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Retraction of articles by H. Zhong *et al.*

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A series of 41 papers by H. Zhong *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 41 papers by H. Zhong *et al.* are retracted. 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	DOI	Refcode
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate	Zhong, Zeng, Liu & Luo (2006*a*)	10.1107/S1600536806041122	KERQEE
cis-Dichlorobis(1,10-phenanthroline)cobalt(II)	Zhong, Zeng & Luo (2006)	10.1107/S1600536806047295	MEQFOE
Tris(quinolin-8-olato-κ^2N,O)cobalt(III) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2006*b*)	10.1107/S1600536806050240	MEQHEW
(8-Quinolinol-κ^2N,O)bis(8-quinolinolato-κ^2N,O)nickel(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2007)	10.1107/S1600536806053232	METVUD
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate	Zhong, Zeng & Luo (2007)	10.1107/S1600536806053530	METQIM
(8-Quinolinol-κ^2N,O)-bis(8-quinolinolato-κ^2N,O)zinc(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')nickel(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*a*)	10.1107/S1600536807004102	YEYGOZ
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')zinc(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*b*)	10.1107/S1600536807004096	YEYGUF
Chloridobis(1,10-phenanthroline-$\kappa N,N'$)copper(I) hexahydrate	Zhong, Zeng, Yang, Luo & Xiao (2007)	10.1107/S160053680700791X	HEGKOU01
Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)	Zhong, Zeng, Yang & Luo (2007*a*)	10.1107/S1600536807017461	ITCPCO01
Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)	Zhong, Zeng, Yang & Luo (2007*b*)	10.1107/S160053680701879X	AVUJEG02
Tetrakis(nitrato-κ^2O,O')bis(4-phenylpyridine-κN)cerium(IV)	Zhong, Zeng, Yang & Luo (2007*c*)	10.1107/S1600536807018831	CICDOI
Bis(4,4′-bipyridine-κ^2N,N')tetrakis(nitrato-κ^2O,O')cerium(IV)	Zhong, Zeng, Yang & Luo (2007*d*)	10.1107/S1600536807021502	YIDNEF
(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)	Zhong, Zeng, Yang, Luo & Xu (2007)	10.1107/S1600536807027171	EDUROL
(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)	Zhong, Yang, Luo & Xu (2007*a*)	10.1107/S1600536807028061	EDUTUT
(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)	Zhong, Yang, Luo & Xu (2007*b*)	10.1107/S1600536807028693	RIGQEE
(1,10-Phenanthroline-κ^2N,N')tris(phenoxyacetato)-$\kappa O;\kappa O;\kappa O,O'$-neodymium(III)	Zhong, Yang, Luo & Xu (2007*c*)	10.1107/S1600536807030371	UDUMEM
Bis(2,2′-bipyridyl-κ^2N,N')bis(thiocyanato-κN)nickel(II)	Zhong, Yang, Luo & Xu (2007*d*)	10.1107/S1600536807031613	YEJGOJ01
Bis(2,2′-bipyridyl-κ^2N,N')bis(isothiocyanato-κN)copper(II)	Zhong, Yang, Luo & Xu (2007*e*)	10.1107/S1600536807033181	UFAPOH
Bis(2,2′-bipyridyl-κ^2N,N')bis(thiocyanato-κN)zinc(II)	Zhong, Yang, Luo & Xu (2007*f*)	10.1107/S1600536807035337	TIGFAR
(1,10-Phenanthroline-κ^2N,N')tris(3-phenylpropanoato-κO)neodymium(III)	Zhong, Yang, Luo & Xu (2007*g*)	10.1107/S1600536807035350	TIGFEV
2-Fluoro-3,5-dinitrobenzamide monohydrate	Zhong, Yang, Xie & Luo (2007*j*)	10.1107/S1600536807038676	VIKGAY
2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)	Zhong, Yang, Xie & Luo (2007*k*)	10.1107/S1600536807039724	KILKIA
1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate	Zhong, Yang, Xie & Luo (2007*l*)	10.1107/S1600536807040779	AFETAH
N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)	Zhong, Yang, Xie & Luo (2007*m*)	10.1107/S160053680704086X	AFINAF
catena-Poly[[bis(μ-anilinoacetato-$\kappa^2O:O'$)bis(μ-anilinoacetato-$\kappa^3O,O':O$)bis[(1,10-phenanthroline-κ^2N,N')samarium(III)]-μ-anilinoacetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*a*)	10.1107/S1600536807043528	PILDAQ
2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate	Zhong, Yang, Xie & Luo (2007*n*)	10.1107/S1600536807045199	XILWIZ
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dineodymium(III)]-di-μ-anilinoacetato]	Zhong, Yang, Xie & Luo (2007*b*)	10.1107/S1600536807048489	WIMWEV
Hexaaquacopper(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*c*)	10.1107/S1600536807049525	TOLSCV01

Table 1 (continued)

Title	Reference	DOI	Refcode
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dilanthanum(III)]-di-μ-anilinoacetato]	Zhong, Yang, Xie & Luo (2007*d*)	10.1107/S1600536807051240	GIMZEI
Hexaaquachromium(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*e*)	10.1107/S1600536807051227	GIMZIM
Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*f*)	10.1107/S1600536807052051	QUKQES01
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*g*)	10.1107/S1600536807053494	NIQLAB
Hexaaquanickel(II) bis(4-aminobenzenesulfonate)	Zhong, Zhong, Xie & Luo (2007*a*)	10.1107/S1600536807054372	HIPZOW
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*h*)	10.1107/S160053680705622X	XIRGOV
Hexaaquazinc(II) bis(4-aminobenzenesulfonate)	Zhong, Zhong, Xie & Luo (2007*b*)	10.1107/S1600536807056498	XIRJEO
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')nickel(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*i*)	10.1107/S1600536807058540	HIQJOH
Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)	Zhong, Xie & Luo (2007)	10.1107/S1600536807058527	HIQJUN
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dieuropium(III)]-di-μ-anilinoacetato]	Zhong, Yang, Duan & Hong (2007)	10.1107/S1600536807060643	YIQMAN
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate	Zhong, Yang, Luo & Li (2007)	10.1107/S1600536807061193	YIQNUI
catena-Poly[[(1,10-phenanthroline-κ^2N,N')praseodymium(III)]-di-μ-phenoxyacetato-$\kappa^4O:O'$-[(1,10-phenanthroline-κ^2N,N')-praseodymium(III)]-di-μ-phenoxyacetato-$\kappa^4O:O'$-di-μ-phenoxyacetato-$\kappa^3O,O':O;\kappa^3O:O,O'$]	Zhong, Yang, Luo & Xu (2008)	10.1107/S1600536807068614	GISJIC

References

Zhong, H., Xie, H.-L. & Luo, C.-J. (2007). *Acta Cryst.* E**63**, m3054.
Zhong, H., Yang, X.-M., Duan, S.-H. & Hong, Y.-P. (2007). *Acta Cryst.* E**63**, m3142–m3143.
Zhong, H., Yang, X.-M., Luo, C.-J. & Li, M.-L. (2007). *Acta Cryst.* E**63**, m3160–m3161.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*a*). *Acta Cryst.* E**63**, m1885–m1886.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*b*). *Acta Cryst.* E**63**, m1909.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*c*). *Acta Cryst.* E**63**, m2019.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*d*). *Acta Cryst.* E**63**, m2062.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*e*). *Acta Cryst.* E**63**, m2141.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*f*). *Acta Cryst.* E**63**, m2208.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*g*). *Acta Cryst.* E**63**, m2209–m2210.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2008). *Acta Cryst.* E**64**, m317–m318.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*a*). *Acta Cryst.* E**63**, m2508–m2509.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*b*). *Acta Cryst.* E**63**, m2680–m2681.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*c*). *Acta Cryst.* E**63**, m2724–m2725.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*d*). *Acta Cryst.* E**63**, m2772–m2773.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*e*). *Acta Cryst.* E**63**, m2774.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*f*). *Acta Cryst.* E**63**, m2825.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*g*). *Acta Cryst.* E**63**, m2895–m2896.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*h*). *Acta Cryst.* E**63**, m2979.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*i*). *Acta Cryst.* E**63**, m3053.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*j*). *Acta Cryst.* E**63**, o3780.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*k*). *Acta Cryst.* E**63**, o3831.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*l*). *Acta Cryst.* E**63**, o3881.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*m*). *Acta Cryst.* E**63**, o3882.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*n*). *Acta Cryst.* E**63**, o4191.
Zhong, H., Zeng, X.-R., Liu, Y.-Q. & Luo, Q.-Y. (2006*a*). *Acta Cryst.* E**62**, m2925–m2927.
Zhong, H., Zeng, X.-R., Liu, Y.-Q. & Luo, Q.-Y. (2006*b*). *Acta Cryst.* E**62**, m3557–m3559.
Zhong, H., Zeng, X.-R., Liu, Y.-Q. & Luo, Q.-Y. (2007). *Acta Cryst.* E**63**, m187–m189.
Zhong, H., Zeng, X.-R. & Luo, Q.-Y. (2006). *Acta Cryst.* E**62**, m3330–m3332.
Zhong, H., Zeng, X.-R. & Luo, Q.-Y. (2007). *Acta Cryst.* E**63**, m221–m223.
Zhong, H., Zeng, X.-R., Luo, Q.-Y., Li, M.-L. & Xiao, S.-Z. (2007). *Acta Cryst.* E**63**, m492–m494.
Zhong, H., Zeng, X.-R., Yang, X.-M. & Luo, Q.-Y. (2007*a*). *Acta Cryst.* E**63**, m1379.
Zhong, H., Zeng, X.-R., Yang, X.-M. & Luo, Q.-Y. (2007*b*). *Acta Cryst.* E**63**, m1445.
Zhong, H., Zeng, X.-R., Yang, X.-M. & Luo, Q.-Y. (2007*c*). *Acta Cryst.* E**63**, m1455.
Zhong, H., Zeng, X.-R., Yang, X.-M. & Luo, Q.-Y. (2007*d*). *Acta Cryst.* E**63**, m1592–m1593.
Zhong, H., Zeng, X.-R., Yang, X.-M., Luo, Q.-Y. & Li, M.-L. (2007*a*). *Acta Cryst.* E**63**, m639–m641.
Zhong, H., Zeng, X.-R., Yang, X.-M., Luo, Q.-Y. & Li, M.-L. (2007*b*). *Acta Cryst.* E**63**, m642–m644.
Zhong, H., Zeng, X.-R., Yang, X.-M., Luo, Q.-Y. & Xiao, S.-Z. (2007). *Acta Cryst.* E**63**, m826–m828.
Zhong, H., Zeng, X.-R., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007). *Acta Cryst.* E**63**, m1868–m1869.
Zhong, H., Zhong, Q. Y., Xie, H.-L. & Luo, C.-J. (2007*a*). *Acta Cryst.* E**63**, m2913–m2914.
Zhong, H., Zhong, Q.-Y., Xie, H.-L. & Luo, C.-J. (2007*b*). *Acta Cryst.* E**63**, m2990.

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catena-Poly[[(acetato-κO)(1,10-phenanthroline-$\kappa^2 N,N'$)copper(II)]-μ-acetato-$\kappa^2 O:O'$]

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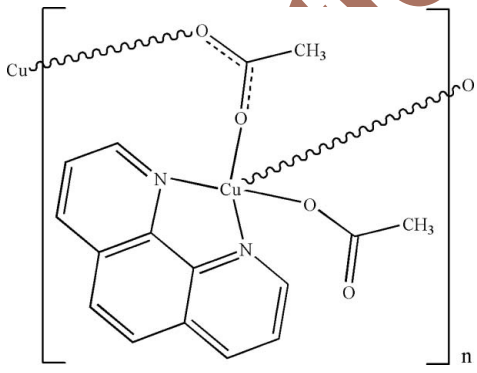
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.045; wR factor = 0.139; data-to-parameter ratio = 12.9.

The title compound, $[Cu(C_2H_3O_2)_2(C_{12}H_8N_2)]_n$, is a polymeric complex involving bridging of Cu^{II} ions by single *syn–anti* acetate ligands. Each Cu atom is five-coordinated by two 1,10-phenanthroline N atoms and three O atoms of acetate ligands in a distorted square-pyramidal geometry. In the crystal structure, C—H···O hydrogen bonds result in the formation of a polymeric ribbon structure.

Related literature

For a related structure, see: Zhong *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Cu(C_2H_3O_2)_2(C_{12}H_8N_2)]$
M_r = 361.83
Monoclinic, $P2_1/n$
a = 8.711 (2) Å
b = 9.1735 (19) Å
c = 16.8974 (15) Å
β = 102.122 (7)°
V = 1320.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.68 mm^{-1}
T = 273 (2) K
0.40 × 0.25 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.555, T_{max} = 0.737
8509 measured reflections
2703 independent reflections
2306 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.139
S = 1.00
2703 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.995 (2)	Cu1—N1	2.000 (3)
Cu1—O2	1.928 (2)	Cu1—N2	1.971 (3)
Cu1—O4^{i}	2.322 (3)		
O1—Cu1—O2	91.40 (11)	O2—Cu1—N1	93.52 (12)
O1—Cu1—O4^{i}	87.00 (10)	O2—Cu1—N2	174.38 (11)
O2—Cu1—O4^{i}	82.67 (10)	O4—Cu1—N1^{i}	138.68 (5)
O1—Cu1—N1	166.03 (11)	O4—Cu1—N2^{i}	125.72 (5)
O1—Cu1—N2	92.68 (10)	N1—Cu1—N2	83.39 (11)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O3^{ii}	0.93	2.50	3.323 (5)	148
C10—H10···O2^{iii}	0.93	2.35	3.250 (4)	164

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2366).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1996). *SMART*, *SAINT* and *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007). *Acta Cryst.* E**63**, m2895–2896.

supplementary materials

Acta Cryst. (2007). E**63**, m2979 [**doi:10.1107/S160053680705622X**]

catena-Poly[[(acetato-κO)(1,10-phenanthroline-$\kappa^2 N,N'$)copper(II)]-μ-acetato-$\kappa^2 O:O'$]

H. Zhong, X.-M. Yang, H.-L. Xie and C.-J. Luo

Comment

The crystal structure of *catena*-poly[[(acetato-κ*O*)(1,10-phenanthroline -$\kappa^2 N,N'$)cobalt(II)]-μ-acetato-$\kappa^2 O:O'$], (II), has previously been reported (Zhong *et al.*, 2007). The crystal structure determination of the title compound, (I), has been carried out in order to elucidate the molecular conformation and to compare it with that of (II). We report herein the crystal structure of (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). It is a polymeric complex involving bridging of Cu^{II} ions by single *syn*-anti acetate ligands. Each Cu atom is five-coordinated by two 1,10-phenanthroline N atoms and three O atoms of acetate ligands within a pyramidal coordination geometry. The Cu—O and Cu—N bond lengths are in the range of [1.928 (2)- 2.322 (3) Å] and [1.971 (3)–2.000 (3) Å], respectively (Table 1), as in (II).

In the crystal structure, C—H···O hydrogen bonds (Table 2, Fig. 2) result in the formation of a polymeric ribbon structure, as in (II).

The both compounds, (I) and (II), are isostructural.

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb. Copper (II) nitrate hexahydrate (295.6 mg, 1 mmol), phen (180.2 mg, 1 mmol), acetic acid (120.1 mg, 2 mmol), ammonia (4 ml, 0.5 mol/l) and distilled water (10 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 453 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small blue crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

Refinement

H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å, for aromatic and methyl H atoms and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where $x = 1.2$ for aromatic H and $x = 1.5$ for methyl H atoms.

Figures

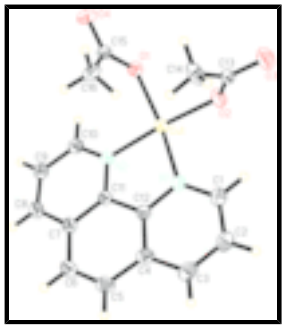

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

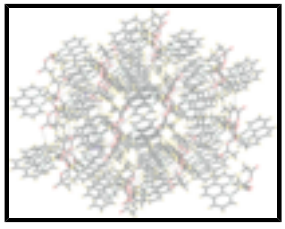

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

catena-Poly[[(acetato-κ*O*)(1,10-phenanthroline-κ^2*N*,*N*')copper(II)]-\ μ-acetato-κ^2*O*:*O*']

Crystal data

$[Cu(C_2H_3O_2)_2(C_{12}H_8N_2)]$	F_{000} = 740
M_r = 361.83	D_x = 1.821 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -p 2yn	Cell parameters from 5704 reflections
a = 8.711 (2) Å	θ = 2.3–27.2°
b = 9.1735 (19) Å	μ = 1.68 mm^{-1}
c = 16.8974 (15) Å	T = 273 (2) K
β = 102.122 (7)°	Prism, blue
V = 1320.2 (4) Å^3	0.40 × 0.25 × 0.19 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2703 independent reflections
Radiation source: fine-focus sealed tube	2306 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.017
T = 273(2) K	θ_{max} = 26.8°
φ and ω scans	θ_{min} = 2.5°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −11→11
T_{min} = 0.555, T_{max} = 0.737	k = −11→11
8509 measured reflections	l = −21→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.139$	$w = 1/[\sigma^2(F_o^2) + (0.1005P)^2 + 1.1936P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
2703 reflections	$\Delta\rho_{max} = 0.82$ e Å^{-3}
210 parameters	$\Delta\rho_{min} = -0.65$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.66503 (4)	0.92787 (4)	0.80316 (2)	0.03415 (18)
O1	0.6877 (3)	0.7351 (3)	0.75211 (13)	0.0399 (5)
O2	0.5486 (3)	1.0051 (3)	0.70218 (14)	0.0476 (6)
O3	0.3284 (4)	1.0281 (4)	0.62141 (18)	0.0637 (8)
O4	0.6212 (3)	0.5046 (3)	0.74809 (16)	0.0476 (6)
N1	0.6079 (3)	1.0938 (3)	0.86819 (17)	0.0358 (6)
N2	0.7954 (3)	0.8671 (3)	0.90786 (15)	0.0343 (6)
C1	0.5192 (4)	1.2110 (4)	0.8466 (2)	0.0440 (8)
H1	0.4792	1.2269	0.7918	0.053*
C2	0.4833 (4)	1.3111 (4)	0.9017 (2)	0.0484 (8)
H2	0.4230	1.3930	0.8838	0.058*
C3	0.5366 (4)	1.2879 (4)	0.9812 (2)	0.0475 (8)
H3	0.5103	1.3517	1.0190	0.057*
C4	0.6325 (4)	1.1664 (4)	1.0066 (2)	0.0380 (7)
C5	0.6981 (4)	1.1337 (4)	1.0885 (2)	0.0451 (8)
H5	0.6742	1.1921	1.1293	0.054*
C6	0.7948 (4)	1.0189 (5)	1.1080 (2)	0.0446 (8)
H6	0.8364	1.0000	1.1623	0.054*

C7	0.8358 (4)	0.9250 (3)	1.0482 (2)	0.0362 (7)
C8	0.9432 (4)	0.8076 (4)	1.0635 (2)	0.0423 (7)
H8	0.9941	0.7865	1.1163	0.051*
C9	0.9723 (4)	0.7260 (4)	1.0017 (2)	0.0443 (8)
H9	1.0433	0.6491	1.0118	0.053*
C10	0.8959 (4)	0.7579 (4)	0.9237 (2)	0.0410 (7)
H10	0.9155	0.7012	0.8813	0.049*
C11	0.7675 (4)	0.9514 (3)	0.96852 (19)	0.0318 (6)
C12	0.6647 (4)	1.0729 (3)	0.94753 (19)	0.0319 (6)
C13	0.4027 (3)	0.9782 (3)	0.68361 (18)	0.0319 (6)
C14	0.3463 (4)	0.8994 (5)	0.7292 (2)	0.0517 (10)
H14A	0.2547	0.9452	0.7411	0.077*
H14B	0.4225	0.8846	0.7786	0.077*
H14C	0.3179	0.8071	0.7035	0.077*
C15	0.6160 (3)	0.6290 (3)	0.77800 (18)	0.0296 (6)
C16	0.5449 (4)	0.6522 (3)	0.8314 (2)	0.0386 (7)
H16A	0.4477	0.5993	0.8203	0.058*
H16B	0.5237	0.7546	0.8336	0.058*
H16C	0.6073	0.6211	0.8823	0.058*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0409 (3)	0.0329 (3)	0.0271 (2)	0.00240 (14)	0.00370 (17)	0.00087 (14)
O1	0.0503 (13)	0.0372 (12)	0.0331 (11)	−0.0041 (10)	0.0109 (10)	−0.0026 (9)
O2	0.0451 (13)	0.0561 (17)	0.0375 (12)	−0.0063 (12)	−0.0003 (10)	0.0114 (12)
O3	0.0552 (16)	0.0710 (18)	0.0552 (17)	−0.0070 (15)	−0.0106 (13)	0.0174 (16)
O4	0.0472 (13)	0.0368 (13)	0.0589 (15)	−0.0047 (10)	0.0117 (12)	−0.0155 (12)
N1	0.0387 (13)	0.0326 (13)	0.0359 (14)	0.0030 (11)	0.0070 (11)	0.0049 (11)
N2	0.0401 (13)	0.0317 (13)	0.0303 (12)	0.0029 (11)	0.0055 (11)	−0.0016 (10)
C1	0.0460 (17)	0.0395 (18)	0.0451 (18)	0.0058 (15)	0.0063 (15)	0.0055 (15)
C2	0.0472 (18)	0.0393 (18)	0.059 (2)	0.0108 (15)	0.0111 (17)	0.0029 (17)
C3	0.0484 (19)	0.0385 (18)	0.059 (2)	0.0075 (15)	0.0182 (17)	−0.0045 (16)
C4	0.0390 (15)	0.0372 (16)	0.0406 (16)	−0.0032 (13)	0.0146 (13)	−0.0042 (14)
C5	0.0536 (19)	0.049 (2)	0.0373 (16)	−0.0021 (17)	0.0194 (15)	−0.0087 (15)
C6	0.0513 (19)	0.054 (2)	0.0290 (15)	0.0005 (17)	0.0090 (14)	−0.0013 (15)
C7	0.0424 (16)	0.0361 (17)	0.0301 (15)	−0.0036 (13)	0.0077 (13)	0.0024 (12)
C8	0.0467 (17)	0.0428 (18)	0.0342 (15)	0.0006 (15)	0.0010 (14)	0.0063 (14)
C9	0.0471 (18)	0.0361 (17)	0.0460 (18)	0.0077 (14)	0.0011 (15)	0.0039 (15)
C10	0.0475 (17)	0.0328 (16)	0.0409 (17)	0.0061 (14)	0.0054 (15)	−0.0035 (13)
C11	0.0362 (15)	0.0284 (14)	0.0307 (14)	−0.0022 (12)	0.0072 (12)	0.0000 (11)
C12	0.0341 (14)	0.0306 (15)	0.0319 (15)	−0.0031 (11)	0.0092 (12)	0.0014 (11)
C13	0.0330 (14)	0.0305 (14)	0.0293 (14)	0.0004 (12)	−0.0002 (12)	0.0000 (12)
C14	0.0379 (17)	0.086 (3)	0.0317 (16)	−0.0186 (18)	0.0077 (14)	0.0186 (18)
C15	0.0308 (13)	0.0266 (13)	0.0300 (14)	0.0003 (11)	0.0031 (11)	−0.0030 (11)
C16	0.0519 (18)	0.0286 (15)	0.0459 (17)	−0.0038 (13)	0.0346 (16)	−0.0047 (13)

Geometric parameters (Å, °)

Cu1—O1	1.995 (2)	C4—C5	1.414 (5)
Cu1—O2	1.928 (2)	C5—C6	1.345 (6)
Cu1—O4^{i}	2.322 (3)	C5—H5	0.9300
Cu1—N1	2.000 (3)	C6—C7	1.429 (5)
Cu1—N2	1.971 (3)	C6—H6	0.9300
O1—C15	1.282 (4)	C7—C11	1.374 (4)
O2—C13	1.268 (4)	C7—C8	1.415 (5)
O3—C13	1.203 (4)	C8—C9	1.350 (5)
O4—C15	1.252 (4)	C8—H8	0.9300
O4—Cu1^{ii}	2.322 (3)	C9—C10	1.378 (5)
N1—C1	1.330 (4)	C9—H9	0.9300
N1—C12	1.342 (4)	C10—H10	0.9300
N2—C10	1.321 (4)	C11—C12	1.427 (4)
N2—C11	1.346 (4)	C13—C14	1.231 (5)
C1—C2	1.389 (5)	C14—H14A	0.9600
C1—H1	0.9300	C14—H14B	0.9600
C2—C3	1.342 (6)	C14—H14C	0.9600
C2—H2	0.9300	C15—C16	1.215 (4)
C3—C4	1.406 (5)	C16—H16A	0.9600
C3—H3	0.9300	C16—H16B	0.9600
C4—C12	1.388 (4)	C16—H16C	0.9600
O1—Cu1—O2	91.40 (11)	C11—C7—C8	116.5 (3)
O1—Cu1—O4^{i}	87.00 (10)	C11—C7—C6	117.7 (3)
O2—Cu1—O4^{i}	82.67 (10)	C8—C7—C6	125.7 (3)
O1—Cu1—N1	166.03 (11)	C9—C8—C7	120.3 (3)
O1—Cu1—N2	92.68 (10)	C9—C8—H8	119.8
O2—Cu1—N1	93.52 (12)	C7—C8—H8	119.8
O2—Cu1—N2	174.38 (11)	C8—C9—C10	119.4 (3)
O4—Cu1—N1^{i}	138.68 (5)	C8—C9—H9	120.3
O4—Cu1—N2^{i}	125.72 (5)	C10—C9—H9	120.3
N1—Cu1—N2	83.39 (11)	N2—C10—C9	121.4 (3)
C15—O1—Cu1	115.19 (19)	N2—C10—H10	119.3
C13—O2—Cu1	117.5 (2)	C9—C10—H10	119.3
C15—O4—Cu1^{ii}	121.8 (2)	N2—C11—C7	122.3 (3)
C1—N1—C12	117.4 (3)	N2—C11—C12	117.6 (3)
C1—N1—Cu1	131.5 (2)	C7—C11—C12	120.1 (3)
C12—N1—Cu1	111.0 (2)	N1—C12—C4	122.9 (3)
C10—N2—C11	120.0 (3)	N1—C12—C11	116.1 (3)
C10—N2—Cu1	129.0 (2)	C4—C12—C11	121.0 (3)
C11—N2—Cu1	111.0 (2)	O3—C13—C14	123.9 (3)
N1—C1—C2	123.4 (3)	O3—C13—O2	118.0 (3)
N1—C1—H1	118.3	C14—C13—O2	118.1 (3)
C2—C1—H1	118.3	C13—C14—H14A	109.5
C3—C2—C1	119.1 (3)	C13—C14—H14B	109.5

C3—C2—H2	120.4	H14A—C14—H14B	109.5
C1—C2—H2	120.4	C13—C14—H14C	109.5
C2—C3—C4	119.3 (3)	H14A—C14—H14C	109.5
C2—C3—H3	120.3	H14B—C14—H14C	109.5
C4—C3—H3	120.3	C16—C15—O4	121.8 (3)
C12—C4—C3	117.8 (3)	C16—C15—O1	118.7 (3)
C12—C4—C5	118.2 (3)	O4—C15—O1	119.5 (3)
C3—C4—C5	124.0 (3)	C15—C16—H16A	109.5
C6—C5—C4	120.6 (3)	C15—C16—H16B	109.5
C6—C5—H5	119.7	H16A—C16—H16B	109.5
C4—C5—H5	119.7	C15—C16—H16C	109.5
C5—C6—C7	122.4 (3)	H16A—C16—H16C	109.5
C5—C6—H6	118.8	H16B—C16—H16C	109.5
C7—C6—H6	118.8		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O3^{iii}	0.93	2.50	3.323 (5)	148
C10—H10···O2^{ii}	0.93	2.35	3.250 (4)	164

Symmetry codes: (iii) −*x*+1/2, *y*+1/2, −*z*+3/2; (ii) −*x*+3/2, *y*−1/2, −*z*+3/2.

Fig. 1

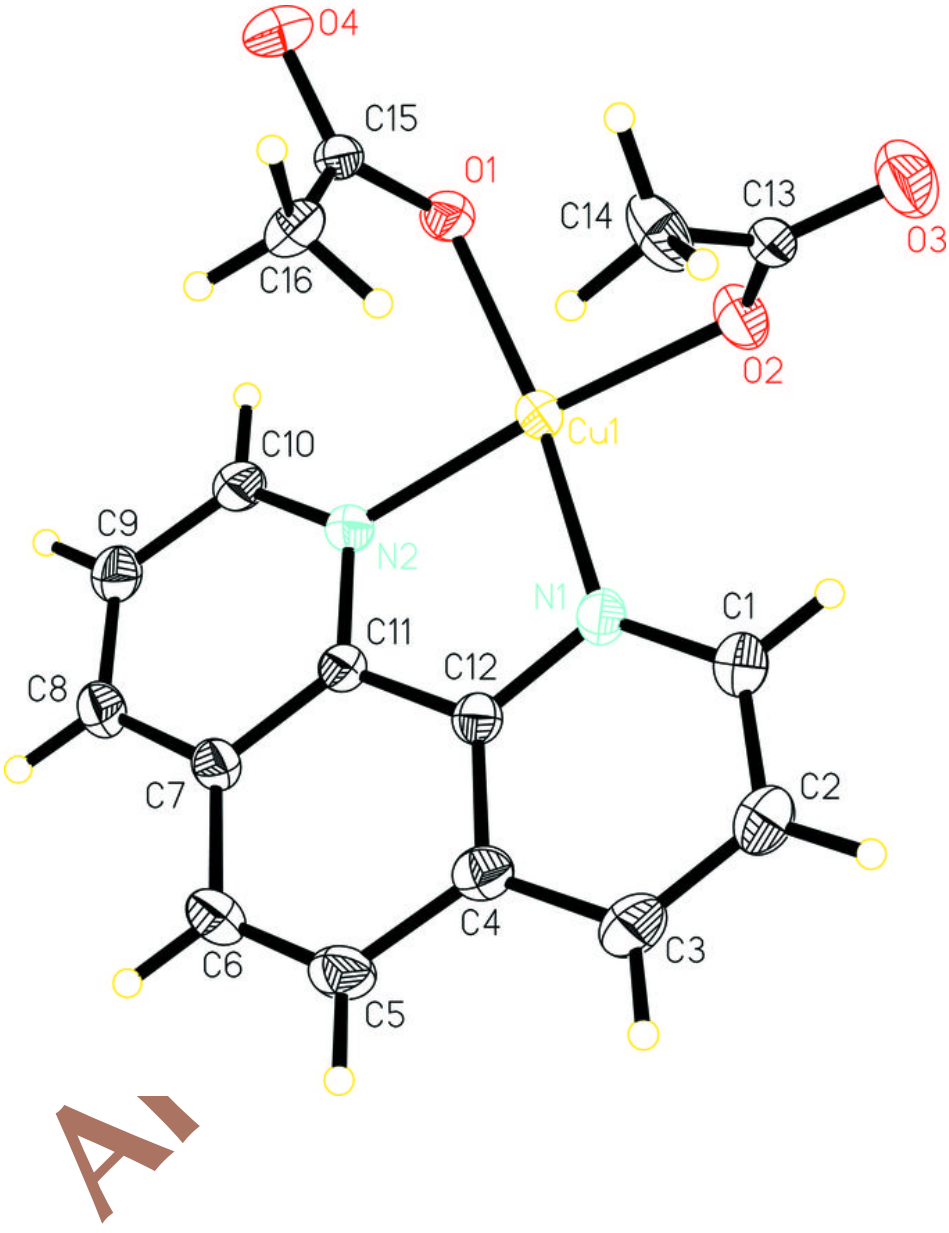
O4
C15
O1
C14
C13
O3
C16
O2
Cu1
C10
C9
N2
N1
C1
C11
C12
C8
C7
C2
C4
C6
C3
C5

Fig. 2