). *Acta Cryst.* E**63**, m2547.
Liu, Y.-Q. & Zeng, X.-R. (2007*b*). *Acta Cryst.* E**63**, m2684.
Liu, Y.-Q., Zeng, X.-R. & Chen, W.-T. (2007). *Acta Cryst.* E**63**, m2462.
Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007*a*). *Acta Cryst.* E**63**, m2396.
Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007*b*). *Acta Cryst.* E**63**, m2854.
Qadeer, G., Rama, N. H. & Chen, W.-T. (2007*a*). *Acta Cryst.* E**63**, o2892.
Qadeer, G., Rama, N. H. & Chen, W.-T. (2007*b*). *Acta Cryst.* E**63**, o2932.
Qiu, X.-Y. (2006). *Acta Cryst.* E**62**, m1190–m1191.
Sui, Y., Fang, X.-N., Hu, P. & Lin, J. (2007). *Acta Cryst.* E**63**, m2135–m2136.
Sui, Y., Fang, X.-N. & Yuan, M.-W. (2007). *Acta Cryst.* E**63**, m2275–m2276.
Sui, Y., Li, X.-F., Huang, G.-S. & Wang, G.-J. (2007). *Acta Cryst.* E**63**, m2093–m2094.
Sui, Y., Sui, Y.-H., Luo, Q.-Y. & Wang, Y.-D. (2007). *Acta Cryst.* E**63**, m2277–m2278.
Sui, Y., Xiao, Y.-A., Fang, X.-N., Zeng, X.-R. & Li, M.-H. (2006). *Acta Cryst.* E**62**, m3205–m3207.
Sui, Y., Zhang, J.-H., Hu, R.-H. & Jiang, R.-Q. (2007). *Acta Cryst.* E**63**, m2256–m2257.
Sui, Y., Zhang, J.-H., Hu, R.-H. & Yin, L.-Y. (2007). *Acta Cryst.* E**63**, m2089–m2090.
Sun, Y.-X. & Gao, G.-Z. (2005). *Acta Cryst.* E**61**, m354–m355.
Wang, Q. & Fang, Z.-N. (2006). *Acta Cryst.* E**62**, m1492–m1493.
Wang, S., Yang, T., Li, Z. & Yu, X. (2009). *Acta Cryst.* E**65**, o2198.
Xiao, Y.-A., Fu, X.-K., Sui, Y., Wu, Q. & Xiong, S.-H. (2008). *Acta Cryst.* E**64**, m806–m807.
Xiao, Y.-A., Sui, Y., Yi, X.-G., Wu, J.-H. & Zhang, L.-P. (2008). *Acta Cryst.* E**64**, m804–m805.
Xiong, Z.-Y. & Liu, L.-J. (2005). *Acta Cryst.* E**61**, m863–m864.
Yang, X.-M. (2007). *Acta Cryst.* E**63**, o4453.
Yang, Y.-M., Lu, P.-C., Zhu, T.-T. & Liu, C.-H. (2007). *Acta Cryst.* E**63**, m1613.
Zhang, P. (2004). *Acta Cryst.* E**60**, m1808–m1810.

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Tetraaqua(1,10-phenanthroline-κ^2N,N')copper(II) naphthalene-1,5-disulfonate dihydrate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.040
wR factor = 0.116
Data-to-parameter ratio = 13.7

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

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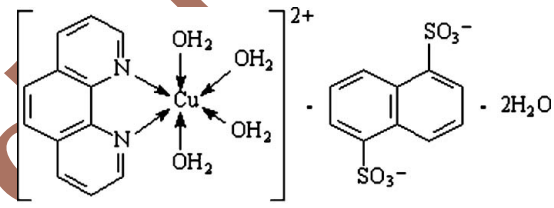
In the title structure, $[Cu(C_{12}H_8N_2)(H_2O)_4](C_{10}H_6S_2O_6)\cdot 2H_2O$, the cation lies on a crystallographic twofold rotation axis and the anion lies on a centre of inversion. The Cu^{II} atom is coordinated by two N atoms of a 1,10-phenanthroline ligand and four O atoms from four water ligands in a distorted octahedral geometry. The unique Cu—O distances are 2.054 (2) and 2.088 (2) Å and the Cu—N distance is 2.073 (2) Å. In the crystal structure, a three-dimensional supramolecular framework is constructed by extensive intermolecular O—H···O hydrogen bonds.

Comment

The structures of some tetraaqua(1,10-phenanthroline)metal ionic complexes (Zhang *et al.*, 1999; Cherni *et al.*, 1999) with different anions have been reported. As a multifunctional ligand, naphthalene-1,5-disulfonate often forms ionic compounds (Cai *et al.*, 2001; Piguet *et al.*, 1989) with other metal complex cations. Here we report the crystal structure of the title naphthalene-1,5-disulfonate ionic complex, (I).



(I)

The structure of (I) is shown in Fig. 1. The cation lies on a crystallographic twofold rotation axis which runs through the Cu^{II} atom and bisects the plane of the 1,10-phenanthroline ligand. The anion has a center of symmetry located at the centre of the naphthalene unit. In the cation, the coordination geometry at the Cu^{II} atom is distorted octahedral, with an N_2O_4 environment consisting of two N atoms of a 1,10-phenanthroline ligand and four O atoms from four water ligands. Selected bond distances and angles are listed in Table 1. In the crystal structure, a three-dimensional supramolecular framework of cations, anions and uncoordinated water molecules (Fig. 2) is formed *via* intermolecular O—H···O hydrogen-bond interactions (Table 2).

Experimental

A mixture of $Cu(NO_3)_2\cdot 3H_2O$ (43 mg, 0.2 mmol), 1,10-phenanthroline (37 mg, 0.2 mmol) and disodium naphthalene-1,5-disulfonate (67 mg, 0.2 mmol) in water (15 ml) was placed in a Teflon-lined stainless steel Parr bomb that was heated at 433 K for 48 h. The bomb

was then cooled to room temperature over a period of 24 h. Blue crystals were isolated in about 15% yield based on Cu.

Crystal data

$[Cu(C_{12}H_8N_2)(H_2O)_4](C_{10}H_6O_6S_2)\cdot 2H_2O$
$M_r = 638.11$
Monoclinic, $C2/c$
$a = 20.562$ (3) Å
$b = 12.4311$ (19) Å
$c = 12.5373$ (18) Å
$\beta = 124.576$ (2)°
$V = 2638.6$ (7) Å^3
$Z = 4$
$D_x = 1.606$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.05$ mm^{-1}
$T = 294$ (2) K
Block, blue
0.24 × 0.22 × 0.22 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.676$, $T_{max} = 0.790$
7258 measured reflections
2676 independent reflections
2166 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 26.4°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.116$
$S = 1.03$
2676 reflections
195 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0621P)^2 + 4.912P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.88$ e Å^{-3}
$\Delta\rho_{min} = -0.57$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.073 (2)	Cu1—O2W	2.054 (2)
Cu1—O1W	2.088 (2)		
N1^i—Cu1—N1	79.75 (13)	O2W—Cu1—N1^i	170.24 (11)
N1^i—Cu1—O1W	95.99 (8)	O2W—Cu1—O1W	88.83 (9)
N1—Cu1—O1W	88.31 (8)	O2W^i—Cu1—O1W	87.45 (9)
O1W—Cu1—O1W^i	174.40 (11)	O2W—Cu1—O2W^i	96.74 (18)
O2W—Cu1—N1	91.95 (11)		

Symmetry code: (i) $-x+1, y, -z+\frac{1}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O2	0.84 (5)	1.90 (3)	2.726 (3)	169 (3)
O1W—H1WB···O1^{ii}	0.85 (5)	1.96 (3)	2.805 (3)	178 (3)
O2W—H2WB···O3W	0.84 (5)	1.85 (5)	2.683 (4)	170 (4)
O2W—H2WA···O3^{ii}	0.84 (5)	1.94 (4)	2.760 (3)	165 (4)
O3W—H3WA···O1^{iii}	0.85 (5)	2.42 (6)	2.915 (5)	118 (5)
O3W—H3WA···O1W^i	0.85 (5)	2.59 (4)	3.299 (4)	142 (6)
O3W—H3WB···O3^{iv}	0.85 (5)	2.01 (8)	2.837 (4)	166 (6)

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

Water H atoms were located in a difference map and were refined with an O—H distance restraint of 0.85 (1) Å. H atoms bound to C atoms were placed in calculated positions (C—H = 0.93 Å) and refined in the riding-model approximation, $U_{iso}(H) = 1.2U_{eq}(C,O)$.

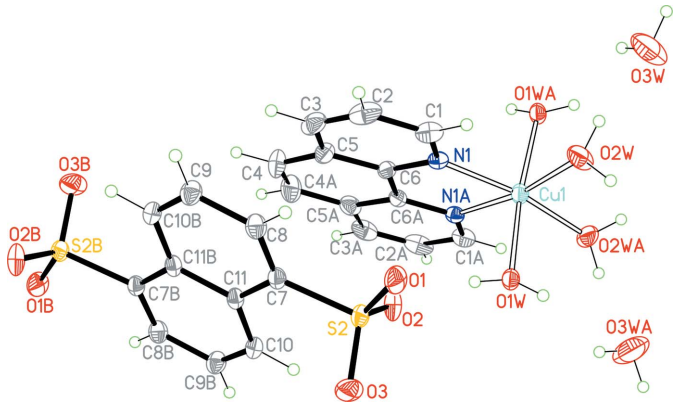


Figure 1
The asymmetric unit of (I), showing displacement ellipsoids at the 30% probability level. [Symmetry codes: (A) $1-x, y, \frac{1}{2}-z$; (B) $\frac{3}{2}-x, \frac{1}{2}-y, 1-z$.]

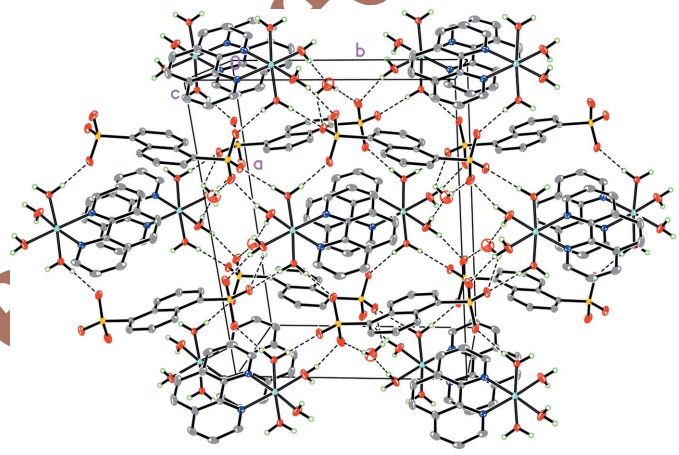


Figure 2
The structure of (I), with hydrogen bonds indicated by dashed lines.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97*; molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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References

Bruker (1998). *SMART* (Version 5.051), *SAINT* (Version 5.01), *SADABS* (Version 2.03) and *SHELXTL* (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Cai, J., Chen, C.-H., Liao, C.-Z., Yao, J.-H., Hu, X.-P. & Chen, X.-M. (2001). *J. Chem. Soc. Dalton Trans.* pp. 1137–1142.
Cherni, S. N., Driss, A. & Jouini, T. (1999). *Acta Cryst.* C**55**, 1248–1250.
Piguet, C., Bernardinelli, G. & Williams, A. F. (1989). *Inorg. Chem.* **28**, 2920–2925.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Zhang, C., Yu, K., Wu, D. & Zhao, C. (1999). *Acta Cryst.* C**55**, 1815–1817.