

Retraction of articles by T. Liu *et al.*

T. Liu,^{a*} Y.-X. Wang,^b Z.-W. Wang,^a Z.-P. Xie^{a,c} and J. Y. Zhu^d

^aCollege of Engineering, Jinggangshan University, Jian 343009, People's Republic of China, ^bCollege of Mathematics and Physics, Jinggangshan University, Jian

343009, People's Republic of China, ^cDepartment of Chemistry, Jiangxi University of Science and Technology, Ganzhou 341000, People's Republic of China, and

^dDepartment of Information Engineering, Jiangxi University of Science and Technology, Nanchang 330013, People's Republic of China

Correspondence e-mail: taoliu07@126.com

Received 20 November 2009; accepted 15 December 2009

A series of 29 papers by Liu *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 29 papers by Liu *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
<i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)</i> <i>(Dihydroxyglyoxime-κ²N,N')bis(I,10-phenanthroline-κ²N,N')copper(II) dinitrate dihydrate</i>	Liu & Xie (2007a) Liu, Wang, Wang & Xie (2007b)	10.1107/S1600536807026852 10.1107/S1600536807028255	EDUMAS EDUVAB
<i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)</i>	Liu & Xie (2007b)	10.1107/S1600536807028735	RIGQAA
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(I,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]</i>	Liu, Wang, Wang & Xie (2007c)	10.1107/S1600536807030917	UDUMIQ
<i>Polymeric KNO₂</i> <i>(Dihydroxyglyoxime-κ²N,N')bis(I,10-phenanthroline-κ²N,N')cobalt(II) dinitrate dihydrate</i>	Liu Wang, Wang & Xie (2007a) Liu, Wang, Wang & Xie (2007d)	10.1107/S1600536807027195 10.1107/S1600536807031224	ICSD 240891 WIHIED
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(I,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]</i>	Liu, Wang, Wang & Xie (2007e)	10.1107/S1600536807032679	WIHQEK
<i>Tetrakis[μ-(2-pyridyloxyacetato-κ²O:O')bis(I,10-phenanthroline-κ²N,N')-(2-pyridyloxyacetato-κO)neodymium(III)]</i>	Liu, Wang, Wang & Xie (2007f)	10.1107/S1600536807035349	TIGDAP
<i>(Dihydroxyglyoxime-κ²N,N')bis(I,10-phenanthroline-κ²N,N')manganese(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007g)	10.1107/S1600536807035076	TIGDET
<i>2-Amino-3,5-dinitrobenzoic acid-ammonium (I/I)</i>	Liu & Zhu (2007j)	10.1107/S1600536807040068	KIKQAX
<i>2-Hydroxy-3,5-dinitrobenzamide monohydrate</i>	Liu & Zhu (2007k)	10.1107/S1600536807039712	KIKQEB
<i>2-(1-Hydroxy-2-pyridyl)acetamide monohydrate</i>	Liu & Zhu (2007l)	10.1107/S1600536807040652	CIKQOD
<i>Bis(2,2'-bipyridine-κN,N')bis(thiocyanato-κN)iron(II)</i>	Liu & Zhu (2007a)	10.1107/S1600536807043486	XIFXOA
<i>catena-Poly[hexakis(μ₂-anilinoacetamide)bis(I,10-phenanthroline)disamarium(III)]</i>	Liu & Zhu (2007b)	10.1107/S1600536807045485	XILNAI
<i>3-Hydroxy-2,4,6-trinitropyridine monohydrate</i>	Liu & Zhu (2007m)	10.1107/S1600536807045230	PILNOO
<i>catena-Poly[hexakis(μ₂-anilinoacetamide)bis(I,10-phenanthroline)-dipraseodymium(III)]</i>	Liu & Zhu (2007c)	10.1107/S1600536807047733	SILZET
<i>catena-Poly[[tetra-μ-anilinoacetamido-bis(I,10-phenanthroline)dicerium(III)-di-μ-anilinoacetamido]</i>	Liu & Zhu (2007d)	10.1107/S1600536807050969	GIMZOS
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)chromium(II)</i>	Liu & Zhu (2007e)	10.1107/S1600536807051756	WINFAB
<i>2-Ammonio-3-carboxy-5-nitrobenzoate monohydrate</i>	Liu & Zhu (2007n)	10.1107/S1600536807048477	GINFEP
<i>2-(Benzoylhydrazinocarbonyl)benzoic acid</i>	Liu & Zhu (2007o)	10.1107/S160053680705204X	TINZIA
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)vanadium(II)</i>	Liu & Zhu (2007f)	10.1107/S1600536807054529	HIPZIQ
<i>catena-Poly[[nitrato-κO](I,10-phenanthroline-κ²N,N')nickel(II)-μ-acetamido-κ²O:N]</i>	Liu & Zhu (2007g)	10.1107/S1600536807056504	XIRGIP
<i>catena-Poly[[nitrato-κO](I,10-phenanthroline-κ²N,N')copper(II)-μ-acetamido-κ²O:N]</i>	Liu & Zhu (2007h)	10.1107/S1600536807059077	HIQROP
<i>catena-Poly[[nitrato-κO](I,10-phenanthroline-κ²N,N')cobalt(II)-μ-acetamido-κ²O:N]</i>	Liu & Zhu (2007i)	10.1107/S1600536807060631	YIQMER
<i>N'-Benzoyl-4-nitronicotinohydrazide</i>	Liu & Zhu (2007p)	10.1107/S1600536807053068	CIPVON
<i>N'-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide</i>	Liu & Zhu (2007q)	10.1107/S1600536807054876	RIRWEV

addenda and errata

Table 1 (continued)

Title	Reference	DOI	Refcode
Ethylenediammonium sulfate	Liu & Zhu (2007r)	10.1107/S1600536807056280	ETDAMS03
Ethylenediammonium perchlorate	Liu & Zhu (2007s)	10.1107/S1600536807059909	HIRYEN
catena-Poly[μ (nitro- κO)(1,10-phenanthroline- $\kappa^2 N,N'$)manganese(II)]- μ -nitroato- $\kappa^2 O:O'$]	Liu & Zhu (2008)	10.1107/S160053680706254X	MIRROV

References

- Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007a). *Acta Cryst.* E63, i170.
Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007b). *Acta Cryst.* E63, m1887–m1888.
Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007c). *Acta Cryst.* E63, m2020–m2021.
Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007d). *Acta Cryst.* E63, m2027–m2028.
Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007e). *Acta Cryst.* E63, m2080–m2081.
Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007f). *Acta Cryst.* E63, m2196–m2197.
Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007g). *Acta Cryst.* E63, m2198–m2199.
Liu, T. & Xie, Z.-P. (2007a). *Acta Cryst.* E63, m1820.
Liu, T. & Xie, Z.-P. (2007b). *Acta Cryst.* E63, m1908.
Liu, T. & Zhu, J. Y. (2007a). *Acta Cryst.* E63, m2506–m2507.
Liu, T. & Zhu, J.-Y. (2007b). *Acta Cryst.* E63, m2592–m2593.
Liu, T. & Zhu, J. Y. (2007c). *Acta Cryst.* E63, m2659–m2660.
Liu, T. & Zhu, J. Y. (2007d). *Acta Cryst.* E63, m2775–m2776.
Liu, T. & Zhu, J. Y. (2007e). *Acta Cryst.* E63, m2809.
Liu, T. & Zhu, J. Y. (2007f). *Acta Cryst.* E63, m2912.
Liu, T. & Zhu, J.-Y. (2007g). *Acta Cryst.* E63, m2977–m2978.
Liu, T. & Zhu, J. Y. (2007h). *Acta Cryst.* E63, m3108.
Liu, T. & Zhu, J. Y. (2007i). *Acta Cryst.* E63, m3144.
Liu, T. & Zhu, J.-Y. (2007j). *Acta Cryst.* E63, o3829.
Liu, T. & Zhu, J. Y. (2007k). *Acta Cryst.* E63, o3830.
Liu, T. & Zhu, J.-Y. (2007l). *Acta Cryst.* E63, o3860.
Liu, T. & Zhu, J. Y. (2007m). *Acta Cryst.* E63, o4112.
Liu, T. & Zhu, J. Y. (2007n). *Acta Cryst.* E63, o4267.
Liu, T. & Zhu, J. Y. (2007o). *Acta Cryst.* E63, o4441.
Liu, T. & Zhu, J. Y. (2007p). *Acta Cryst.* E63, o4527.
Liu, T. & Zhu, J. Y. (2007q). *Acta Cryst.* E63, o4574.
Liu, T. & Zhu, J.-Y. (2007r). *Acta Cryst.* E63, o4660.
Liu, T. & Zhu, J. Y. (2007s). *Acta Cryst.* E63, o4874.
Liu, T. & Zhu, J. Y. (2008). *Acta Cryst.* E64, m28.

2-(1-Hydroxy-2-pyridyl)acetamide monohydrate

T. Liu^{a*} and J.-Y. Zhu^b
^aCollege of Engineering, Jinggangshan University, Jian 343009, People's Republic of China, and ^bDepartment of Information Engineering, Jiangxi University of Science and Technology, Nanchang 330013, People's Republic of China

Correspondence e-mail: taoliu07@126.com

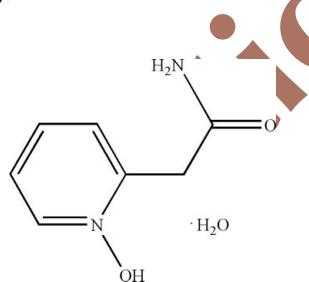
Received 16 August 2007; accepted 16 August 2007

 Key indicators: single-crystal X-ray study; $T = 273\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$; R factor = 0.055; wR factor = 0.187; data-to-parameter ratio = 12.7.

In the crystal structure of the title complex, $\text{C}_7\text{H}_7\text{N}_2\text{O}_2\cdot\text{H}_2\text{O}$, intermolecular $\text{O}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds result in the formation of a supramolecular network structure; intramolecular $\text{O}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds are also present.

Related literature

For general background, see: Desiraju (1995, 1997); Braga *et al.* (1998); Zaworotko (1997); Braga & Grepioni (2000); Moulton & Zaworotko (2001); Pan *et al.* (2001); Ma *et al.* (2001); Prior & Rosseinsky (2001). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

 $\text{C}_7\text{H}_7\text{N}_2\text{O}_2\cdot\text{H}_2\text{O}$
 $M_r = 169.16$

 Monoclinic, $P2_1/n$
 $a = 12.998 (3)\text{ \AA}$
 $b = 4.0992 (11)\text{ \AA}$
 $c = 15.581 (4)\text{ \AA}$
 $\beta = 114.159 (5)^\circ$
 $V = 757.5 (3)\text{ \AA}^3$
 $Z = 4$

 Mo $K\alpha$ radiation

 $\mu = 0.12\text{ mm}^{-1}$
 $T = 273 (2)\text{ K}$
 $0.64 \times 0.13 \times 0.09\text{ mm}$

Data collection

 Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.929$, $T_{\max} = 0.990$

 4820 measured reflections
1611 independent reflections
896 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.054$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.187$
 $S = 1.00$
1611 reflections
127 parameters
7 restraints

 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.56\text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.21\text{ e \AA}^{-3}$
Table 1

 Hydrogen-bond geometry (\AA , $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O3—H3B \cdots N1	0.86 (4)	2.58 (4)	3.404 (3)	163 (4)
O3—H3B \cdots O1	0.86 (4)	1.89 (4)	2.715 (3)	162 (4)
O1—H1A \cdots O3	0.82	1.93	2.715 (3)	161
N2—H2A \cdots O2 ⁱ	0.883 (18)	2.076 (18)	2.951 (3)	171 (3)
N2—H2B \cdots O3 ⁱⁱ	0.887 (17)	2.11 (2)	2.888 (4)	146 (3)
O3—H3A \cdots O1 ⁱⁱⁱ	0.86 (2)	2.61 (3)	3.282 (4)	137 (3)
O3—H3A \cdots O1 ^{iv}	0.86 (2)	2.34 (2)	3.063 (3)	142 (3)

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

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*.

We thank the Youth Program of Jinggangshan University for financial support of this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2312).

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.
- Braga, D., Grepioni, F. & Desiraju, G. R. (1998). *Chem. Rev.* **98**, 1375–1386.
- Braga, D. & Grepioni, F. (2000). *Acc. Chem. Res.* **33**, 601–608.
- Desiraju, G. R. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 2311–2315.
- Desiraju, G. R. (1997). *J. Chem. Soc. Chem. Commun.* pp. 1475–1476.
- Ma, B. Q., Gao, S., Sun, H. L. & Xu, G. X. (2001). *J. Chem. Soc. Dalton Trans.* pp. 130–133.
- Moulton, B. & Zaworotko, M. J. (2001). *Chem. Rev.* **101**, 1629–1658.
- Pan, L., Ching, N. & Huang, X. Y. (2001). *Chem. Eur. J.* **7**, 4431–4437.
- Prior, T. J. & Rosseinsky, M. J. (2001). *Chem. Commun.* pp. 1222–1223.
- 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.
- Zaworotko, M. J. (1997). *Nature (London)*, **386**, 220–226.

supplementary materials

Article retracted

Acta Cryst. (2007). E63, o3860 [doi:10.1107/S1600536807040652]

2-(1-Hydroxy-2-pyridyl)acetamide monohydrate

T. Liu and J.-Y. Zhu

Comment

In the synthesis of crystal structures by design, the assembly of molecular units in predefined arrangements is a key goal (Desiraju, 1995, 1997; Braga *et al.*, 1998). Due to hydrogen-bonding interactions are of critical importance in biological systems, organic materials and coordination chemistry, hydrogen-bonding is currently the best tool in achieving this goal (Zaworotko, 1997; Braga & Grepioni, 2000). Supramolecular architectures are of considerable contemporary interest by virtue of their potential applications in various fields (Moulton & Zaworotko, 2001; Pan *et al.*, 2001; Ma *et al.*, 2001; Prior & Rosseinsky, 2001). We originally attempted to synthesize complexes featuring La metal chains by reaction of the lanthanum(III) ion with 1-hydroxy-2-acetylaminopyridine ligand. Unfortunately, we obtained only the title compound, (I), and we report herein its crystal structure.

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). It contains one ($C_7H_7N_2O_2$) molecule and one water molecule.

In the crystal structure, intramolecular O—H···O and O—H···N and intermolecular O—H···O and N—H···O hydrogen bonds (Table 1) result in the formation of a supramolecular network structure (Fig. 2).

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb. Lanthanum (III) nitrate hexahydrate (216.4 mg, 0.5 mmol), 1-hydroxy-2-acetylaminopyridine (151.2 mg, 1 mmol) and distilled water (3 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 443 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 colorless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

Refinement

H3A, H3B (for OH₂) and H2A, H2B (for NH₂) were located in difference syntheses and refined isotropically [O—H = 0.86 (2) and 0.86 (4) Å, $U_{iso}(H) = 0.099$ (14) and 0.121 (17) Å²; N—H = 0.883 (18) and 0.887 (17) Å, $U_{iso}(H) = 0.088$ (11) and 0.086 (11) Å²]. The remaining H atoms were positioned geometrically, with O—H = 0.82 Å (for OH) and C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C,O)$, where $x = 1.2$ for aromatic H and $x = 1.5$ for OH H atoms.

supplementary materials

Figures

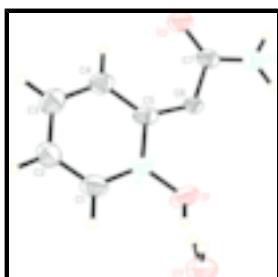


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

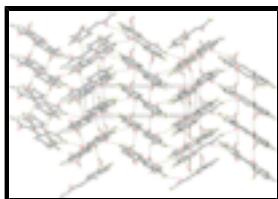


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

2-(1-Hydroxy-2-pyridyl)acetamide monohydrate

Crystal data

$C_7H_7N_2O_2 \cdot H_2O$

$F_{000} = 356$

$M_r = 169.16$

$D_x = 1.483 \text{ Mg m}^{-3}$

Monoclinic, $P2_1/n$

Mo $K\alpha$ radiation

Hall symbol: -P 2yn

$\lambda = 0.71073 \text{ \AA}$

$a = 12.998 (3) \text{ \AA}$

Cell parameters from 1902 reflections

$b = 4.0992 (11) \text{ \AA}$

$\theta = 2.7\text{--}28.0^\circ$

$c = 15.581 (4) \text{ \AA}$

$\mu = 0.12 \text{ mm}^{-1}$

$\beta = 114.159 (5)^\circ$

$T = 273 (2) \text{ K}$

$V = 757.5 (3) \text{ \AA}^3$

Prism, colourless

$Z = 4$

$0.64 \times 0.13 \times 0.09 \text{ mm}$

Data collection

Bruker SMART CCD area-detector
diffractometer

1611 independent reflections

Radiation source: fine-focus sealed tube

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

Monochromator: graphite

$R_{\text{int}} = 0.054$

$T = 273(2) \text{ K}$

$\theta_{\max} = 27.0^\circ$

φ and ω scans

$\theta_{\min} = 2.9^\circ$

Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)

$h = -16 \rightarrow 15$

$T_{\min} = 0.929, T_{\max} = 0.990$

$k = -5 \rightarrow 4$

4820 measured reflections

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.055$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.187$	$w = 1/[\sigma^2(F_o^2) + (0.1181P)^2 + 0.01P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1611 reflections	$\Delta\rho_{\text{max}} = 0.56 \text{ e \AA}^{-3}$
127 parameters	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
7 restraints	Extinction correction: SHELXTL (Siemens, 1996), $F_c^* = kF_c[1 + 0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.050 (19)

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.63246 (18)	0.9693 (6)	0.06578 (17)	0.0777 (8)
H1A	0.6007	0.8559	0.0909	0.117*
O2	0.82022 (17)	1.1177 (6)	-0.13760 (13)	0.0687 (7)
O3	0.5047 (2)	0.5292 (7)	0.10867 (16)	0.0724 (7)
H3A	0.507 (3)	0.354 (5)	0.079 (2)	0.099 (14)*
H3B	0.551 (3)	0.631 (7)	0.092 (3)	0.121 (17)*
N1	0.73275 (19)	0.8485 (6)	0.08390 (17)	0.0551 (7)
N2	0.6565 (2)	1.3944 (7)	-0.19117 (18)	0.0645 (8)
H2A	0.660 (3)	1.481 (8)	-0.2419 (18)	0.088 (11)*
H2B	0.597 (2)	1.479 (8)	-0.185 (2)	0.086 (11)*
C1	0.7882 (3)	0.6667 (8)	0.1618 (2)	0.0651 (9)
H1	0.7541	0.6275	0.2028	0.078*
C2	0.8904 (3)	0.5416 (8)	0.1817 (2)	0.0643 (9)
H2	0.9268	0.4154	0.2353	0.077*
C3	0.9408 (3)	0.6049 (8)	0.1203 (2)	0.0651 (9)

supplementary materials

H3	1.0123	0.5230	0.1330	0.078*
C4	0.8851 (2)	0.7890 (8)	0.0404 (2)	0.0567 (8)
H4	0.9188	0.8263	-0.0011	0.068*
C5	0.7793 (2)	0.9193 (7)	0.02133 (19)	0.0507 (7)
C6	0.71272 (18)	1.1137 (6)	-0.05215 (15)	0.0363 (6)
C7	0.7356 (2)	1.2057 (7)	-0.12975 (19)	0.0523 (8)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0782 (15)	0.0862 (17)	0.0987 (17)	0.0263 (12)	0.0668 (14)	0.0342 (13)
O2	0.0629 (13)	0.0955 (18)	0.0645 (14)	-0.0075 (11)	0.0432 (11)	-0.0086 (11)
O3	0.0850 (16)	0.0765 (17)	0.0741 (15)	0.0080 (13)	0.0512 (13)	0.0056 (13)
N1	0.0585 (14)	0.0589 (15)	0.0633 (15)	0.0061 (11)	0.0406 (12)	0.0056 (12)
N2	0.0637 (17)	0.083 (2)	0.0563 (16)	-0.0042 (14)	0.0336 (14)	0.0096 (14)
C1	0.082 (2)	0.065 (2)	0.0635 (18)	0.0092 (16)	0.0453 (17)	0.0103 (16)
C2	0.0676 (19)	0.066 (2)	0.0581 (18)	0.0012 (15)	0.0241 (15)	0.0017 (15)
C3	0.0515 (16)	0.065 (2)	0.078 (2)	-0.0033 (14)	0.0250 (16)	-0.0090 (17)
C4	0.0501 (15)	0.068 (2)	0.0609 (17)	-0.0097 (13)	0.0311 (14)	-0.0064 (15)
C5	0.0550 (15)	0.0537 (17)	0.0552 (16)	-0.0160 (13)	0.0346 (13)	-0.0148 (13)
C6	0.0392 (12)	0.0416 (14)	0.0351 (12)	-0.0058 (10)	0.0223 (10)	0.0023 (10)
C7	0.0545 (16)	0.0630 (18)	0.0484 (15)	-0.0183 (14)	0.0302 (13)	-0.0124 (14)

Geometric parameters (\AA , $^\circ$)

O1—N1	1.313 (3)	C1—C2	1.337 (4)
O1—H1A	0.8200	C1—H1	0.9300
O2—C7	1.210 (3)	C2—C3	1.386 (4)
O3—H3A	0.86 (2)	C2—H2	0.9300
O3—H3B	0.86 (4)	C3—C4	1.381 (4)
N1—C1	1.353 (4)	C3—H3	0.9300
N1—C5	1.373 (3)	C4—C5	1.388 (4)
N2—C7	1.329 (4)	C4—H4	0.9300
N2—H2A	0.883 (18)	C5—C6	1.373 (4)
N2—H2B	0.887 (17)	C6—C7	1.410 (3)
N1—O1—H1A	109.5	C4—C3—C2	120.2 (3)
H3A—O3—H3B	94 (3)	C4—C3—H3	119.9
O1—N1—C1	121.2 (2)	C2—C3—H3	119.9
O1—N1—C5	117.1 (2)	C3—C4—C5	120.7 (3)
C1—N1—C5	121.7 (2)	C3—C4—H4	119.6
C7—N2—H2B	127 (2)	C5—C4—H4	119.6
C7—N2—H2A	125 (2)	C6—C5—N1	113.8 (2)
H2B—N2—H2A	108 (2)	C6—C5—C4	129.3 (2)
C2—C1—N1	122.3 (3)	N1—C5—C4	116.9 (3)
C2—C1—H1	118.9	C5—C6—C7	126.0 (2)
N1—C1—H1	118.9	O2—C7—N2	124.6 (3)
C1—C2—C3	118.2 (3)	O2—C7—C6	121.8 (3)
C1—C2—H2	120.9	N2—C7—C6	113.6 (2)

C3—C2—H2 120.9

Hydrogen-bond geometry (\AA , $^\circ$)

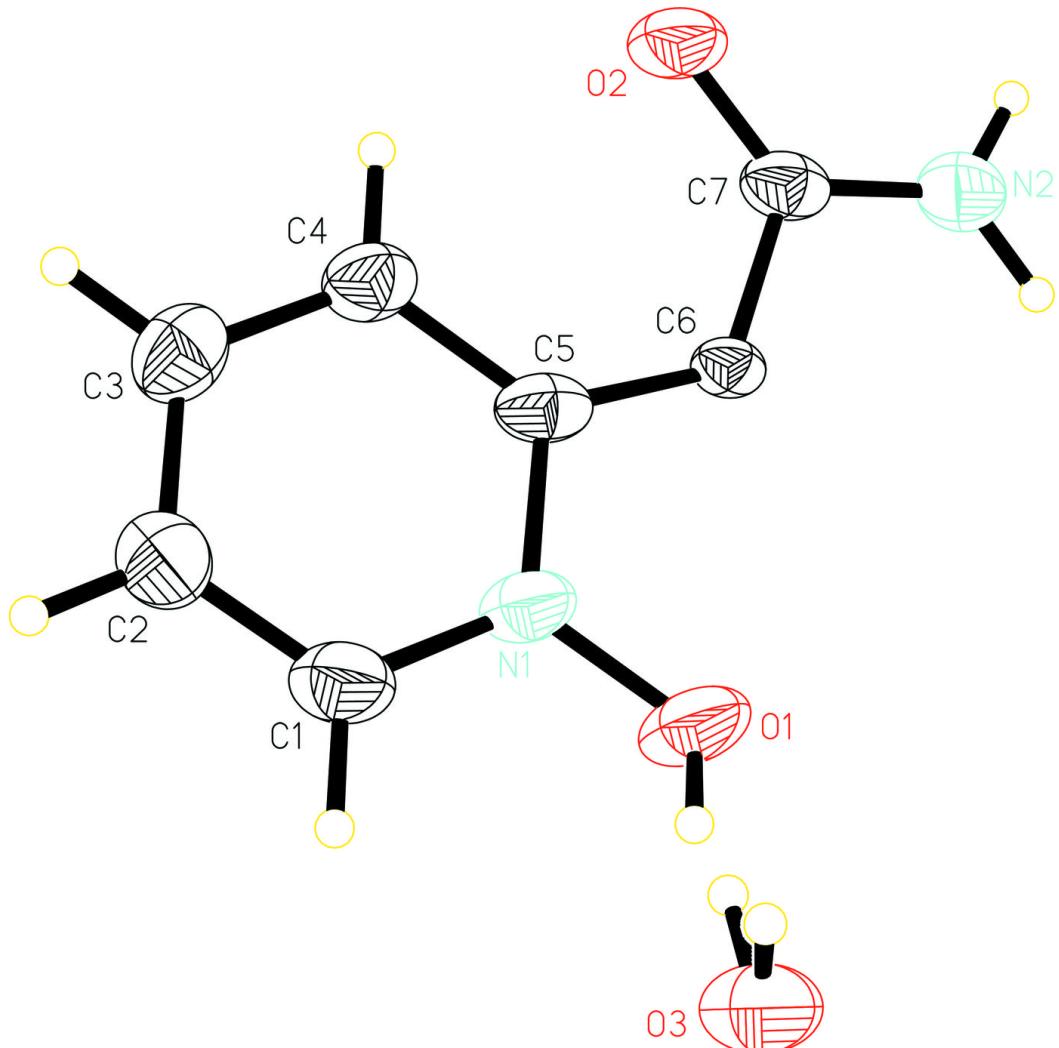
$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
O3—H3B···N1	0.86 (4)	2.58 (4)	3.404 (3)	163 (4)
O3—H3B···O1	0.86 (4)	1.89 (4)	2.715 (3)	162 (4)
O1—H1A···O3	0.82	1.93	2.715 (3)	161
N2—H2A···O2 ⁱ	0.883 (18)	2.076 (18)	2.951 (3)	171 (3)
N2—H2B···O3 ⁱⁱ	0.887 (17)	2.11 (2)	2.888 (4)	146 (3)
O3—H3A···O1 ⁱⁱⁱ	0.86 (2)	2.61 (3)	3.282 (4)	137 (3)
O3—H3A···O1 ^{iv}	0.86 (2)	2.34 (2)	3.063 (3)	142 (3)

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

Article retracted

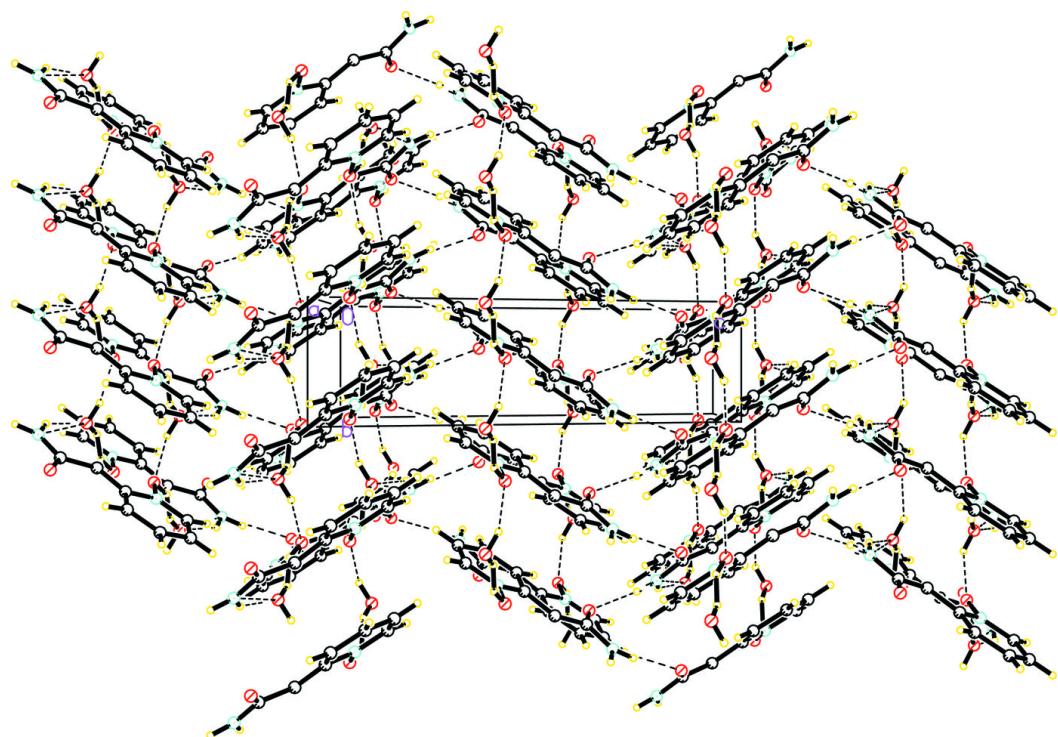
supplementary materials

Fig. 1



Ari

Fig. 2



Article re-