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

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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
Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)	Liu & Xie (2007*a*)	10.1107/S1600536807026852	EDUMAS
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*b*)	10.1107/S1600536807028255	EDUVAB
Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)	Liu & Xie (2007*b*)	10.1107/S1600536807028735	RIGQAA
Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]	Liu, Wang, Wang & Xie (2007*c*)	10.1107/S1600536807030917	UDUMIQ
Polymeric $KNOF_2$	Liu Wang, Wang & Xie (2007*a*)	10.1107/S1600536807027195	ICSD 240891
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')cobalt(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*d*)	10.1107/S1600536807031224	WIHJED
Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]	Liu, Wang, Wang & Xie (2007*e*)	10.1107/S1600536807032679	WIHQEK
Tetrakis[μ-(2-pyridyloxy)acetato-$\kappa^2O:O'$]bis{(1,10-phenanthroline-κ^2N,N')-[(2-pyridyloxy)acetato-κO]neodymium(III)}	Liu, Wang, Wang & Xie (2007*f*)	10.1107/S1600536807035349	TIGDAP
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')manganese(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*g*)	10.1107/S1600536807035076	TIGDET
2-Amino-3,5-dinitrobenzoic acid–ammonia (1/1)	Liu & Zhu (2007*j*)	10.1107/S1600536807040068	KIKQAX
2-Hydroxy-3,5-dinitrobenzamide monohydrate	Liu & Zhu (2007*k*)	10.1107/S1600536807039712	KIKQEB
2-(1-Hydroxy-2-pyridyl)acetamide monohydrate	Liu & Zhu (2007*l*)	10.1107/S1600536807040652	CIKQOD
Bis(2,2′-bipyridine-κN,N′)bis(thiocyanato-κN)iron(II)	Liu & Zhu (2007*a*)	10.1107/S1600536807043486	XIFXOA
catena-Poly[hexakis(μ_2-anilinoacetamide)bis(1,10-phenanthroline)disamarium(III]	Liu & Zhu (2007*b*)	10.1107/S1600536807045485	XILNAI
3-Hydroxy-2,4,6-trinitropyridine monohydrate	Liu & Zhu (2007*m*)	10.1107/S1600536807045230	PILNOO
catena-Poly[hexakis(μ_2-anilinoacetamide)bis(1,10-phenanthroline)-dipraseodymium(III)]	Liu & Zhu (2007*c*)	10.1107/S1600536807047733	SILZET
catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10-phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]	Liu & Zhu (2007*d*)	10.1107/S1600536807050969	GIMZOS
Tetrakis(pyridine-κN)bis(thiocyanato-κN)chromium(II)	Liu & Zhu (2007*e*)	10.1107/S1600536807051756	WINFAB
2-Ammonio-3-carboxy-5-nitrobenzoate monohydrate	Liu & Zhu (2007*n*)	10.1107/S1600536807048477	GINFEP
2-(Benzoylhydrazinocarbonyl)benzoic acid	Liu & Zhu (2007*o*)	10.1107/S160053680705204X	TINZIA
Tetrakis(pyridine-κN)bis(thiocyanato-κN)vanadium(II)	Liu & Zhu (2007*f*)	10.1107/S1600536807054529	HIPZIQ
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')nickel(II)]-μ-acetamido-$\kappa^2O:N$]	Liu & Zhu (2007*g*)	10.1107/S1600536807056504	XIRGIP
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-acetamido-$\kappa^2O:N$]	Liu & Zhu (2007*h*)	10.1107/S1600536807059077	HIQROP
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-acetamidato-$\kappa^2O:N$]	Liu & Zhu (2007*i*)	10.1107/S1600536807060631	YIQMER
N′-Benzoyl-4-nitronicotinohydrazide	Liu & Zhu (2007*p*)	10.1107/S1600536807053068	CIPVON
N′-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide	Liu & Zhu (2007*q*)	10.1107/S1600536807054876	RIRWEV

 doi:10.1107/S1600536809049976

Table 1 (continued)

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

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3-Hydroxy-2,4,6-trinitropyridine monohydrate

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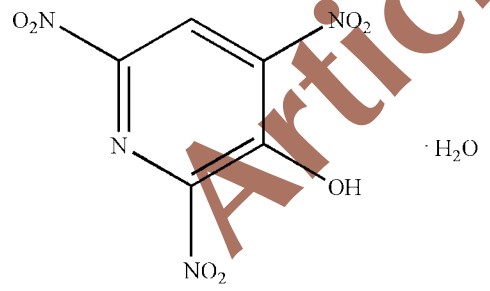
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.056; wR factor = 0.192; data-to-parameter ratio = 11.3.

In the crystal structure of the title compound, $C_5H_2N_4O_7\cdot H_2O$, intermolecular O—H···O hydrogen bonds result in the formation of a supramolecular network structure; intramolecular O—H···O and O—H···N hydrogen bonds are also present.

Related literature

For general background, see: Carter *et al.* (1998); Lowe *et al.* (1999); Pai *et al.* (2000); Swarnabala & Rajasekharan (1998); Zhao *et al.* (2005). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_5H_2N_4O_7\cdot H_2O$
M_r = 248.12
Monoclinic, $C2/c$
a = 25.103 (2) Å
b = 6.4103 (17) Å
c = 12.2307 (11) Å
β = 111.897 (4)°
V = 1826.1 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 273 (2) K
0.24 × 0.15 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.959, T_{max} = 0.975
5964 measured reflections
1841 independent reflections
955 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.192
S = 1.02
1841 reflections
163 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O6	0.82	1.80	2.533 (3)	148
O1—H1···N4	0.82	2.32	2.800 (4)	118
O8—H8B···O3	0.85 (3)	2.024 (19)	2.816 (4)	155 (4)
O1—H1···O6^{i}	0.82	2.23	2.857 (4)	134
O8—H8A···O1^{ii}	0.85 (3)	2.134 (17)	2.934 (4)	157 (4)
O8—H8A···O2^{ii}	0.85 (3)	2.57 (3)	3.242 (4)	137 (4)

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

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: HK2325).

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supplementary materials

Acta Cryst. (2007). E**63**, o4112 [**doi:10.1107/S1600536807045230**]

3-Hydroxy-2,4,6-trinitropyridine monohydrate

T. Liu and J. Y. Zhu

Comment

Due to pyridyl groups are one of the most important classes of biological ligands, the coordination of metal–pyridyl groups complexes are of critical importance in biological systems, organic materials and coordination chemistry. Recently, pyridyl groups with variable coordination modes have been used to construct metal–organic supramolecular structures (Carter *et al.*, 1998; Lowe *et al.*, 1999; Pai *et al.*, 2000; Swarnabala & Rajasekharan, 1998; Zhao *et al.*, 2005). We originally attempted to synthesize complexes featuring Nd metal chains by reaction of the neodymium(III) ion with 3-hydroxy-2,4,6-trinitropyridine 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 $C_5H_2N_4O_7$ molecule and one H_2O molecule.

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

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb. Neodymium(III) nitrate hexahydrate (219.1 mg, 0.5 mmol), 3-hydroxy-2,4,6-trinitropyridine (230.2 mg, 1 mmol) and distilled water (8 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

H8A and H8B (for OH_2) were located were located in difference syntheses and refined isotropically [O—H = 0.85 (3) and 0.85 (3) Å, U_{iso}(H) = 0.092 (16) and 0.15 (2) Å^2]. 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.

Figures

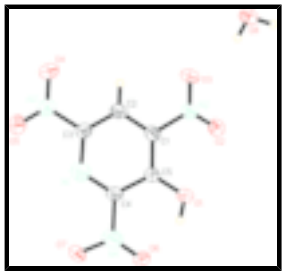

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

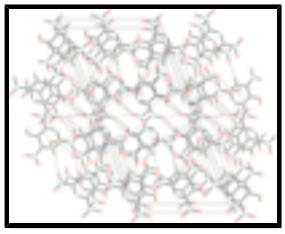

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

3-hydroxy-2,4,6-trinitropyridine monohydrate

Crystal data

$C_5H_2N_4O_7 \cdot H_2O$	F_{000} = 1008
M_r = 248.12	D_x = 1.805 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 1493 reflections
a = 25.103 (2) Å	θ = 2.8–26.8°
b = 6.4103 (17) Å	μ = 0.18 mm^{-1}
c = 12.2307 (11) Å	*T* = 273 (2) K
β = 111.897 (4)°	Prism, colourless
V = 1826.1 (5) Å^3	0.24 × 0.15 × 0.14 mm
Z = 8	

Data collection

Bruker SMART CCD area-detector diffractometer	1841 independent reflections
Radiation source: fine-focus sealed tube	955 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 273(2) K	θ_{max} = 26.6°
φ and ω scans	θ_{min} = 3.6°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −31→31
T_{min} = 0.959, T_{max} = 0.975	*k* = −7→8
5964 measured reflections	*l* = −15→15

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.056$

$wR(F^2) = 0.192$

$S = 1.03$

1841 reflections

163 parameters

3 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

$w = 1/[\sigma^2(F_o^2) + (0.1224P)^2 + 0.3617P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.56$ e Å^{-3}

$\Delta\rho_{min} = -0.45$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$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}
O1	0.40218 (10)	0.2101 (5)	0.7293 (2)	0.0667 (8)
H1	0.4369	0.2174	0.7461	0.100*
O2	0.29261 (11)	0.1309 (5)	0.6307 (2)	0.0726 (8)
O3	0.24198 (10)	0.3054 (5)	0.7038 (2)	0.0707 (8)
O4	0.30592 (11)	0.3719 (5)	1.1123 (2)	0.0767 (8)
O5	0.39222 (13)	0.3006 (5)	1.2180 (2)	0.0890 (10)
O6	0.50769 (12)	0.2168 (6)	0.8601 (2)	0.0954 (12)
O7	0.53307 (10)	0.2528 (4)	1.0474 (2)	0.0630 (7)
O8	0.13152 (11)	0.2710 (4)	0.5274 (3)	0.0665 (8)
H8A	0.1318 (19)	0.287 (7)	0.4587 (15)	0.092 (16)*
H8B	0.1671 (6)	0.297 (10)	0.563 (3)	0.15 (2)*
N1	0.42327 (15)	0.2687 (5)	1.0332 (3)	0.0692 (9)
N2	0.28669 (12)	0.2259 (5)	0.7093 (2)	0.0563 (8)
N3	0.35432 (14)	0.3203 (5)	1.1253 (3)	0.0598 (8)
N4	0.49590 (14)	0.2382 (6)	0.9437 (3)	0.0779 (10)
C1	0.33555 (14)	0.2442 (5)	0.8198 (3)	0.0481 (8)

C2	0.32265 (14)	0.2744 (5)	0.9165 (3)	0.0480 (8)
H2	0.2848	0.2878	0.9109	0.058*
C3	0.36664 (14)	0.2841 (5)	1.0210 (3)	0.0492 (8)
C4	0.43536 (13)	0.2449 (5)	0.9352 (3)	0.0489 (8)
C5	0.39105 (14)	0.2309 (5)	0.8244 (3)	0.0480 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0352 (13)	0.113 (2)	0.0514 (14)	−0.0003 (12)	0.0153 (11)	−0.0023 (12)
O2	0.0502 (15)	0.109 (2)	0.0540 (14)	−0.0057 (14)	0.0138 (12)	−0.0143 (14)
O3	0.0319 (13)	0.110 (2)	0.0648 (16)	0.0097 (12)	0.0122 (11)	0.0058 (13)
O4	0.0545 (17)	0.112 (2)	0.0726 (17)	0.0047 (15)	0.0344 (14)	−0.0079 (15)
O5	0.072 (2)	0.145 (3)	0.0465 (16)	0.0151 (17)	0.0180 (15)	−0.0027 (15)
O6	0.0408 (15)	0.202 (4)	0.0491 (16)	0.0026 (16)	0.0234 (13)	0.0010 (16)
O7	0.0355 (14)	0.0908 (19)	0.0513 (14)	−0.0015 (11)	0.0030 (11)	−0.0005 (11)
O8	0.0378 (14)	0.0893 (19)	0.0668 (18)	−0.0018 (12)	0.0131 (12)	−0.0036 (14)
N1	0.062 (2)	0.076 (2)	0.069 (2)	−0.0007 (15)	0.0238 (17)	0.0008 (15)
N2	0.0366 (16)	0.080 (2)	0.0485 (17)	−0.0058 (13)	0.0118 (13)	0.0061 (14)
N3	0.056 (2)	0.073 (2)	0.0537 (18)	−0.0009 (15)	0.0242 (16)	−0.0046 (13)
N4	0.052 (2)	0.098 (3)	0.077 (2)	−0.0010 (16)	0.016 (2)	0.0065 (17)
C1	0.0391 (18)	0.057 (2)	0.0431 (17)	−0.0001 (13)	0.0100 (14)	0.0041 (13)
C2	0.0362 (18)	0.0538 (19)	0.0544 (19)	0.0019 (13)	0.0173 (15)	0.0044 (13)
C3	0.0435 (19)	0.0597 (19)	0.0484 (18)	0.0023 (14)	0.0216 (15)	0.0011 (14)
C4	0.0344 (17)	0.064 (2)	0.0502 (19)	0.0004 (14)	0.0178 (15)	0.0016 (14)
C5	0.0371 (17)	0.065 (2)	0.0426 (17)	0.0012 (14)	0.0159 (14)	−0.0012 (13)

Geometric parameters (Å, °)

O1—C5	1.300 (4)	N1—C4	1.350 (5)
O1—H1	0.8200	N1—C3	1.377 (5)
O2—N2	1.193 (4)	N2—C1	1.453 (4)
O3—N2	1.212 (4)	N3—C3	1.440 (4)
O4—N3	1.211 (4)	N4—C4	1.485 (5)
O5—N3	1.184 (4)	C1—C2	1.351 (5)
O6—N4	1.174 (4)	C1—C5	1.376 (5)
O7—N4	1.268 (4)	C2—C3	1.343 (5)
O8—H8A	0.85 (3)	C2—H2	0.9300
O8—H8B	0.85 (3)	C4—C5	1.399 (5)
C5—O1—H1	109.5	C2—C1—N2	115.6 (3)
H8A—O8—H8B	95 (4)	C5—C1—N2	121.6 (3)
H8B—O8—H8A	95 (4)	C3—C2—C1	117.3 (3)
C4—N1—C3	118.5 (3)	C3—C2—H2	121.3
O2—N2—O3	124.2 (3)	C1—C2—H2	121.3
O2—N2—C1	118.4 (3)	C2—C3—N1	123.3 (3)
O3—N2—C1	117.4 (3)	C2—C3—N3	118.6 (3)
O5—N3—O4	124.4 (3)	N1—C3—N3	118.1 (3)
O5—N3—C3	118.0 (3)	N1—C4—C5	120.4 (3)

O4—N3—C3	117.6 (3)	N1—C4—N4	120.3 (3)
O6—N4—O7	123.4 (3)	C5—C4—N4	119.3 (3)
O6—N4—C4	121.8 (3)	O1—C5—C1	121.5 (3)
O7—N4—C4	114.8 (3)	O1—C5—C4	121.0 (3)
C2—C1—C5	122.9 (3)	C1—C5—C4	117.6 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O6	0.82	1.80	2.533 (3)	148
O1—H1···N4	0.82	2.32	2.800 (4)	118
O8—H8B···O3	0.85 (3)	2.024 (19)	2.816 (4)	155 (4)
O1—H1···O6^{i}	0.82	2.23	2.857 (4)	134
O8—H8A···O1^{ii}	0.85 (3)	2.134 (17)	2.934 (4)	157 (4)
O8—H8A···O2^{ii}	0.85 (3)	2.57 (3)	3.242 (4)	137 (4)

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

Fig. 1

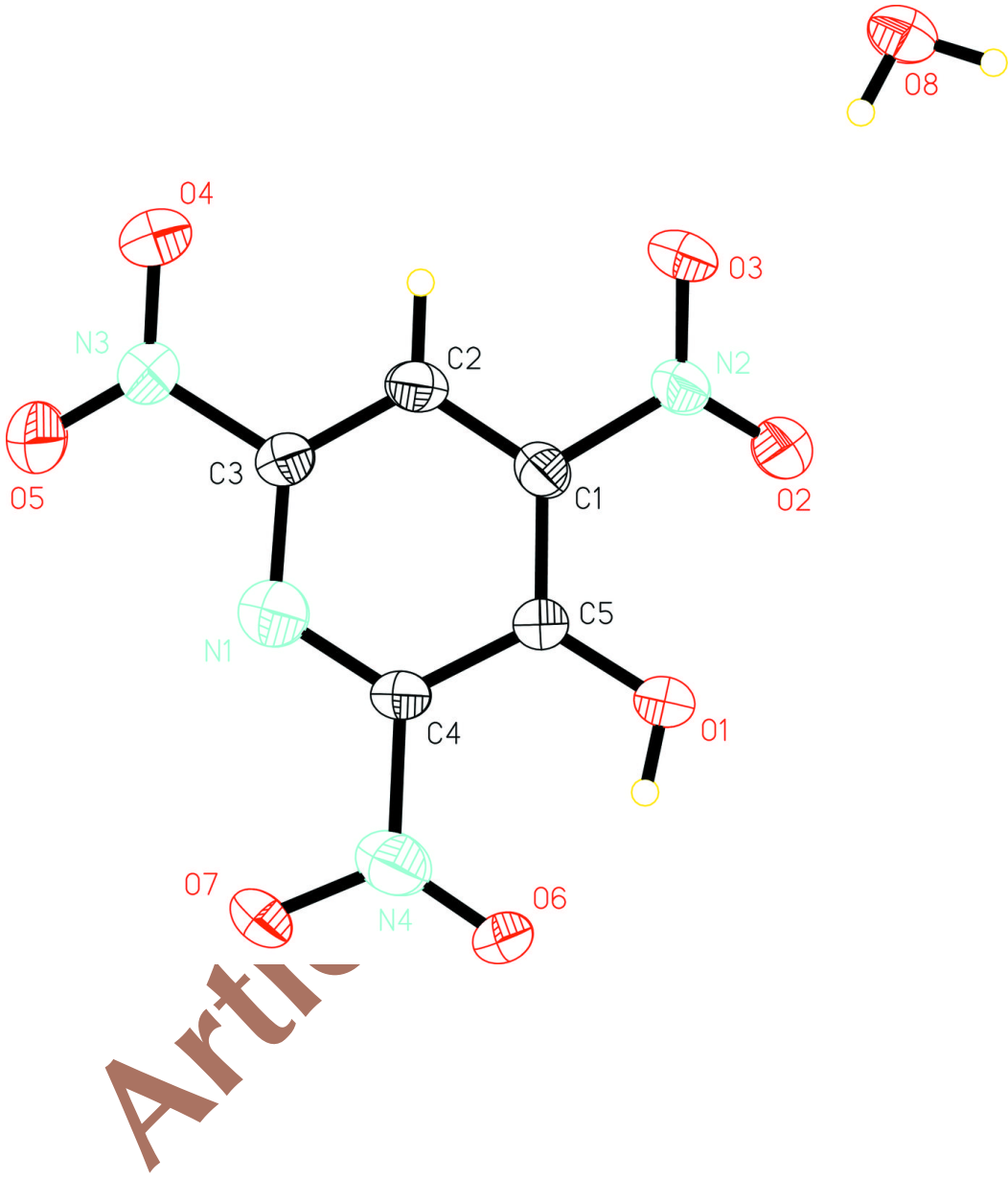

Fig. 2