

## Retraction of articles

This article reports the retraction of articles published in *Acta Crystallographica Section E* between 2007 and 2009.

After further thorough investigation (see Harrison *et al.*, 2010), 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	DOI	Refcode
<i>catena</i> -Poly[[ <i>aqua</i> (pyrazine-2-carboxylato)iron(II)]- $\mu$ -pyrazine-2-carboxylato] Poly[[ <i>aquabis</i> ( $\mu$ -pyrazine-2-carboxylato)nickel(II)]	Hao & Liu (2007)	10.1107/S1600536806053207	NEVLWU
<i>catena</i> -Poly[[2,2'-bipyridine)cobalt(II)]- $\mu$ -imidazole-4,5-dicarboxylato- $\kappa^4N^1, O^5, N^3, O^2$ ]	Hao, Mu & Liu (2007)	10.1107/S1600536806054225	TEVQUH
Poly[[ <i>aqua</i> (2,2-bipyridyl)( $\mu_3$ -pyridine-3,4-dicarboxylato)manganese(II)] monohydrate]	Li, Dong <i>et al.</i> (2007)	10.1107/S1600536807014420	XIBPAA
Poly[chlorido- $\mu_3$ -1,2,4-triazolato-nickel(II)]	Li, Niu <i>et al.</i> (2007)	10.1107/S1600536807023586	GIGYAX
Poly[[ $\mu_3$ -carbonyldibenzene-3,3',4,4'-tetracarboxylato)tetrakis(1,10-phenanthroline)-dicadmium(II)] dihydrate]	Gao, Wang & Hao (2007a)	10.1107/S1600536807025962	WIGTEM
Tetraaquaabis(4,4'-bipyridine)iron(II) pyridine-2,6-dicarboxylate tetrahydrate	Gao, Wang & Niu (2007a)	10.1107/S1600536807028425	EDUNUN
<i>catena</i> -Poly[[2,2'-bipyridine)cobalt(II)]- $\mu$ -imidazole-4,5-dicarboxylato]	Gao, Wang & Niu (2007b)	10.1107/S1600536807027973	EDUPAV
<i>catena</i> -Poly[[ <i>aqua</i> (pyrazine-2-carboxylato)cobalt(II)]- $\mu$ -pyrazine-2-carboxylato]	Hao, Bao & Yu (2007)	10.1107/S1600536807027699	EDURUR
Poly[[ $\mu_3$ -carbonyldibenzene-3,3',4,4'-tetracarboxylato)tetrakis(1,10-phenanthroline)-dicadmium(II)] dihydrate]	Gao, Wang, Niu & Hao (2007a)	10.1107/S1600536807027961	ODOJIA01
<i>catena</i> -Poly[[ <i>aqua</i> (2,2-bipyridine)iron(II)]- $\mu_3$ -pyridine-3,4-dicarboxylato] monohydrate]	Hao & Yu (2007a)	10.1107/S160053680702867X	RIGRUV
<i>catena</i> -Poly[[ <i>diaqua</i> (6-carboxypyridine-2-carboxylato- $\kappa^3O, N, O'$ )gadolinium(III)]- $\mu$ -pyridine-2,6-dicarboxylato- $\kappa^4N, O, O':O''$ ] tetrahydrate]	Hao & Yu (2007b)	10.1107/S1600536807029789	MIGDOW
Poly[[ <i>aqua</i> (pyrazine-2-carboxylato)copper(II)]- $\mu$ -pyrazine-2-carboxylato]	Gao, Wang, Niu & Hao (2007b)	10.1107/S1600536807030528	MIGKUJ
cyclo-Tetrakis[ $\mu$ -N-(2-hydroxybenzoyl)-N'-(2-hydroxy-3-methoxybenzylidene)hydrazinate(2-)]tetracobalt(II) N,N-dimethylformamide tetrasolvate	Gao, Wang & Niu (2007c)	10.1107/S1600536807033338	UDUXOH
Poly[chlorido( $\mu_3$ -1,2,4-triazolato)manganese(II)]	Gao, Wang & Hao (2007b)	10.1107/S1600536807032886	UDUZAV
<i>catena</i> -Poly[[ <i>aqua</i> (pyrazine-2-carboxylato- $\kappa^2N^1, O$ )zinc(II)]- $\mu$ -pyrazine-2-carboxylato- $\kappa^2N^1, O:N^4$ ]	Gao, Wang, Niu & Hao (2007c)	10.1107/S1600536807033041	UDUZEZ
cyclo-Tetrakis[ $\mu$ -N-(2-hydroxybenzoyl)-N'-(2-hydroxy-3-methoxybenzylidene)hydrazinate(2-)]tetracobalt(II) N,N-dimethylformamide tetrasolvate	Gao, Wang & Niu (2007d)	10.1107/S1600536807034514	TIFZIS
<i>catena</i> -Poly[[ <i>diaqua</i> (6-carboxypyridine-2-carboxylato)terbium(III)]- $\mu$ -pyridine-2,6-dicarboxylato] tetrahydrate]	Hao & Yu (2007c)	10.1107/S1600536807034629	TIFZUE
<i>catena</i> -Poly[[ <i>aqua</i> (pyrazine-2-carboxylato- $\kappa^2N^1, O$ )manganese(II)]- $\mu$ -pyrazine-2-carboxylato- $\kappa^2N^1, O:N^4$ ]	Gao, Wang, Niu & Hao (2007d)	10.1107/S1600536807034496	TIGBER
Poly[chlorido- $\mu_3$ -1,2,4-triazolato-iron(II)]	Gao, Wang & Hao (2007c)	10.1107/S1600536807036239	TIGHIB
Tetraaquaabis(4,4'-bipyridine)manganese(II) pyridine-2,6-dicarboxylate tetrahydrate	Gao, Wang & Niu (2007e)	10.1107/S160053680703766X	AFEGIC
Poly[chlorido( $\mu_3$ -1,2,4-triazolato)copper(II)]	Gao, Wang & Niu (2007f)	10.1107/S1600536807040007	VIKBAT
<i>catena</i> -Poly[[2,2'-bipyridine)nickel(II)]- $\mu$ -imidazole-4,5-dicarboxylato]	Hao & Yu (2007d)	10.1107/S1600536807040330	VIKCOI
Poly[[2,2'-bipyridine)cadmium(II)]- $\mu_3$ -pyridine-2,4-dicarboxylato] monohydrate]	Li, Wang & Liu (2007)	10.1107/S160053680704202X	XIKVOD
Poly[[ <i>aqua</i> ( $\mu_3$ -benzene-1,3-dicarboxylato- $\kappa^4O':O'':O''')$ bis(imidazole- $\kappa$ N)palladium(II)]	Hao & Yu (2007e)	10.1107/S1600536807044315	SILKII
Tetraaquaabis(4,4'-bipyridine)cobalt(II) pyridine-2,6-dicarboxylate tetrahydrate	Guan, Gao, Wang & Wang (2007a)	10.1107/S1600536807046107	XILPOY
cyclo-Tetrakis[ $\mu$ -N-(2-hydroxybenzoyl)-N'-(2-hydroxy-3-methoxybenzylidene)hydrazinate(2-)]tetracobalt(II) N,N-dimethylformamide tetrasolvate	Guan, Gao, Wang & Wang (2007b)	10.1107/S1600536807048325	SILZOD
Bis(cyanido- $\kappa$ C)bis(1,10-phenanthroline- $\kappa^2N, N'$ )chromium(III) bis(azido- $\kappa$ N)[N,N'-(o-phenylene)bis(pyridine-2-carboxamide)- $\kappa^2N$ ]chromate(III) monohydrate	Guan, Gao, Wang & Wang (2007c)	10.1107/S1600536807049872	GIMVUU
Tris[2-(propyliminomethyl)phenolato- $\kappa^2N, O$ ]iron(III)	Hao, Mu & Kong (2008a)	10.1107/S1600536808018540	MODFIV
Bis[ $\mu$ -2,2'-ethane-1,2-diybis(nitratomethylidene)]diphenolato]bis[(thiocyanato- $\kappa$ N)-iron(III)]	Hao, Mu & Kong (2008b)	10.1107/S1600536808021892	YODCAW
<i>catena</i> -Poly[[ <i>aqua</i> (2,2'-bipyridine- $\kappa^2N, N'$ )copper(II)]- $\mu$ -5-nitrosophthalato- $\kappa^3O^1, O^1':O^3$ ]	Hao & Liu (2008)	10.1107/S1600536808035150	COLVEF
Tetrakis( $\mu$ -2,4-difluorobenzoato)bis[(2,2'-bipyridine)(2,4-difluorobenzoato)terbium(III)]	Hao & Liu (2009)	10.1107/S1600536808043936	WOQLAQ

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## catena-Poly[[aqua(2,2'-bipyridine- $\kappa^2N,N'$ )copper(II)]- $\mu$ -5-nitroisophthalato- $\kappa^3O^1,O^1':O^3$ ]

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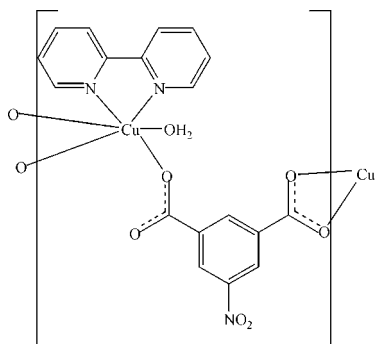
Received 28 September 2008; accepted 28 October 2008

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(C-C) = 0.005$  Å;  $R$  factor = 0.042;  $wR$  factor = 0.123; data-to-parameter ratio = 12.5.

In the asymmetric unit of the title compound,  $[Cu(C_8H_3NO_6)(C_{10}H_8N_2)(H_2O)]_n$ , there are two symmetry-independent one-dimensional coordination polymers related by a non-crystallographic inversion center. Within the polymers, the  $Cu^{II}$  atoms, coordinated by the water molecule and the chelating 2,2'-bipyridine ligands, are bridged by 5-nitrobenzene-1,3-dicarboxylate dianions which act as tridentate ligands; the carboxylate groups exhibit monodentate and symmetric bidentate coordination modes. The  $Cu^{II}$  atoms show a strongly distorted octahedral coordination geometry. In the crystal structure, the two symmetry-independent coordination polymers form another one-dimensional polymeric structure *via* O—H...O hydrogen bonds between coordinated water molecules and carboxylate groups.

### Related literature

For the uses of carboxylic acids in materials science, see: Church & Halvorson (1959), and in biological systems, see: Okabe & Oya (2000); Kim *et al.* (2001).



### Experimental

#### Crystal data

$[Cu(C_8H_3NO_6)(C_{10}H_8N_2)(H_2O)]$   
 $M_r = 446.85$   
 Monoclinic,  $P2_1/n$   
 $a = 10.1326$  (10) Å  
 $b = 23.263$  (3) Å  
 $c = 15.6087$  (15) Å  
 $\beta = 97.28$  (2)°  
 $V = 3649.6$  (7) Å<sup>3</sup>  
 $Z = 8$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.25$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 $0.12 \times 0.10 \times 0.08$  mm

#### Data collection

Bruker APEXII CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2001)  
 $T_{min} = 0.865$ ,  $T_{max} = 0.907$   
 18862 measured reflections  
 6694 independent reflections  
 5089 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.025$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.123$   
 $S = 1.00$   
 6694 reflections  
 535 parameters  
 6 restraints  
 H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{max} = 0.83$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.40$  e Å<sup>-3</sup>

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O12-H1W\cdots O2^i$	0.83 (4)	1.98 (2)	2.742 (3)	153 (4)
$O1-H4W\cdots O10^{ii}$	0.82 (3)	1.95 (2)	2.724 (3)	158 (4)
$O12-H2W\cdots O5$	0.82 (4)	2.07 (3)	2.760 (3)	141 (4)
$O1-H3W\cdots O13$	0.83 (3)	2.13 (3)	2.778 (3)	135 (4)

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); 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: GK2170).

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## supporting information

*Acta Cryst.* (2008). E64, m1500 [doi:10.1107/S1600536808035150]

***catena*-Poly[[aqua(2,2'-bipyridine- $\kappa^2N,N'$ )copper(II)]- $\mu$ -5-nitroisophthalato- $\kappa^3O^1,O^1':O^3$ ]**

**Lujiang Hao and Xia Liu**

### S1. Comment

In recent years, carboxylic acids have been widely used as polydentate ligands, which can coordinate to transition or rare earth ions yielding complexes with interesting properties that are useful in materials science (Church & Halvorson, 1959) and in biological systems (Okabe & Oya, 2000). For example, Kim *et al.* (2001) focused on the syntheses of transition metal complexes containing benzene carboxylate and rigid aromatic pyridine ligands in order to study their electronic conductivity and magnetic properties. The importance of transition metal dicarboxylate complexes motivated us to pursue synthetic strategies for these compounds, using 5-nitroisophthalic acid as a polydentate ligand. Here we report the synthesis and X-ray crystal structure analysis of the title compound.

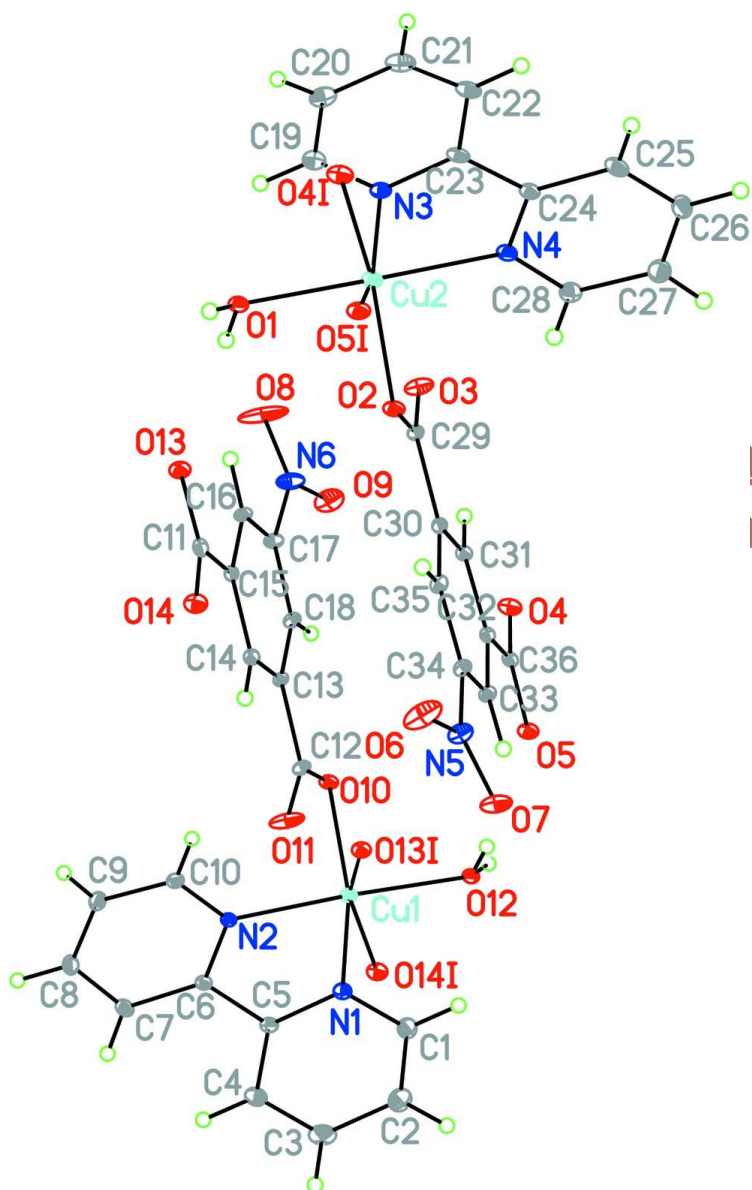
The molecular structure of the title compound is shown in Fig. 1. The title compound,  $[\text{Cu}(\text{C}_8\text{H}_3\text{NO}_6)(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]_n$  is a one-dimensional coordination polymer (Fig. 2). There are two symmetry independent 1D polymers in the crystal. The Cu(II) atom shows a strongly disordered coordination geometry. It is coordinated by two carboxylate groups from two different 5-nitroisophthalate ligands, 2,2'-bipyridyl and water molecule. The carboxylate groups act in a monodentate and bidentate coordination modes. The symmetry independent polymeric chains are linked via O-H $\cdots$ O hydrogen bonds (Table 1).

### S2. Experimental

A mixture of copper dichloride (0.5 mmol), 2,2'-bipyridine (0.5 mmol), and 5-nitroisophthalic acid (0.5 mmol) in H<sub>2</sub>O (8 ml) and ethanol (8 ml) was sealed in a 25 ml Teflon-lined stainless steel autoclave and kept at 413 K for three days. Blue crystals were obtained after cooling to room temperature (yield 27%). Anal. Calc. for C<sub>18</sub>H<sub>13</sub>CuN<sub>3</sub>O<sub>7</sub>: C 48.34, H 2.91, N 10.74%; Found: C 48.30, H 2.84, N 10.69%.

### S3. Refinement

The H atoms of water molecule were located from difference Fourier maps and were refined with distance restraints:  $d(\text{H}-\text{H}) = 1.38(2) \text{ \AA}$ ,  $d(\text{O}-\text{H}) = 0.88(2) \text{ \AA}$ , and with a fixed  $U_{\text{iso}}$  of  $0.080 \text{ \AA}^2$ . All other H atoms were placed in calculated positions with a C—H bond distance of  $0.93 \text{ \AA}$  and refined in the riding model approximation with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$  of the carrier atom.

**Figure 1**

A view of the title structure showing the atomic numbering scheme and 30% probability displacement ellipsoids.

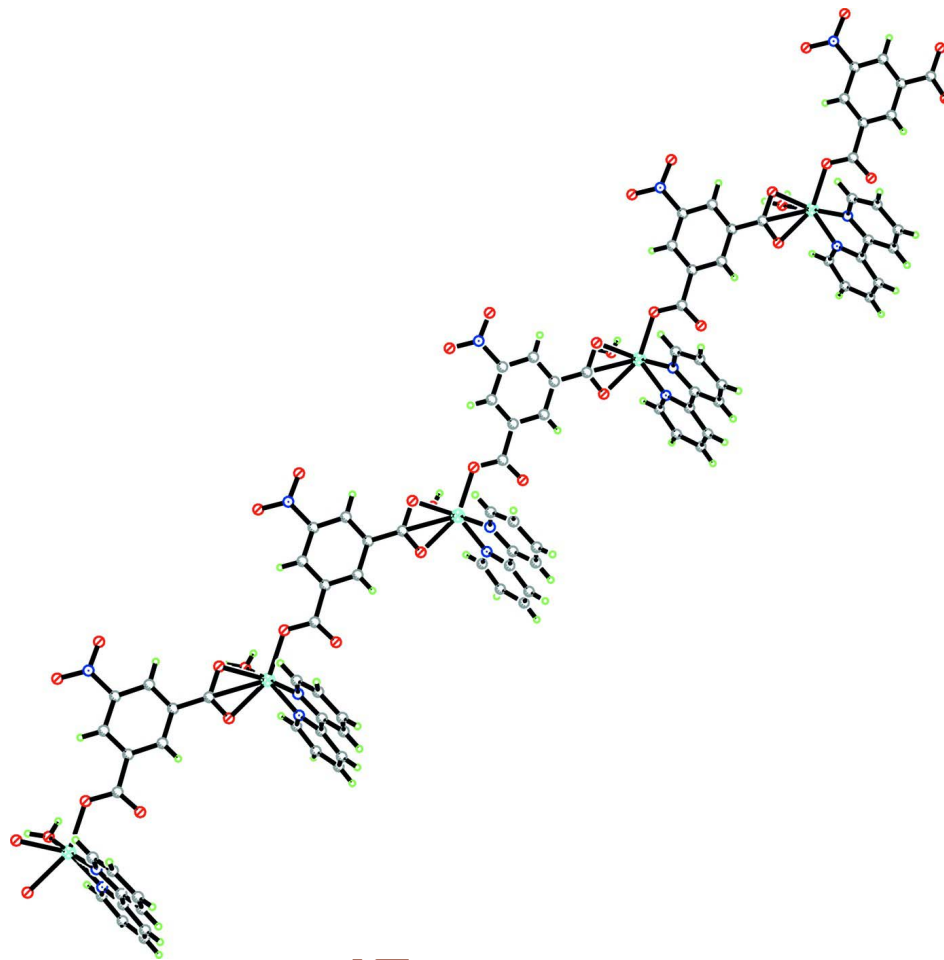


Figure 2

One of the symmetry-independent coordination polymers

**catena-Poly[[aqua(2,2'-bipyridine- $\kappa^2N,N'$ )copper(II)]- $\mu$ -5-nitroisophthalato- $\kappa^3O^1,O^1':O^3$ ]**

*Crystal data*

[Cu(C<sub>8</sub>H<sub>3</sub>NO<sub>6</sub>)(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)(H<sub>2</sub>O)]

$M_r = 446.85$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 10.1326$  (10) Å

$b = 23.263$  (3) Å

$c = 15.6087$  (15) Å

$\beta = 97.28$  (2)°

$V = 3649.6$  (7) Å<sup>3</sup>

$Z = 8$

$F(000) = 1816$

$D_x = 1.627$  Mg m<sup>-3</sup>

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

Cell parameters from 6694 reflections

$\theta = 1.8$ – $25.5$ °

$\mu = 1.25$  mm<sup>-1</sup>

$T = 293$  K

Block, blue

$0.12 \times 0.10 \times 0.08$  mm

*Data collection*

Bruker APEXII CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2001)

$T_{\min} = 0.865$ ,  $T_{\max} = 0.907$

18862 measured reflections

6694 independent reflections

5089 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.025$   
 $\theta_{\text{max}} = 25.5^\circ$ ,  $\theta_{\text{min}} = 1.8^\circ$

$h = -12 \rightarrow 10$   
 $k = -28 \rightarrow 22$   
 $l = -18 \rightarrow 18$

### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.124$   
 $S = 1.00$   
 6694 reflections  
 535 parameters  
 6 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  
 $w = 1/[\sigma^2(F_o^2) + (0.075P)^2 + 2.4671P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.003$   
 $\Delta\rho_{\text{max}} = 0.83 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.40 \text{ e } \text{\AA}^{-3}$

### 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	1.16168 (4)	0.154431 (15)	0.85573 (3)	0.02711 (13)
Cu2	0.12372 (4)	0.354405 (16)	0.93350 (3)	0.03053 (13)
C1	1.1959 (4)	0.07213 (16)	1.0079 (2)	0.0457 (9)
H1	1.2145	0.1048	1.0416	0.055*
C2	1.2039 (5)	0.0193 (2)	1.0471 (3)	0.0635 (13)
H2	1.2268	0.0161	1.1065	0.076*
C3	1.1773 (5)	-0.02890 (18)	0.9970 (3)	0.0634 (13)
H3	1.1810	-0.0651	1.0224	0.076*
C4	1.1452 (4)	-0.02334 (16)	0.9089 (3)	0.0481 (10)
H4	1.1282	-0.0556	0.8741	0.058*
C5	1.1388 (3)	0.03117 (13)	0.8732 (2)	0.0291 (7)
C6	1.1072 (3)	0.04138 (13)	0.7785 (2)	0.0266 (7)
C7	1.0796 (3)	-0.00183 (15)	0.7180 (2)	0.0376 (8)
H7	1.0788	-0.0401	0.7354	0.045*
C8	1.0527 (4)	0.01249 (16)	0.6306 (2)	0.0408 (9)
H8	1.0328	-0.0160	0.5891	0.049*
C9	1.0562 (4)	0.06932 (16)	0.6068 (2)	0.0415 (9)
H9	1.0383	0.0800	0.5491	0.050*
C10	1.0866 (3)	0.11017 (14)	0.6700 (2)	0.0337 (8)
H10	1.0889	0.1486	0.6536	0.040*
C11	0.3761 (3)	0.19406 (14)	0.8105 (2)	0.0284 (7)

C12	0.8756 (3)	0.17568 (14)	0.8380 (2)	0.0286 (7)
C13	0.7500 (3)	0.20954 (13)	0.80617 (19)	0.0232 (6)
C14	0.6258 (3)	0.18759 (13)	0.8202 (2)	0.0252 (6)
H14	0.6213	0.1526	0.8484	0.030*
C15	0.5081 (3)	0.21767 (13)	0.79223 (19)	0.0228 (6)
C16	0.5143 (3)	0.27058 (14)	0.7520 (2)	0.0287 (7)
H16	0.4375	0.2912	0.7332	0.034*
C17	0.6391 (3)	0.29176 (14)	0.7409 (2)	0.0300 (7)
C18	0.7573 (3)	0.26273 (13)	0.7665 (2)	0.0268 (7)
H18	0.8388	0.2784	0.7574	0.032*
C19	0.0858 (4)	0.43908 (16)	0.7844 (3)	0.0419 (9)
H19	0.0717	0.4066	0.7497	0.050*
C20	0.0710 (4)	0.49282 (18)	0.7464 (3)	0.0506 (10)
H20	0.0493	0.4965	0.6869	0.061*
C21	0.0891 (4)	0.54045 (17)	0.7982 (3)	0.0530 (11)
H21	0.0801	0.5770	0.7741	0.064*
C22	0.1206 (3)	0.53393 (15)	0.8859 (3)	0.0437 (9)
H22	0.1312	0.5660	0.9217	0.052*
C23	0.1365 (3)	0.47885 (13)	0.9207 (2)	0.0331 (8)
C24	0.1701 (3)	0.46692 (14)	1.0141 (2)	0.0312 (7)
C25	0.1994 (4)	0.50930 (15)	1.0773 (3)	0.0450 (10)
H25	0.1976	0.5480	1.0620	0.054*
C26	0.2313 (4)	0.49311 (18)	1.1632 (3)	0.0505 (10)
H26	0.2502	0.5209	1.2059	0.061*
C27	0.2346 (4)	0.43618 (19)	1.1844 (3)	0.0502 (10)
H27	0.2573	0.4245	1.2414	0.060*
C28	0.2036 (4)	0.39641 (17)	1.1200 (2)	0.0423 (9)
H28	0.2048	0.3577	1.1348	0.051*
C29	0.4118 (3)	0.33262 (14)	0.9445 (2)	0.0276 (7)
C30	0.5355 (3)	0.29913 (13)	0.9800 (2)	0.0245 (7)
C31	0.6609 (3)	0.31950 (13)	0.9659 (2)	0.0247 (6)
H31	0.6668	0.3529	0.9339	0.030*
C32	0.7773 (3)	0.29078 (12)	0.9988 (2)	0.0230 (6)
C33	0.7701 (3)	0.24090 (13)	1.0462 (2)	0.0281 (7)
H33	0.8466	0.2213	1.0687	0.034*
C34	0.6445 (3)	0.22111 (13)	1.0589 (2)	0.0274 (7)
C35	0.5281 (3)	0.24928 (14)	1.0278 (2)	0.0273 (7)
H35	0.4461	0.2350	1.0387	0.033*
C36	0.9110 (3)	0.31370 (13)	0.9804 (2)	0.0265 (7)
N1	1.1618 (3)	0.07821 (11)	0.92194 (18)	0.0308 (6)
N2	1.1133 (2)	0.09711 (10)	0.75448 (17)	0.0256 (6)
N3	0.1197 (3)	0.43222 (12)	0.86995 (18)	0.0310 (6)
N4	0.1716 (3)	0.41090 (11)	1.03653 (19)	0.0315 (6)
N5	0.6350 (3)	0.16771 (13)	1.1080 (2)	0.0421 (8)
N6	0.6481 (4)	0.34942 (14)	0.7038 (2)	0.0526 (9)
O1	0.0918 (2)	0.30549 (9)	0.81941 (17)	0.0320 (5)
O2	0.3006 (2)	0.31188 (9)	0.96166 (16)	0.0358 (6)
O3	0.4241 (3)	0.37683 (12)	0.90419 (19)	0.0532 (7)



O4	0.9139 (2)	0.35925 (10)	0.93797 (18)	0.0392 (6)
O5	1.0167 (2)	0.28721 (10)	1.00723 (16)	0.0360 (6)
O6	0.5265 (3)	0.14511 (15)	1.1064 (3)	0.0852 (13)
O7	0.7369 (3)	0.14842 (12)	1.1487 (2)	0.0579 (8)
O8	0.5457 (3)	0.37104 (19)	0.6687 (4)	0.128 (2)
O9	0.7554 (3)	0.37294 (13)	0.7091 (2)	0.0734 (10)
O10	0.9862 (2)	0.19817 (9)	0.82626 (16)	0.0328 (5)
O11	0.8637 (3)	0.12791 (13)	0.8686 (2)	0.0653 (9)
O12	1.1948 (2)	0.20384 (9)	0.97015 (16)	0.0319 (5)
O13	0.2693 (2)	0.22031 (10)	0.78406 (16)	0.0369 (6)
O14	0.3736 (2)	0.14837 (10)	0.85273 (17)	0.0390 (6)
H1W	1.245 (4)	0.2303 (13)	0.960 (3)	0.080*
H2W	1.132 (3)	0.2151 (17)	0.994 (3)	0.080*
H3W	0.157 (3)	0.2969 (18)	0.795 (3)	0.080*
H4W	0.042 (4)	0.2781 (13)	0.824 (3)	0.080*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.0215 (2)	0.0234 (2)	0.0363 (2)	0.00148 (15)	0.00314 (16)	0.00163 (15)
Cu2	0.0210 (2)	0.0245 (2)	0.0466 (3)	0.00113 (15)	0.00654 (18)	0.00113 (16)
C1	0.065 (3)	0.041 (2)	0.031 (2)	0.0004 (19)	0.0076 (18)	0.0047 (16)
C2	0.096 (4)	0.060 (3)	0.033 (2)	0.006 (3)	0.007 (2)	0.014 (2)
C3	0.092 (4)	0.040 (2)	0.059 (3)	0.004 (2)	0.012 (3)	0.031 (2)
C4	0.063 (3)	0.0273 (18)	0.053 (3)	-0.0023 (17)	0.005 (2)	0.0101 (16)
C5	0.0230 (16)	0.0246 (16)	0.0396 (19)	-0.0009 (12)	0.0039 (14)	0.0044 (13)
C6	0.0201 (15)	0.0235 (15)	0.0361 (18)	-0.0006 (12)	0.0037 (13)	0.0017 (13)
C7	0.0313 (18)	0.0270 (17)	0.054 (2)	-0.0024 (14)	0.0052 (16)	-0.0048 (16)
C8	0.036 (2)	0.043 (2)	0.042 (2)	-0.0019 (16)	0.0012 (16)	-0.0122 (16)
C9	0.041 (2)	0.048 (2)	0.034 (2)	0.0023 (17)	-0.0006 (16)	-0.0037 (16)
C10	0.0362 (19)	0.0319 (17)	0.0323 (19)	0.0054 (14)	0.0015 (15)	0.0049 (14)
C11	0.0197 (16)	0.0332 (17)	0.0332 (18)	-0.0034 (13)	0.0071 (13)	-0.0116 (14)
C12	0.0172 (16)	0.0347 (18)	0.0332 (18)	0.0028 (13)	0.0008 (13)	0.0056 (14)
C13	0.0147 (14)	0.0287 (16)	0.0257 (16)	0.0017 (12)	0.0008 (12)	0.0000 (12)
C14	0.0219 (16)	0.0261 (15)	0.0283 (16)	-0.0010 (12)	0.0054 (13)	-0.0006 (13)
C15	0.0156 (14)	0.0280 (15)	0.0252 (16)	-0.0013 (12)	0.0041 (12)	-0.0061 (12)
C16	0.0173 (15)	0.0372 (18)	0.0314 (18)	0.0093 (13)	0.0027 (13)	0.0019 (14)
C17	0.0269 (17)	0.0298 (16)	0.0343 (18)	0.0035 (13)	0.0078 (14)	0.0110 (13)
C18	0.0156 (14)	0.0337 (17)	0.0314 (18)	-0.0016 (12)	0.0039 (12)	0.0049 (13)
C19	0.040 (2)	0.040 (2)	0.049 (2)	0.0029 (16)	0.0137 (17)	0.0071 (17)
C20	0.043 (2)	0.058 (3)	0.052 (2)	0.0069 (19)	0.0135 (19)	0.024 (2)
C21	0.040 (2)	0.034 (2)	0.088 (3)	0.0026 (17)	0.021 (2)	0.027 (2)
C22	0.031 (2)	0.0237 (17)	0.078 (3)	0.0018 (14)	0.0160 (19)	0.0050 (18)
C23	0.0160 (15)	0.0232 (16)	0.062 (2)	0.0000 (12)	0.0137 (15)	0.0010 (15)
C24	0.0149 (15)	0.0292 (17)	0.051 (2)	-0.0005 (12)	0.0090 (14)	-0.0043 (15)
C25	0.032 (2)	0.0279 (18)	0.077 (3)	-0.0019 (15)	0.0121 (19)	-0.0106 (18)
C26	0.034 (2)	0.059 (3)	0.058 (3)	-0.0019 (18)	0.0037 (19)	-0.021 (2)
C27	0.039 (2)	0.064 (3)	0.048 (2)	0.0050 (19)	0.0075 (18)	-0.006 (2)

C28	0.037 (2)	0.043 (2)	0.047 (2)	0.0056 (17)	0.0058 (17)	-0.0007 (17)
C29	0.0166 (15)	0.0327 (17)	0.0326 (18)	0.0031 (13)	-0.0002 (13)	-0.0046 (14)
C30	0.0155 (15)	0.0300 (16)	0.0279 (17)	0.0005 (12)	0.0024 (12)	-0.0048 (12)
C31	0.0192 (15)	0.0241 (15)	0.0312 (17)	-0.0012 (12)	0.0053 (12)	-0.0004 (12)
C32	0.0156 (15)	0.0266 (15)	0.0276 (16)	-0.0004 (11)	0.0059 (12)	-0.0043 (12)
C33	0.0187 (15)	0.0345 (17)	0.0305 (18)	0.0020 (13)	0.0017 (13)	0.0005 (13)
C34	0.0216 (16)	0.0316 (16)	0.0288 (17)	-0.0020 (13)	0.0027 (13)	0.0043 (13)
C35	0.0175 (15)	0.0342 (17)	0.0307 (18)	-0.0059 (13)	0.0050 (13)	0.0015 (13)
C36	0.0140 (15)	0.0294 (16)	0.0370 (18)	0.0009 (12)	0.0073 (13)	-0.0085 (14)
N1	0.0305 (15)	0.0280 (14)	0.0347 (16)	-0.0011 (11)	0.0068 (12)	0.0048 (11)
N2	0.0213 (13)	0.0233 (13)	0.0320 (15)	0.0026 (10)	0.0030 (11)	-0.0005 (11)
N3	0.0216 (14)	0.0277 (14)	0.0446 (18)	0.0022 (11)	0.0075 (12)	0.0052 (12)
N4	0.0239 (14)	0.0268 (14)	0.0445 (18)	0.0028 (11)	0.0071 (12)	-0.0015 (12)
N5	0.0325 (17)	0.0448 (18)	0.0488 (19)	-0.0039 (14)	0.0042 (14)	0.0181 (14)
N6	0.044 (2)	0.049 (2)	0.068 (2)	0.0143 (16)	0.0185 (17)	0.0321 (17)
O1	0.0243 (12)	0.0261 (12)	0.0455 (14)	0.0024 (9)	0.0044 (10)	-0.0001 (10)
O2	0.0148 (11)	0.0301 (12)	0.0621 (16)	0.0023 (9)	0.0033 (10)	-0.0029 (11)
O3	0.0327 (14)	0.0511 (17)	0.075 (2)	0.0086 (12)	0.0035 (13)	0.0290 (15)
O4	0.0241 (12)	0.0291 (12)	0.0669 (17)	-0.0021 (9)	0.0153 (12)	0.0085 (11)
O5	0.0157 (11)	0.0366 (12)	0.0564 (16)	0.0029 (9)	0.0072 (10)	-0.0003 (11)
O6	0.0464 (19)	0.086 (2)	0.116 (3)	-0.0290 (17)	-0.0150 (19)	0.065 (2)
O7	0.0401 (16)	0.0511 (17)	0.083 (2)	0.0105 (13)	0.0080 (15)	0.0336 (15)
O8	0.046 (2)	0.117 (3)	0.226 (5)	0.037 (2)	0.036 (3)	0.131 (4)
O9	0.061 (2)	0.0534 (18)	0.102 (3)	-0.0163 (16)	-0.0027 (19)	0.0388 (18)
O10	0.0121 (10)	0.0274 (11)	0.0583 (15)	0.0017 (8)	0.0015 (10)	-0.0021 (10)
O11	0.0313 (15)	0.0648 (19)	0.101 (2)	0.0135 (13)	0.0130 (15)	0.0564 (18)
O12	0.0267 (12)	0.0261 (11)	0.0415 (14)	0.0039 (9)	-0.0003 (10)	-0.0027 (10)
O13	0.0157 (11)	0.0404 (13)	0.0550 (16)	0.0031 (10)	0.0066 (10)	-0.0012 (11)
O14	0.0223 (12)	0.0378 (14)	0.0583 (16)	-0.0027 (10)	0.0103 (11)	0.0048 (11)

*Geometric parameters (Å, °)*

Cu1—O10	2.049 (2)	C19—N3	1.345 (5)
Cu1—N1	2.052 (3)	C19—C20	1.384 (5)
Cu1—N2	2.078 (3)	C19—H19	0.9300
Cu1—O12	2.115 (2)	C20—C21	1.371 (6)
Cu1—O14 <sup>i</sup>	2.158 (2)	C20—H20	0.9300
Cu1—O13 <sup>i</sup>	2.258 (2)	C21—C22	1.374 (6)
Cu2—O2	2.046 (2)	C21—H21	0.9300
Cu2—N3	2.062 (3)	C22—C23	1.393 (5)
Cu2—N4	2.086 (3)	C22—H22	0.9300
Cu2—O1	2.104 (2)	C23—N3	1.341 (4)
Cu2—O4 <sup>ii</sup>	2.139 (2)	C23—C24	1.481 (5)
Cu2—O5 <sup>ii</sup>	2.294 (2)	C24—N4	1.349 (4)
C1—N1	1.350 (5)	C24—C25	1.400 (5)
C1—C2	1.372 (6)	C25—C26	1.391 (6)
C1—H1	0.9300	C25—H25	0.9300
C2—C3	1.373 (6)	C26—C27	1.364 (6)

C2—H2	0.9300	C26—H26	0.9300
C3—C4	1.379 (6)	C27—C28	1.373 (6)
C3—H3	0.9300	C27—H27	0.9300
C4—C5	1.383 (5)	C28—N4	1.346 (5)
C4—H4	0.9300	C28—H28	0.9300
C5—N1	1.337 (4)	C29—O3	1.220 (4)
C5—C6	1.491 (5)	C29—O2	1.284 (4)
C6—N2	1.353 (4)	C29—C30	1.520 (4)
C6—C7	1.383 (5)	C30—C35	1.386 (4)
C7—C8	1.398 (5)	C30—C31	1.400 (4)
C7—H7	0.9300	C31—C32	1.395 (4)
C8—C9	1.375 (5)	C31—H31	0.9300
C8—H8	0.9300	C32—C33	1.382 (4)
C9—C10	1.375 (5)	C32—C36	1.518 (4)
C9—H9	0.9300	C33—C34	1.391 (4)
C10—N2	1.347 (4)	C33—H33	0.9300
C10—H10	0.9300	C34—C35	1.383 (4)
C11—O14	1.253 (4)	C34—N5	1.470 (4)
C11—O13	1.265 (4)	C35—H35	0.9300
C11—C15	1.506 (4)	C36—O4	1.252 (4)
C12—O11	1.222 (4)	C36—O5	1.260 (4)
C12—O10	1.271 (4)	N5—O6	1.216 (4)
C12—C13	1.525 (4)	N5—O7	1.226 (4)
C13—C18	1.390 (4)	N6—O9	1.211 (4)
C13—C14	1.401 (4)	N6—O8	1.218 (4)
C14—C15	1.404 (4)	O1—H3W	0.83 (3)
C14—H14	0.9300	O1—H4W	0.82 (3)
C15—C16	1.387 (4)	O4—Cu2 <sup>i</sup>	2.139 (2)
C16—C17	1.388 (5)	O5—Cu2 <sup>i</sup>	2.294 (2)
C16—H16	0.9300	O12—H1W	0.82 (4)
C17—C18	1.389 (4)	O12—H2W	0.82 (4)
C17—N6	1.468 (4)	O13—Cu1 <sup>ii</sup>	2.258 (2)
C18—H18	0.9300	O14—Cu1 <sup>ii</sup>	2.158 (2)
O10—Cu1—N1	119.16 (10)	N3—C19—C20	122.2 (4)
O10—Cu1—N2	91.92 (10)	N3—C19—H19	118.9
N1—Cu1—N2	79.26 (10)	C20—C19—H19	118.9
O10—Cu1—O12	87.71 (9)	C21—C20—C19	118.5 (4)
N1—Cu1—O12	93.12 (10)	C21—C20—H20	120.7
N2—Cu1—O12	171.06 (10)	C19—C20—H20	120.7
O10—Cu1—O14 <sup>i</sup>	149.84 (9)	C20—C21—C22	119.7 (3)
N1—Cu1—O14 <sup>i</sup>	90.99 (10)	C20—C21—H21	120.1
N2—Cu1—O14 <sup>i</sup>	94.65 (10)	C22—C21—H21	120.1
O12—Cu1—O14 <sup>i</sup>	90.11 (10)	C21—C22—C23	119.4 (4)
O10—Cu1—O13 <sup>i</sup>	90.66 (9)	C21—C22—H22	120.3
N1—Cu1—O13 <sup>i</sup>	150.04 (10)	C23—C22—H22	120.3
N2—Cu1—O13 <sup>i</sup>	98.11 (10)	N3—C23—C22	120.9 (4)
O12—Cu1—O13 <sup>i</sup>	90.83 (9)	N3—C23—C24	115.2 (3)

O14 <sup>i</sup> —Cu1—O13 <sup>i</sup>	59.29 (8)	C22—C23—C24	123.8 (3)
O2—Cu2—N3	119.41 (10)	N4—C24—C25	120.2 (3)
O2—Cu2—N4	91.57 (10)	N4—C24—C23	115.5 (3)
N3—Cu2—N4	78.83 (11)	C25—C24—C23	124.3 (3)
O2—Cu2—O1	87.52 (9)	C26—C25—C24	119.4 (4)
N3—Cu2—O1	94.37 (10)	C26—C25—H25	120.3
N4—Cu2—O1	171.62 (10)	C24—C25—H25	120.3
O2—Cu2—O4 <sup>ii</sup>	149.99 (9)	C27—C26—C25	119.5 (4)
N3—Cu2—O4 <sup>ii</sup>	90.60 (9)	C27—C26—H26	120.3
N4—Cu2—O4 <sup>ii</sup>	94.38 (10)	C25—C26—H26	120.3
O1—Cu2—O4 <sup>ii</sup>	90.54 (10)	C26—C27—C28	118.7 (4)
O2—Cu2—O5 <sup>ii</sup>	91.14 (9)	C26—C27—H27	120.6
N3—Cu2—O5 <sup>ii</sup>	149.09 (9)	C28—C27—H27	120.6
N4—Cu2—O5 <sup>ii</sup>	96.95 (10)	N4—C28—C27	123.0 (4)
O1—Cu2—O5 <sup>ii</sup>	91.40 (9)	N4—C28—H28	118.5
O4 <sup>ii</sup> —Cu2—O5 <sup>ii</sup>	58.96 (8)	C27—C28—H28	118.5
N1—C1—C2	122.1 (4)	O3—C29—O2	125.0 (3)
N1—C1—H1	119.0	O3—C29—C30	119.1 (3)
C2—C1—H1	119.0	O2—C29—C30	115.9 (3)
C1—C2—C3	118.7 (4)	C35—C30—C31	118.7 (3)
C1—C2—H2	120.6	C35—C30—C29	121.8 (3)
C3—C2—H2	120.6	C31—C30—C29	119.5 (3)
C2—C3—C4	119.7 (4)	C32—C31—C30	121.5 (3)
C2—C3—H3	120.1	C32—C31—H31	119.3
C4—C3—H3	120.1	C30—C31—H31	119.3
C3—C4—C5	118.8 (4)	C33—C32—C31	120.0 (3)
C3—C4—H4	120.6	C33—C32—C36	120.3 (3)
C5—C4—H4	120.6	C31—C32—C36	119.7 (3)
N1—C5—C4	121.7 (3)	C32—C33—C34	117.7 (3)
N1—C5—C6	115.7 (3)	C32—C33—H33	121.1
C4—C5—C6	122.6 (3)	C34—C33—H33	121.1
N2—C6—C7	121.3 (3)	C35—C34—C33	123.2 (3)
N2—C6—C5	114.6 (3)	C35—C34—N5	118.3 (3)
C7—C6—C5	124.1 (3)	C33—C34—N5	118.4 (3)
C6—C7—C8	119.4 (3)	C34—C35—C30	118.9 (3)
C6—C7—H7	120.3	C34—C35—H35	120.5
C8—C7—H7	120.3	C30—C35—H35	120.5
C9—C8—C7	118.9 (3)	O4—C36—O5	121.0 (3)
C9—C8—H8	120.5	O4—C36—C32	118.6 (3)
C7—C8—H8	120.5	O5—C36—C32	120.4 (3)
C8—C9—C10	118.8 (3)	O4—C36—Cu2 <sup>i</sup>	57.03 (16)
C8—C9—H9	120.6	O5—C36—Cu2 <sup>i</sup>	64.09 (16)
C10—C9—H9	120.6	C32—C36—Cu2 <sup>i</sup>	174.0 (2)
N2—C10—C9	123.0 (3)	C5—N1—C1	119.0 (3)
N2—C10—H10	118.5	C5—N1—Cu1	115.6 (2)
C9—C10—H10	118.5	C1—N1—Cu1	125.1 (2)
O14—C11—O13	120.5 (3)	C10—N2—C6	118.5 (3)
O14—C11—C15	119.1 (3)	C10—N2—Cu1	126.8 (2)

O13—C11—C15	120.4 (3)	C6—N2—Cu1	114.8 (2)
O14—C11—Cu1 <sup>ii</sup>	58.05 (16)	C23—N3—C19	119.2 (3)
O13—C11—Cu1 <sup>ii</sup>	62.60 (17)	C23—N3—Cu2	115.6 (2)
C15—C11—Cu1 <sup>ii</sup>	174.8 (2)	C19—N3—Cu2	124.6 (2)
O11—C12—O10	124.3 (3)	C28—N4—C24	119.1 (3)
O11—C12—C13	118.5 (3)	C28—N4—Cu2	126.4 (2)
O10—C12—C13	117.1 (3)	C24—N4—Cu2	114.5 (2)
C18—C13—C14	119.6 (3)	O6—N5—O7	123.5 (3)
C18—C13—C12	121.0 (3)	O6—N5—C34	118.3 (3)
C14—C13—C12	119.4 (3)	O7—N5—C34	118.2 (3)
C13—C14—C15	121.0 (3)	O9—N6—O8	123.4 (3)
C13—C14—H14	119.5	O9—N6—C17	119.1 (3)
C15—C14—H14	119.5	O8—N6—C17	117.6 (4)
C16—C15—C14	119.8 (3)	Cu2—O1—H3W	118 (3)
C16—C15—C11	120.1 (3)	Cu2—O1—H4W	112 (3)
C14—C15—C11	120.0 (3)	H3W—O1—H4W	113 (4)
C15—C16—C17	117.8 (3)	C29—O2—Cu2	122.8 (2)
C15—C16—H16	121.1	C36—O4—Cu2 <sup>i</sup>	93.58 (18)
C17—C16—H16	121.1	C36—O5—Cu2 <sup>i</sup>	86.30 (19)
C16—C17—C18	123.9 (3)	C12—O10—Cu1	121.3 (2)
C16—C17—N6	118.4 (3)	Cu1—O12—H1W	106 (3)
C18—C17—N6	117.6 (3)	Cu1—O12—H2W	121 (3)
C13—C18—C17	117.9 (3)	H1W—O12—H2W	112 (4)
C13—C18—H18	121.0	C11—O13—Cu1 <sup>ii</sup>	87.6 (2)
C17—C18—H18	121.0	C11—O14—Cu1 <sup>ii</sup>	92.45 (19)

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

#### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O12—H1W $\cdots$ O2 <sup>i</sup>	0.83 (4)	1.98 (2)	2.742 (3)	153 (4)
O1—H4W $\cdots$ O10 <sup>ii</sup>	0.82 (3)	1.95 (2)	2.724 (3)	158 (4)
O12—H2W $\cdots$ O5	0.82 (4)	2.07 (3)	2.760 (3)	141 (4)
O1—H3W $\cdots$ O13	0.83 (3)	2.13 (3)	2.778 (3)	135 (4)

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