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Retraction of articles

This article reports the retraction of 39 articles published in *Acta Crystallographica Section E* between 2004 and 2009.

After thorough investigation (see Harrison *et al.*, 2010), 39 additional articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	Retracted by	DOI	Refcode
trans-Bis{1-[3-(cyclohexylamino)propyliminomethyl]-2-naphtholato}copper(II) dichloride dihydrate	Zhang (2004)	Journal	10.1107/S1600536804028296	BIPDUA
Bis(4-bromo-2-formylphenolato-κ^2O,O')copper(II)	Sun & Gao (2005)	Author	10.1107/S160053680500187X	FEYSUY
Bis(salicylaldehydo)zinc(II)	Xiong & Liu (2005)	Journal	10.1107/S1600536805010913	GAMDUU
Bis(4-bromo-2-formylphenolato-κ^2O,O')zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
Bis(2-formylphenolato-κ^2O,O')nickel(II)	Li & Chen (2006)	Journal	10.1107/S1600536806012931	IDAZAP
Bis(2-formylphenolato)cobalt(II)	Qiu (2006)	Journal	10.1107/S1600536806015704	GEJDUV
Bis(2-formylphenolato-κ^2O,O')manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraaqua(1,10-phenanthroline-κ^2N,N')copper(II) naphthalene-1,5-disulfonate dihydrate	Liu *et al.* (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraaqua(1,10-phenanthroline-κ^2N,N')nickel(II) naphthalene-1,5-disulfonate dihydrate	Liu & Fan (2006)	Author	10.1107/S1600536806035410	KERBEP
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratolutetium(III)copper(II)	Sui *et al.* (2006)	Journal	10.1107/S160053680604565X	HESPEP
Bis(2-formylphenolato-κ^2O,O')iron(II)	Yang *et al.* (2007)	Author	10.1107/S1600536807021721	PIFCAJ
2,6-Dimethoxybenzohydrazide	Qadeer *et al.* (2007*a*)	Journal	10.1107/S1600536807022593	PIFHES
2-(2,4-Dichlorophenylsulfanyl)acetohydrazide	Qadeer *et al.* (2007*b*)	Journal	10.1107/S1600536807022891	YIFSOW
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoeuropium(III)zinc(II)	Hu *et al.* (2007)	Author	10.1107/S1600536807031121	WIHKEE
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratocerium(III)zinc(II)	Sui, Zhang, Hu & Yin (2007)	Author	10.1107/S1600536807032564	WIHREL
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)zinc(II)	Chen *et al.* (2007)	Author	10.1107/S1600536807032540	WIHRIP
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)nickel(II)	Sui, Li *et al.* (2007)	Author	10.1107/S1600536807032618	UFACUA
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(methanol-1κO)-μ-nitrato-1:2κ^2O:O′-dinitrato-1κ^4O,O'-cerium(III)zinc(II)	Sui, Fang, Hu & Lin (2007)	Author	10.1107/S1600536807033314	UDUYIC
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratosamarium(III)nickel(II)	Sui, Zhang, Hu & Jiang (2007)	Author	10.1107/S1600536807037130	AFECEU
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratopraseodymium(III)zinc(II)	Sui, Fang & Yuan (2007)	Author	10.1107/S1600536807037488	AFICEY
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratolutetium(III)zinc(II)	Sui, Sui *et al.* (2007)	Author	10.1107/S1600536807037737	AFEFOH
catena-Poly[[chloridonickel(II)]-di-μ-chlorido-[chloridonickel(II)]-μ-4,4′-methylenebis(3,5-dimethylpyrazole)-κ^2N^2:$N^{2'}$]	Huang & Chen (2007)	Author	10.1107/S1600536807039384	VIJYOD
{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}zinc(II)	Liu *et al.* (2007*a*)	Author	10.1107/S1600536807040640	DIKYUS
trans-Bis(ethylenediamine-κ^2N,N')bis(nitrato-κO)zinc(II)	Liu, Zeng & Chen (2007)	Author	10.1107/S1600536807042390	XIKYEW
[N,N′-(o-Phenylene)bis(picolinamido)-κ^4N,N',N'',N''']cobalt(II)	Liu & Zeng (2007*a*)	Author	10.1107/S1600536807044571	XILFII
[N,N′-(o-Phenylene)dipicolinamide-κ^4N]nickel(II)	Liu & Zeng (2007*b*)	Author	10.1107/S1600536807048386	WINWEW
{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}manganese(II)	Liu *et al.* (2007*b*)	Author	10.1107/S1600536807052993	VIQPIV
N-(2-Amino-3-pyridyl)urea monohydrate	Li *et al.* (2007)	Author	10.1107/S1600536807047526	SIMFEA
N-(2-Fluorophenyl)carbamic acid monohydrate	Yang (2007)	Author	10.1107/S1600536807052464	WINMOW
Aqua(dimethylglyoxime-κ^2N,N')(3,5-dinitro-2-oxidobenzoato-κ^2O^1,O^2)-copper(II)	Liu & Wen (2007)	Author	10.1107/S1600536807054244	HIQCAM
μ-Acetato-tri-μ-ferrocenecarboxylatobis[(N,N-dimethylformamide)-copper(II)]	Liu, Lin *et al.* (2007)	Journal	10.1107/S1600536807059041	HIQQEE

 doi:10.1107/S1600536809054300

Table 1 (continued)

Title	Reference	Retracted by	DOI	Refcode
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoeuropium(III)zinc(II)	Hu *et al.* (2008)	Author	10.1107/S160053680706151X	MIRPAF
Bis(4-chloro-2-formylphenolato)nickel(II)	Li *et al.* (2008)	Author	10.1107/S1600536807056309	RISTET
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoterbium(III)zinc(II)	Chen *et al.* (2008)	Author	10.1107/S1600536808006958	QIXHIP
Bis(2-ethoxy-6-formylphenolato-κ^2O^1,O^6)nickel(II)	Han (2008)	Journal	10.1107/S160053680800809X	QIXLIT
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoholmium(III)zinc(II)	Xiao, Sui *et al.* (2008)	Author	10.1107/S1600536808013743	BIZTUA
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoholmium(III)nickel(II)	Xiao, Fu *et al.* (2008)	Author	10.1107/S1600536808013755	BIZVAI
Hydrogen-bonding patterns in the cocrystal terephthalic acid–4,4′-bipyridine (2/1)	Wang *et al.* (2009)	Journal	10.1107/S160053680903236X	DUCZEH
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(ethanol-1κO)-μ-nitrato-1:2κ^2O:O′-dinitrato-1κ^4O,O′-samarium(III)zinc(II)	Huang *et al.* (2009)	Journal	10.1107/S1600536809033558	YUCWAV

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N-(2-Amino-3-pyridyl)urea monohydrate

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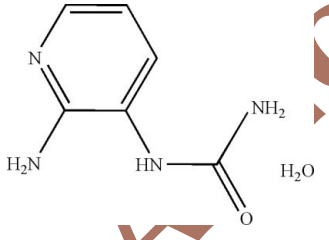
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.006 Å; H-atom completeness 91%; R factor = 0.058; wR factor = 0.177; data-to-parameter ratio = 11.9.

In the crystal structure of the title compound, $C_6H_9N_4O\cdot H_2O$, intermolecular O—H···N and N—H···O hydrogen bonds result in the formation of a supramolecular network structure; intramolecular O—H···N hydrogen bonds are also present.

Related literature

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



Experimental

Crystal data

$C_6H_9N_4O\cdot H_2O$
M_r = 171.19
Monoclinic, $P2_1/n$
a = 12.8769 (14) Å
b = 4.002 (2) Å
c = 15.4412 (17) Å
β = 114.084 (3)°
V = 726.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 273 (2) K
0.64 × 0.13 × 0.09 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.927, T_{max} = 0.989
4336 measured reflections
1400 independent reflections
871 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.178
S = 1.07
1400 reflections
118 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H5B···N2	0.85 (4)	1.85 (2)	2.674 (5)	160 (4)
O2—H5B···N1	0.85 (4)	2.78 (3)	3.439 (6)	135 (3)
N2—H2A···O2^{i}	0.86	2.39	3.248 (4)	174
N3—H3A···O2^{i}	0.86	2.15	2.941 (4)	153
N4—H4A···O1^{ii}	0.86	2.06	2.920 (4)	179
N4—H4B···O2^{i}	0.86	2.05	2.860 (5)	156
O2—H5A···N2^{iii}	0.848 (19)	2.26 (3)	3.018 (4)	149 (4)
O2—H5A···N2^{iv}	0.848 (19)	2.68 (5)	3.242 (5)	125 (5)

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2332).

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supplementary materials

Acta Cryst. (2007). E**63**, o4228 [**doi:10.1107/S1600536807047526**]

N-(2-Amino-3-pyridyl)urea monohydrate

N.-G. Li, R.-M. Tao and B.-F. Fu

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 *N*-(1-amino-2-pyridyl)-carbamide ligand. Unfortunately, we obtained only the title compound, (I), and 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 *N*-(2-amino-3-pyridyl)urea molecule and one H_2O molecule.

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

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), *N*-(1-amino-2-pyridyl)carbamide (163.2 mg, 1 mmol) and distilled water (5 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 colorless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

Refinement

H5A and H5B (for H_2O) were located in difference syntheses and refined isotropically [O—H = 0.894 (18) and 0.855 (18) Å, U_{iso}(H) = 0.107 (18) and 0.085 (12) Å^2]. The remaining H atoms were positioned geometrically, with N—H = 0.86 Å (for NH and NH_2) and C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,*N*).

Figures

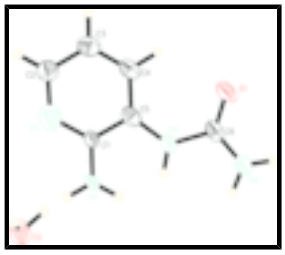

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

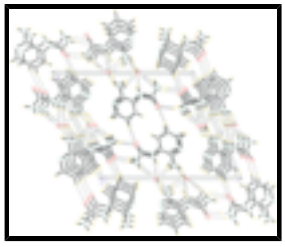

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

N-(2-Amino-3-pyridyl)urea monohydrate

Crystal data

$C_6H_9N_4O\cdot H_2O$	F_{000} = 364
M_r = 171.19	D_x = 1.565 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 1898 reflections
a = 12.8769 (14) Å	θ = 2.6–27.9°
b = 4.002 (2) Å	μ = 0.12 mm^{-1}
c = 15.4412 (17) Å	T = 273 (2) K
β = 114.084 (3)°	Prism, colorless
V = 726.4 (4) Å^3	0.64 × 0.13 × 0.09 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	1400 independent reflections
Radiation source: fine-focus sealed tube	871 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.053
T = 273(2) K	θ_{max} = 26.0°
φ and ω scans	θ_{min} = 2.9°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −15→15
T_{min} = 0.927, T_{max} = 0.989	k = −4→4
4336 measured reflections	l = −19→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.058$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.178$	$w = 1/[\sigma^2(F_o^2) + (0.1781P)^2 + 0.01P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
1400 reflections	$\Delta\rho_{max} = 0.53$ e Å^{-3}
118 parameters	$\Delta\rho_{min} = -0.44$ e Å^{-3}
3 restraints	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.10 (4)

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.8205 (2)	1.1190 (8)	−0.13722 (18)	0.0666 (10)
O2	0.5041 (3)	0.5300 (9)	0.1084 (2)	0.0721 (10)
C1	0.7325 (3)	0.8489 (8)	0.0830 (2)	0.0412 (9)
N2	0.6334 (2)	0.9690 (8)	0.0666 (2)	0.0584 (10)
H2A	0.5989	1.0920	0.0175	0.070*
H2B	0.6016	0.9260	0.1047	0.070*
N3	0.7135 (3)	1.1140 (8)	−0.0520 (2)	0.0520 (9)
H3A	0.6512	1.1879	−0.0512	0.062*
N4	0.6563 (3)	1.3945 (9)	−0.1916 (2)	0.0644 (11)
H4A	0.6634	1.4634	−0.2417	0.077*
H4B	0.5972	1.4486	−0.1820	0.077*
N1	0.7876 (4)	0.6668 (11)	0.1628 (3)	0.0887 (14)
C2	0.8910 (3)	0.5406 (11)	0.1824 (3)	0.0642 (11)
H2	0.9287	0.4131	0.2366	0.077*
C3	0.9400 (3)	0.6060 (10)	0.1192 (3)	0.0626 (12)

H3	1.0118	0.5217	0.1310	0.075*
C4	0.8848 (3)	0.7896 (10)	0.0414 (3)	0.0571 (11)
H4	0.9186	0.8293	−0.0006	0.069*
C5	0.7800 (3)	0.9194 (9)	0.0226 (3)	0.0506 (10)
C6	0.7367 (3)	1.2042 (10)	−0.1291 (2)	0.0515 (10)
H5A	0.515 (4)	0.341 (6)	0.089 (4)	0.07 (2)*
H5B	0.552 (3)	0.629 (8)	0.092 (3)	0.053 (11)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0620 (17)	0.091 (2)	0.0634 (18)	−0.0063 (14)	0.0423 (15)	−0.0087 (14)
O2	0.084 (2)	0.075 (2)	0.075 (2)	0.0057 (17)	0.0501 (17)	0.0045 (17)
C1	0.0478 (18)	0.0396 (18)	0.0463 (17)	0.0045 (13)	0.0294 (15)	0.0072 (14)
N2	0.0616 (18)	0.065 (2)	0.074 (2)	0.0238 (15)	0.0526 (16)	0.0318 (16)
N3	0.0535 (17)	0.059 (2)	0.0526 (18)	−0.0043 (14)	0.0314 (15)	0.0008 (14)
N4	0.068 (2)	0.079 (2)	0.058 (2)	−0.0069 (18)	0.0375 (18)	0.0049 (17)
N1	0.109 (3)	0.082 (3)	0.089 (3)	0.004 (2)	0.055 (3)	0.004 (2)
C2	0.065 (2)	0.063 (3)	0.066 (2)	0.005 (2)	0.028 (2)	0.003 (2)
C3	0.052 (2)	0.067 (3)	0.068 (3)	−0.0031 (18)	0.024 (2)	−0.007 (2)
C4	0.051 (2)	0.063 (2)	0.068 (2)	−0.0097 (17)	0.0342 (19)	−0.006 (2)
C5	0.056 (2)	0.049 (2)	0.055 (2)	−0.0137 (16)	0.0305 (17)	−0.0113 (17)
C6	0.055 (2)	0.060 (2)	0.0471 (19)	−0.0189 (17)	0.0289 (17)	−0.0116 (17)

Geometric parameters (Å, °)

O1—C6	1.187 (4)	N4—C6	1.330 (5)
O2—H5A	0.848 (19)	N4—H4A	0.8600
O2—H5B	0.85 (4)	N4—H4B	0.8600
C1—N2	1.288 (4)	N1—C2	1.338 (6)
C1—C5	1.337 (4)	C2—C3	1.386 (6)
C1—N1	1.356 (5)	C2—H2	0.9300
N2—H2A	0.8600	C3—C4	1.339 (6)
N2—H2B	0.8600	C3—H3	0.9300
N3—C5	1.364 (5)	C4—C5	1.363 (5)
N3—C6	1.387 (4)	C4—H4	0.9300
N3—H3A	0.8600		
H5A—O2—H5B	94 (2)	N1—C2—H2	121.1
N2—C1—C5	118.8 (3)	C3—C2—H2	121.1
N2—C1—N1	119.2 (3)	C4—C3—C2	120.6 (4)
C5—C1—N1	121.9 (3)	C4—C3—H3	119.7
C1—N2—H2A	120.0	C2—C3—H3	119.7
C1—N2—H2B	120.0	C3—C4—C5	121.1 (4)
H2A—N2—H2B	120.0	C3—C4—H4	119.4
C5—N3—C6	126.4 (3)	C5—C4—H4	119.4
C5—N3—H3A	116.8	C1—C5—C4	117.8 (4)
C6—N3—H3A	116.8	C1—C5—N3	113.7 (3)
C6—N4—H4A	120.0	C4—C5—N3	128.5 (3)

C6—N4—H4B	120.0	O1—C6—N4	124.0 (3)
H4A—N4—H4B	120.0	O1—C6—N3	122.6 (4)
C2—N1—C1	120.7 (4)	N4—C6—N3	113.3 (3)
N1—C2—C3	117.8 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H5B···N2	0.85 (4)	1.85 (2)	2.674 (5)	160 (4)
O2—H5B···N1	0.85 (4)	2.78 (3)	3.439 (6)	135 (3)
N2—H2A···O2^{i}	0.86	2.39	3.248 (4)	174
N3—H3A···O2^{i}	0.86	2.15	2.941 (4)	153
N4—H4A···O1^{ii}	0.86	2.06	2.920 (4)	179
N4—H4B···O2^{i}	0.86	2.05	2.860 (5)	156
O2—H5A···N2^{iii}	0.848 (19)	2.26 (3)	3.018 (4)	149 (4)
O2—H5A···N2^{iv}	0.848 (19)	2.68 (5)	3.242 (5)	125 (5)

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

Fig. 1

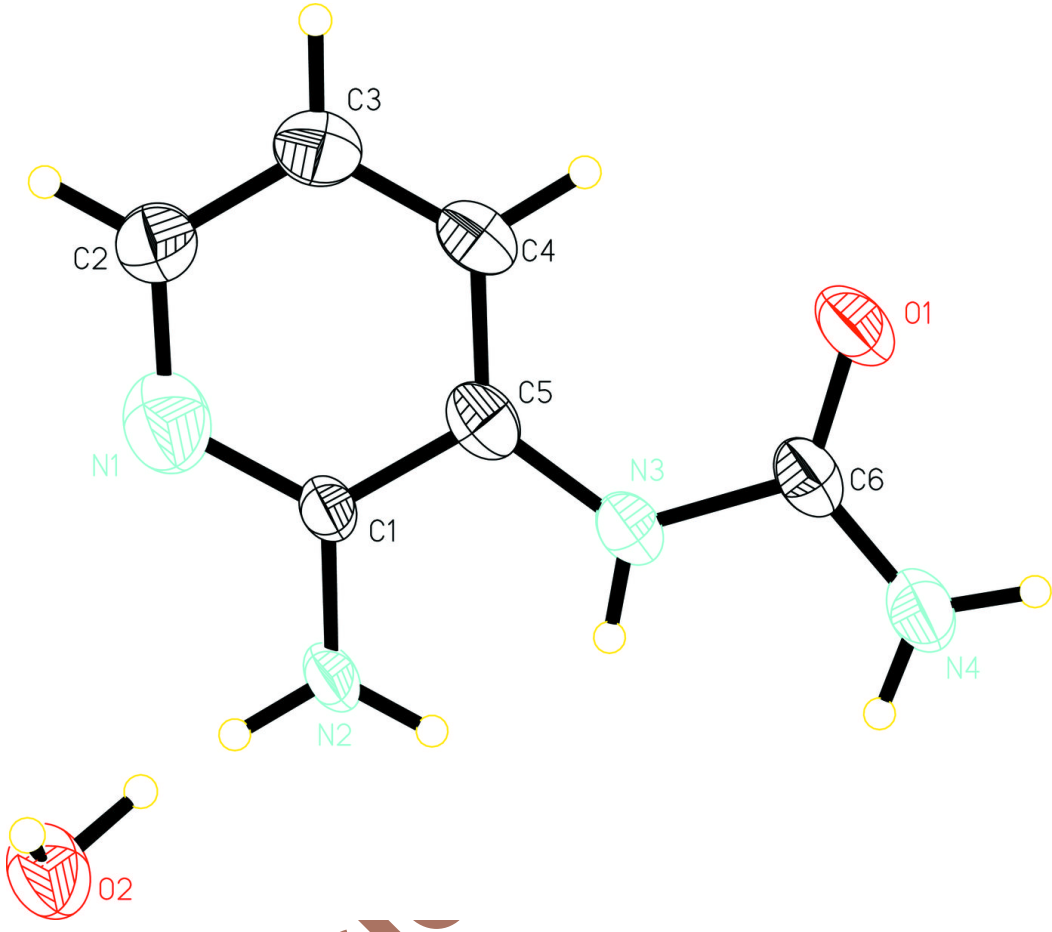

Fig. 2