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

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.

Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Aqua(dimethylglyoxime-κ^2N,N')-(3,5-dinitro-2-oxidobenzoato-κ^2O^1,O^2)-copper(II)

Yin-Qiu Liu[a]* and He-Rui Wen[b]

[a]College of Chemistry and Chemical Engineering, JiangXi Province Key Laboratory of Coordination Chemistry, JingGangShan University, 343009 Ji'an, JiangXi, People's Republic of China, and [b]Chemistry Department, GanNan Teachers' College, 343009 GanZhou, JiangXi, People's Republic of China
Correspondence e-mail: liuyiqja@163.com

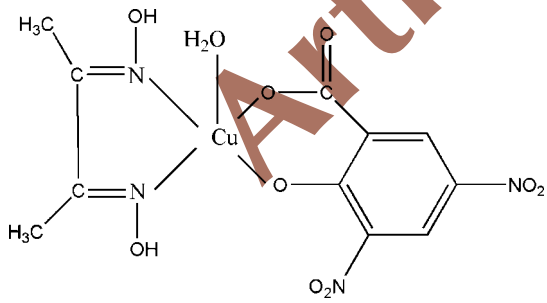
Received 27 October 2007; accepted 29 October 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.027; wR factor = 0.076; data-to-parameter ratio = 11.5.

The title complex, $[Cu(C_7H_2N_2O_7)(C_4H_8N_2O_2)(H_2O)]$, is a mononuclear copper(II) compound. The Cu^{II} ion is five-coordinated in a distorted pyramidal geometry by two N atoms from one dimethylglyoxime molecule, two O atoms from one 3,5-dinitro-2-oxidobenzoate ligand and one O atom from a water molecule. Strong hydrogen bonds connect adjacent molecules into a three-dimensional network.

Related literature

For a copper(II) structure of the same coordination geometry, see: Sui *et al.* (2006).



Experimental

Crystal data

$[Cu(C_7H_2N_2O_7)(C_4H_8N_2O_2)(H_2O)]$
M_r = 423.80
Monoclinic, $P2_1/c$
a = 12.476 (2) Å
b = 7.0786 (14) Å
c = 17.929 (4) Å
β = 103.014 (3)°
V = 1542.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.48 mm^{-1}
T = 293 (2) K
0.30 × 0.28 × 0.23 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
9276 measured reflections
2824 independent reflections
2426 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.076
S = 1.01
2824 reflections
245 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O9—H9···O10^{i}	0.82	1.86	2.675 (2)	175
O8—H8···O7	0.82	2.15	2.745 (2)	130
O8—H8···O4	0.82	2.23	2.987 (2)	154
O10—H10E···O5^{ii}	0.818 (14)	1.877 (15)	2.691 (2)	173 (3)
O10—H10D···O6^{i}	0.82 (2)	1.932 (14)	2.670 (2)	149 (3)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

The authors are grateful for support from the Key Laboratory of Coordination Chemistry, JingGangShan University, China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2336).

References

Bruker (1997). *SMART*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SAINT*. Version 7.06A. Bruker AXS Inc., Madison, Wisconsin, USA.
Sui, A.-X., Zhu, G. & Tang, Z.-X. (2006). *Acta Cryst.* E**62**, m1592–m1594.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1996). *SAINT* and *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

supplementary materials

Acta Cryst. (2007). E**63**, m2928 [**doi:10.1107/S1600536807054244**]

Aqua(dimethylglyoxime-κ^2N,N')(3,5-dinitro-2-oxidobenzoato-κ^2O^1,O^2)copper(II)

Y.-Q. Liu and H.-R. Wen

Comment

As shown in Fig. 1, (I) crystallizes as discrete molecular species. Each copper(II) ion is five-coordinated in a distorted pyramidal geometry by two N atoms from one dimethylglyoxime molecule, two O atoms from one 2-hydroxy-3,5-dinitrobenzoic acid molecule and one O atom from a water molecule. Atoms O6, O7, N3 and N4 located at the base of the pyramid are approximately coplanar with the central Cu1 ion, the maximum deviation from the least-squares plane through all five atoms being 0.081 Å for Cu1, O10 locating at the apex of the pyramid shows a slightly longer bond to Cu1 than O7 and O8. Strong hydrogen bonds are found between adjacent molecules, which including: O(9)—H(9)···O(10)^1 (symmetry code 1: −*x*,-*y* + 1,-*z*); O(10)—H(10E)···O(5)^2 (symmetry code 2:*x*,*y* − 1,*z*) and O(10)—H(10D)···O(6)^1.

Experimental

A mixture of dimethylglyoxime (0.116 g, 0.001 mol), 2-hydroxy-3,5-dinitrobenzoic acid (0.228 g, 0.001 mol) and $CuSO_4·5H_2O$ (0.250 g, 0.001 mol) in the mole ratio of 1:1:1 was added to 15 ml me thanol, The mixture was heated at 408 K for two days in a closed steel chamber with liner. Crystals of (I) were obtained after reaction mixture cooled to room temperature, untouched in the air.

Refinement

The H atoms bonding to C atoms and O atoms of hydroxyl group were located at calculated positions and refined as riding on their parent atoms with the bond length fixed to 0.93 Å for C—H and 0.82 Å for O—H, U_{iso}(H) being 1.2 times U_{eq}(C) and U_{iso}(H) being 1.5 times U_{eq}(O); The H atoms bonding to O atoms of water molecules are found in electron density map and refined with bond lengths fixed to 0.82 Å and with U_{iso}(H) = 1.5 times U_{eq}(O).

Figures

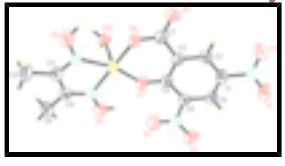


Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids for the non-hydrogen atoms.

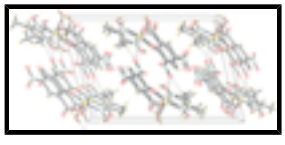


Fig. 2. The packing diagram of (I), viewed along the *b* axis. Hydrogen bonds are shown as dash lines.

Aqua(dimethylglyoxime-κ^2N,N')(3,5-dinitro-2-oxidobenzoato- κ^2O^1,O^2)copper(II)

Crystal data

$[Cu(C_7H_2N_2O_7)(C_4H_8N_2O_2)(H_2O)]$

$M_r = 423.80$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 12.476$ (2) Å

$b = 7.0786$ (14) Å

$c = 17.929$ (4) Å

$\beta = 103.014$ (3)°

$V = 1542.7$ (5) Å^3

$Z = 4$

$F_{000} = 860.0$

$D_x = 1.825$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 7646 reflections

$\theta = 1.0$–$28.3°$

$\mu = 1.48$ mm^{-1}

$T = 293$ (2) K

Block, green

0.30 × 0.28 × 0.23 mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293(2)$ K

φ and ω scans

Absorption correction: none

9276 measured reflections

2824 independent reflections

2426 reflections with $I > 2\sigma(I)$

$R_{int} = 0.019$

$\theta_{max} = 25.5°$

$\theta_{min} = 2.3°$

$h = -14\rightarrow15$

$k = -8\rightarrow8$

$l = -21\rightarrow21$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.028$

$wR(F^2) = 0.076$

$S = 1.01$

2824 reflections

245 parameters

2 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2 + 0.7936P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.009$

$\Delta\rho_{max} = 0.24$ e Å^{-3}

$\Delta\rho_{min} = -0.37$ e Å^{-3}

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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.38551 (19)	0.8248 (3)	−0.15661 (11)	0.0404 (5)
C2	0.29055 (18)	0.8483 (3)	−0.12966 (12)	0.0401 (5)
H2	0.2493	0.9582	−0.1412	0.048*
C3	0.25689 (17)	0.7102 (3)	−0.08585 (12)	0.0363 (4)
C4	0.31727 (17)	0.5362 (3)	−0.07025 (11)	0.0350 (4)
C5	0.41421 (17)	0.5223 (3)	−0.09927 (11)	0.0353 (4)
C6	0.44863 (18)	0.6661 (3)	−0.14088 (11)	0.0384 (5)
H6	0.5136	0.6546	−0.1578	0.046*
C7	0.15805 (18)	0.7568 (3)	−0.05472 (13)	0.0411 (5)
C8	0.2461 (2)	−0.0793 (4)	0.17133 (16)	0.0591 (7)
H8A	0.2924	−0.1435	0.1434	0.089*
H8B	0.1793	−0.1496	0.1677	0.089*
H8C	0.2838	−0.0685	0.2241	0.089*
C9	0.21941 (18)	0.1124 (3)	0.13856 (13)	0.0410 (5)
C10	0.1053 (2)	0.2011 (4)	0.23823 (15)	0.0652 (7)
H10A	0.0880	0.3172	0.2606	0.098*
H10B	0.1617	0.1356	0.2742	0.098*
H10C	0.0407	0.1236	0.2254	0.098*
C11	0.14519 (18)	0.2433 (3)	0.16737 (13)	0.0433 (5)
Cu1	0.19075 (2)	0.41715 (4)	0.035805 (15)	0.04118 (11)
H10D	−0.0046 (14)	0.236 (4)	−0.0242 (14)	0.062*
N1	0.41829 (19)	0.9717 (3)	−0.20416 (11)	0.0530 (5)
N2	0.48523 (15)	0.3558 (3)	−0.08565 (10)	0.0426 (4)
N3	0.25563 (15)	0.1820 (3)	0.08278 (10)	0.0407 (4)
N4	0.11864 (16)	0.3920 (3)	0.12651 (11)	0.0427 (4)
O1	0.50885 (18)	0.9593 (3)	−0.21873 (12)	0.0732 (6)
O2	0.35331 (19)	1.0994 (3)	−0.22715 (13)	0.0824 (7)
O3	0.57503 (15)	0.3662 (3)	−0.10244 (12)	0.0686 (5)
O4	0.45639 (15)	0.2139 (2)	−0.05650 (11)	0.0628 (5)
O5	0.10172 (14)	0.8950 (2)	−0.08023 (11)	0.0537 (4)
O6	0.13474 (13)	0.6566 (2)	−0.00051 (10)	0.0496 (4)
O7	0.28662 (14)	0.3991 (2)	−0.03241 (10)	0.0486 (4)
O8	0.32359 (15)	0.0709 (2)	0.05102 (10)	0.0514 (4)

H8	0.3401	0.1273	0.0152	0.077*
O9	0.05087 (16)	0.5146 (3)	0.15476 (10)	0.0601 (5)
H9	0.0242	0.5917	0.1216	0.090*
O10	0.04730 (13)	0.2463 (2)	−0.04495 (10)	0.0461 (4)
H10E	0.067 (2)	0.1386 (16)	−0.0517 (17)	0.069*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0492 (13)	0.0408 (12)	0.0330 (10)	−0.0073 (10)	0.0130 (9)	0.0008 (9)
C2	0.0439 (13)	0.0342 (11)	0.0425 (11)	0.0011 (9)	0.0102 (10)	0.0015 (9)
C3	0.0377 (11)	0.0316 (10)	0.0413 (11)	0.0015 (8)	0.0127 (9)	−0.0009 (8)
C4	0.0385 (12)	0.0318 (10)	0.0371 (10)	0.0007 (8)	0.0132 (9)	−0.0024 (8)
C5	0.0369 (11)	0.0362 (11)	0.0336 (10)	0.0015 (9)	0.0099 (9)	−0.0050 (8)
C6	0.0385 (12)	0.0461 (12)	0.0337 (10)	−0.0043 (9)	0.0146 (9)	−0.0061 (9)
C7	0.0422 (12)	0.0291 (10)	0.0549 (13)	0.0027 (9)	0.0173 (10)	−0.0021 (9)
C8	0.0606 (17)	0.0538 (16)	0.0655 (16)	0.0111 (12)	0.0195 (13)	0.0209 (12)
C9	0.0358 (12)	0.0430 (12)	0.0433 (12)	0.0000 (9)	0.0072 (9)	0.0055 (9)
C10	0.0740 (19)	0.0716 (19)	0.0599 (16)	0.0073 (15)	0.0355 (14)	0.0187 (14)
C11	0.0404 (12)	0.0474 (13)	0.0449 (12)	0.0006 (10)	0.0157 (10)	0.0055 (10)
Cu1	0.04485 (19)	0.03550 (16)	0.04994 (18)	0.00842 (11)	0.02486 (13)	0.00724 (11)
N1	0.0602 (14)	0.0563 (13)	0.0437 (11)	−0.0084 (11)	0.0142 (10)	0.0097 (10)
N2	0.0414 (11)	0.0446 (10)	0.0451 (10)	0.0068 (8)	0.0167 (8)	−0.0052 (8)
N3	0.0374 (10)	0.0410 (10)	0.0463 (10)	0.0078 (8)	0.0144 (8)	0.0034 (8)
N4	0.0437 (11)	0.0441 (11)	0.0459 (10)	0.0050 (8)	0.0217 (8)	0.0015 (8)
O1	0.0728 (13)	0.0851 (15)	0.0731 (13)	−0.0076 (11)	0.0406 (11)	0.0216 (11)
O2	0.0788 (15)	0.0783 (15)	0.0921 (15)	0.0053 (12)	0.0232 (12)	0.0472 (12)
O3	0.0457 (11)	0.0734 (13)	0.0959 (15)	0.0171 (9)	0.0354 (10)	0.0108 (11)
O4	0.0661 (12)	0.0438 (10)	0.0892 (13)	0.0153 (9)	0.0395 (10)	0.0101 (9)
O5	0.0490 (10)	0.0368 (9)	0.0795 (12)	0.0138 (7)	0.0231 (9)	0.0081 (8)
O6	0.0509 (10)	0.0398 (8)	0.0691 (10)	0.0115 (7)	0.0363 (8)	0.0090 (8)
O7	0.0551 (10)	0.0344 (8)	0.0677 (11)	0.0114 (7)	0.0378 (9)	0.0112 (7)
O8	0.0528 (10)	0.0488 (10)	0.0588 (10)	0.0178 (8)	0.0256 (8)	0.0069 (7)
O9	0.0734 (13)	0.0563 (11)	0.0623 (11)	0.0224 (9)	0.0396 (10)	0.0081 (9)
O10	0.0425 (9)	0.0378 (8)	0.0638 (10)	0.0084 (7)	0.0239 (8)	0.0006 (8)

Geometric parameters (Å, °)

C1—C6	1.364 (3)	C10—C11	1.495 (3)
C1—C2	1.387 (3)	C10—H10A	0.9600
C1—N1	1.461 (3)	C10—H10B	0.9600
C2—C3	1.378 (3)	C10—H10C	0.9600
C2—H2	0.9300	C11—N4	1.282 (3)
C3—C4	1.438 (3)	Cu1—O6	1.8922 (16)
C3—C7	1.500 (3)	Cu1—O7	1.8978 (16)
C4—O7	1.290 (3)	Cu1—N3	1.9566 (18)
C4—C5	1.424 (3)	Cu1—N4	2.0359 (19)
C5—C6	1.386 (3)	Cu1—O10	2.3652 (18)
C5—N2	1.461 (3)	N1—O1	1.219 (3)

C6—H6	0.9300	N1—O2	1.222 (3)
C7—O5	1.231 (3)	N2—O4	1.223 (3)
C7—O6	1.288 (3)	N2—O3	1.226 (3)
C8—C9	1.486 (3)	N3—O8	1.370 (2)
C8—H8A	0.9600	N4—O9	1.385 (2)
C8—H8B	0.9600	O8—H8	0.8200
C8—H8C	0.9600	O9—H9	0.8200
C9—N3	1.285 (3)	O10—H10D	0.82 (2)
C9—C11	1.483 (3)	O10—H10E	0.818 (14)
C6—C1—C2	121.7 (2)	H10A—C10—H10C	109.5
C6—C1—N1	118.9 (2)	H10B—C10—H10C	109.5
C2—C1—N1	119.4 (2)	N4—C11—C9	114.51 (19)
C1—C2—C3	120.5 (2)	N4—C11—C10	123.9 (2)
C1—C2—H2	119.8	C9—C11—C10	121.6 (2)
C3—C2—H2	119.8	O6—Cu1—O7	94.35 (6)
C2—C3—C4	120.4 (2)	O6—Cu1—N3	174.35 (8)
C2—C3—C7	115.96 (19)	O7—Cu1—N3	87.74 (7)
C4—C3—C7	123.67 (18)	O6—Cu1—N4	99.09 (7)
O7—C4—C5	121.14 (19)	O7—Cu1—N4	164.78 (7)
O7—C4—C3	122.82 (19)	N3—Cu1—N4	78.23 (7)
C5—C4—C3	116.04 (19)	O6—Cu1—O10	94.44 (7)
C6—C5—C4	122.52 (19)	O7—Cu1—O10	94.07 (7)
C6—C5—N2	115.62 (19)	N3—Cu1—O10	90.64 (7)
C4—C5—N2	121.85 (19)	N4—Cu1—O10	91.98 (7)
C1—C6—C5	118.8 (2)	O1—N1—O2	123.9 (2)
C1—C6—H6	120.6	O1—N1—C1	117.9 (2)
C5—C6—H6	120.6	O2—N1—C1	118.2 (2)
O5—C7—O6	120.7 (2)	O4—N2—O3	121.8 (2)
O5—C7—C3	119.0 (2)	O4—N2—C5	120.52 (18)
O6—C7—C3	120.26 (19)	O3—N2—C5	117.6 (2)
C9—C8—H8A	109.5	C9—N3—O8	117.55 (18)
C9—C8—H8B	109.5	C9—N3—Cu1	118.50 (15)
H8A—C8—H8B	109.5	O8—N3—Cu1	122.95 (13)
C9—C8—H8C	109.5	C11—N4—O9	113.93 (18)
H8A—C8—H8C	109.5	C11—N4—Cu1	115.12 (15)
H8B—C8—H8C	109.5	O9—N4—Cu1	130.79 (14)
N3—C9—C11	112.86 (19)	C7—O6—Cu1	128.62 (14)
N3—C9—C8	124.8 (2)	C4—O7—Cu1	126.36 (13)
C11—C9—C8	122.3 (2)	N3—O8—H8	109.5
C11—C10—H10A	109.5	N4—O9—H9	109.5
C11—C10—H10B	109.5	Cu1—O10—H10D	109.4 (19)
H10A—C10—H10B	109.5	Cu1—O10—H10E	111 (2)
C11—C10—H10C	109.5	H10D—O10—H10E	106 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O9—H9···O10^{i}	0.82	1.86	2.675 (2)	175
O8—H8···O7	0.82	2.15	2.745 (2)	130

O8—H8···O4	0.82	2.23	2.987 (2)	154
O10—H10E···O5^{ii}	0.818 (14)	1.877 (15)	2.691 (2)	173 (3)
O10—H10D···O6^{i}	0.82 (2)	1.932 (14)	2.670 (2)	149 (3)

Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) *x*, *y*−1, *z*.

Fig. 1

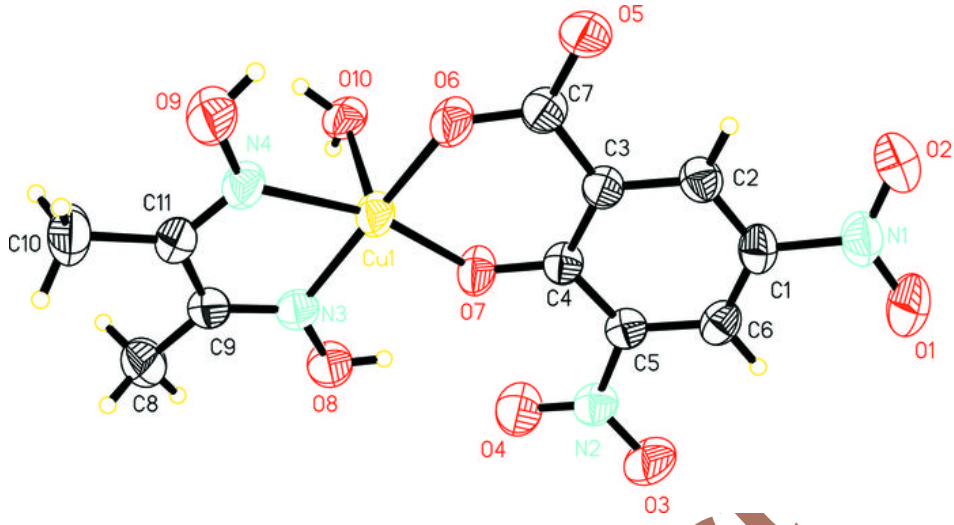


Fig. 2