

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

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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
<i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)</i>	Liu & Xie (2007a)	10.1107/S1600536807026852	EDUMAS
<i>(Dihydroxyglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')copper(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007b)	10.1107/S1600536807028255	EDUVAB
<i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)</i>	Liu & Xie (2007b)	10.1107/S1600536807028735	RIGQAA
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]</i>	Liu, Wang, Wang & Xie (2007c)	10.1107/S1600536807030917	UDUMIQ
<i>Polymeric KNOF₂</i>	Liu Wang, Wang & Xie (2007a)	10.1107/S1600536807027195	ICSD 240891
<i>(Dihydroxyglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')cobalt(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007d)	10.1107/S1600536807031224	WIHJED
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]</i>	Liu, Wang, Wang & Xie (2007e)	10.1107/S1600536807032679	WIHQEK
<i>Tetrakis[μ-(2-pyridyloxy)acetato-κ²O:O']bis[(1,10-phenanthroline-κ²N,N')-(2-pyridyloxy)acetato-κO]neodymium(III)]</i>	Liu, Wang, Wang & Xie (2007f)	10.1107/S1600536807035349	TIGDAP
<i>(Dihydroxyglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')manganese(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007g)	10.1107/S1600536807035076	TIGDET
<i>2-Amino-3,5-dinitrobenzoic acid-ammonia (1/1)</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(1,10-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(1,10-phenanthroline)-dipraseodymium(III)]</i>	Liu & Zhu (2007c)	10.1107/S1600536807047733	SILZET
<i>catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10-phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]</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[[nitrate-κO](1,10-phenanthroline-κ²N,N')nickel(II)]-μ-acetamido-κ²O:N]</i>	Liu & Zhu (2007g)	10.1107/S1600536807056504	XIRGIP
<i>catena-Poly[[nitrate-κO](1,10-phenanthroline-κ²N,N')copper(II)]-μ-acetamido-κ²O:N]</i>	Liu & Zhu (2007h)	10.1107/S1600536807059077	HIQROP
<i>catena-Poly[[nitrate-κO](1,10-phenanthroline-κ²N,N')cobalt(II)]-μ-acetamidato-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

Table 1 (continued)

Title	Reference	DOI	Refcode
<i>Ethylenediammonium sulfate</i>	Liu & Zhu (2007r)	10.1107/S1600536807056280	ETDAMS03
<i>Ethylenediammonium perchlorate</i>	Liu & Zhu (2007s)	10.1107/S1600536807059909	HIRYEN
<i>catena-Poly[[[nitrate-κO](1,10-phenanthroline-κ²N,N')manganese(II)]-μ-nitrate-κ²O:O']</i>	Liu & Zhu (2008)	10.1107/S160053680706254X	MIRROV

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2-Amino-3,5-dinitrobenzoic acid–
ammonia (1/1)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

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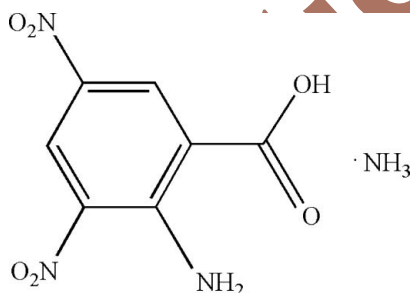
Received 9 August 2007; accepted 13 August 2007

Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.052; wR factor = 0.182; data-to-parameter ratio = 11.4.

The title complex, $\text{C}_7\text{H}_5\text{N}_3\text{O}_6 \cdot \text{NH}_3$, contains one 2-amino-3,5-dinitrobenzoic acid molecule and one ammonia molecule. In the crystal structure, intermolecular $\text{N}-\text{H} \cdots \text{N}$ and $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds result in the formation of a supramolecular network structure; intramolecular $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds are also present.

Related literature

For general background, see: Desiraju (1995, 1997); Braga *et al.* (1998); McCann *et al.* (1996, 1995); Wai *et al.* (1990); Yaghi *et al.* (1996); Min & Lee (2002); Maira *et al.* (2001). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 \cdot \text{NH}_3$
 $M_r = 244.17$
 Monoclinic, $C2/c$
 $a = 24.825$ (14) Å
 $b = 6.594$ (3) Å
 $c = 12.0862$ (16) Å
 $\beta = 111.262$ (5)°

$V = 1843.8$ (14) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.16$ mm⁻¹
 $T = 273$ (2) K
 $0.24 \times 0.15 \times 0.14$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.964$, $T_{\max} = 0.978$

6167 measured reflections
 1907 independent reflections
 979 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.182$
 $S = 1.00$
 1907 reflections
 168 parameters
 6 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.44$ e Å⁻³
 $\Delta\rho_{\min} = -0.25$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{N4}-\text{H4C} \cdots \text{O3}^i$	0.799 (16)	2.62 (3)	3.201 (4)	130 (3)
$\text{N4}-\text{H4C} \cdots \text{N3}^i$	0.799 (16)	2.141 (19)	2.910 (4)	161 (3)
$\text{N4}-\text{H4A} \cdots \text{O4}^{ii}$	0.778 (16)	2.048 (18)	2.822 (4)	173 (3)
$\text{N3}-\text{H3B} \cdots \text{O2}^i$	0.86	2.07	2.820 (4)	145
$\text{N3}-\text{H3A} \cdots \text{N4}^i$	0.86	2.23	2.910 (4)	135
$\text{N4}-\text{H4B} \cdots \text{O2}$	0.82 (4)	2.52 (4)	3.012 (4)	120 (3)
$\text{N4}-\text{H4B} \cdots \text{O1}$	0.82 (4)	1.737 (18)	2.554 (3)	175 (6)
$\text{N3}-\text{H3A} \cdots \text{O3}$	0.86	2.00	2.602 (3)	126
$\text{N3}-\text{H3B} \cdots \text{O2}$	0.86	1.84	2.501 (3)	133

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

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT (Siemens, 1996); 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: HK2309).

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supplementary materials

Article retracted

Acta Cryst. (2007). E63, o3829 [doi:10.1107/S1600536807040068]

2-Amino-3,5-dinitrobenzoic acid-ammonia (1/1)

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 carboxyl groups are one of the most important classes of biological ligands, the coordination of metal-carboxyl groups complexes are of critical importance in biological systems, organic materials and coordination chemistry. Recently, carboxyl groups with variable coordination modes have been used to construct metal-organic supramolecular structures (McCann *et al.*, 1996; McCann *et al.*, 1995; Wai *et al.*, 1990; Yaghi *et al.*, 1996; Min & Lee 2002; Maira *et al.*, 2001). We originally attempted to synthesize complexes featuring Nd metal chains by reaction of the neodymium(III) ion with 2-amino-3,5-dinitrobenzoic acid 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 (C₇H₅N₃O₆) molecule and one ammonia molecule.

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

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), 2-amino-3,5-dinitrobenzoic acid (227.2 mg, 1 mmol), ammonia (0.5 mol/l, 2 ml) and distilled water (6 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

H4A, H4B and H4C (for NH₃) were located in difference syntheses and refined isotropically [N—H = 0.778 (16)–0.82 (4) Å and $U_{\text{iso}}(\text{H}) = 0.069 (4)–0.083 (12) \text{ \AA}^2$]. The remaining H atoms were positioned geometrically, with O—H = 0.82 Å (for OH), N—H = 0.86 Å (for NH₂) and C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C}, \text{N}, \text{O})$, where $x = 1.5$ for OH H, and $x = 1.2$ for all other H atoms.

Figures

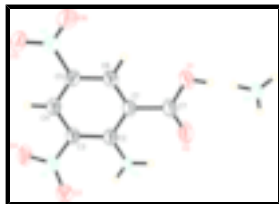


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

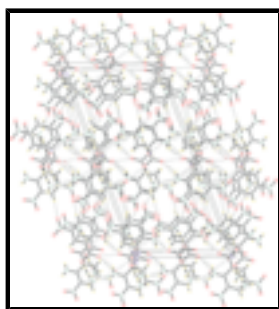


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

2-Amino-3,5-dinitrobenzoic acid–ammonia (1/1)

Crystal data

$C_7H_5N_3O_6 \cdot N_1H_3$

$M_r = 244.17$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 24.825\ (14)\ \text{\AA}$

$b = 6.594\ (3)\ \text{\AA}$

$c = 12.0862\ (16)\ \text{\AA}$

$\beta = 111.262\ (5)^\circ$

$V = 1843.8\ (14)\ \text{\AA}^3$

$Z = 8$

$F_{000} = 1008$

$D_x = 1.759\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

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

Cell parameters from 1487 reflections

$\theta = 3.0\text{--}26.8^\circ$

$\mu = 0.16\ \text{mm}^{-1}$

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

Prism, colorless

$0.24 \times 0.15 \times 0.14\ \text{mm}$

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

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

φ and ω scans

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

$T_{\min} = 0.964$, $T_{\max} = 0.978$

6167 measured reflections

1907 independent reflections

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

$R_{\text{int}} = 0.030$

$\theta_{\max} = 26.7^\circ$

$\theta_{\min} = 3.2^\circ$

$h = -31 \rightarrow 31$

$k = -8 \rightarrow 8$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.052$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.182$	$w = 1/[\sigma^2(F_o^2) + (0.1152P)^2 + 0.02P]$
$S = 1.00$	where $P = (F_o^2 + 2F_c^2)/3$
1907 reflections	$(\Delta/\sigma)_{\max} < 0.001$
168 parameters	$\Delta\rho_{\max} = 0.44 \text{ e } \text{\AA}^{-3}$
6 restraints	$\Delta\rho_{\min} = -0.25 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 1997), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.0065 (17)

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.53274 (9)	0.2533 (4)	1.04676 (19)	0.0731 (7)
H1	0.5650	0.2393	1.0435	0.110*
O2	0.50729 (11)	0.2169 (5)	0.8598 (2)	0.1064 (11)
O3	0.29271 (9)	0.1316 (4)	0.63188 (18)	0.0808 (8)
O4	0.24242 (9)	0.3056 (4)	0.7047 (2)	0.0792 (8)
O5	0.30605 (10)	0.3709 (4)	1.1124 (2)	0.0863 (8)
O6	0.39263 (12)	0.2999 (5)	1.2184 (2)	0.0986 (10)
N1	0.28701 (11)	0.2278 (4)	0.7102 (2)	0.0606 (7)
N2	0.35427 (12)	0.3209 (4)	1.1251 (2)	0.0662 (8)
N3	0.40261 (9)	0.2101 (4)	0.73014 (18)	0.0557 (7)
H3A	0.3750	0.2048	0.6620	0.067*
H3B	0.4379	0.2017	0.7348	0.067*
N4	0.63149 (11)	0.2285 (4)	1.0268 (2)	0.0568 (7)
C1	0.43521 (12)	0.2456 (4)	0.9345 (2)	0.0546 (8)
C2	0.39110 (13)	0.2306 (5)	0.8246 (3)	0.0571 (8)

supplementary materials

C3	0.33508 (12)	0.2443 (4)	0.8191 (3)	0.0536 (7)
C4	0.32277 (12)	0.2740 (4)	0.9167 (2)	0.0557 (8)
H4	0.2847	0.2875	0.9122	0.067*
C5	0.36697 (13)	0.2838 (4)	1.0218 (2)	0.0544 (7)
C6	0.42248 (13)	0.2684 (5)	1.0317 (3)	0.0561 (8)
H6	0.4519	0.2737	1.1060	0.067*
C7	0.49499 (13)	0.2388 (5)	0.9438 (3)	0.0631 (8)
H4A	0.6614 (9)	0.228 (5)	1.078 (2)	0.074 (11)*
H4C	0.6283 (13)	0.205 (5)	0.9598 (16)	0.083 (12)*
H4B	0.6006 (11)	0.242 (12)	1.036 (4)	0.069 (4)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0398 (13)	0.1105 (19)	0.0614 (14)	-0.0010 (12)	0.0094 (11)	-0.0005 (11)
O2	0.0449 (14)	0.216 (3)	0.0616 (15)	0.0038 (15)	0.0227 (12)	0.0008 (15)
O3	0.0561 (14)	0.122 (2)	0.0605 (13)	-0.0053 (13)	0.0163 (11)	-0.0104 (13)
O4	0.0376 (13)	0.126 (2)	0.0702 (15)	0.0098 (12)	0.0144 (11)	0.0057 (13)
O5	0.0611 (16)	0.128 (2)	0.0805 (15)	0.0064 (13)	0.0389 (13)	-0.0095 (14)
O6	0.078 (2)	0.164 (3)	0.0521 (14)	0.0105 (16)	0.0222 (14)	-0.0059 (14)
N1	0.0416 (15)	0.0910 (19)	0.0474 (14)	-0.0014 (12)	0.0141 (11)	0.0051 (12)
N2	0.0572 (18)	0.085 (2)	0.0593 (16)	0.0009 (14)	0.0248 (15)	-0.0027 (13)
N3	0.0239 (11)	0.111 (2)	0.0325 (11)	0.0005 (10)	0.0105 (9)	-0.0036 (11)
N4	0.0288 (13)	0.0847 (19)	0.0506 (16)	0.0018 (12)	0.0068 (12)	0.0018 (13)
C1	0.0385 (16)	0.073 (2)	0.0517 (17)	-0.0004 (13)	0.0160 (14)	0.0004 (13)
C2	0.0434 (16)	0.075 (2)	0.0527 (17)	0.0018 (13)	0.0172 (14)	0.0010 (13)
C3	0.0401 (16)	0.0689 (19)	0.0501 (16)	-0.0014 (12)	0.0145 (13)	0.0037 (13)
C4	0.0444 (17)	0.0661 (19)	0.0570 (18)	0.0023 (12)	0.0189 (15)	0.0048 (13)
C5	0.0502 (17)	0.0672 (19)	0.0493 (16)	0.0027 (13)	0.0223 (14)	0.0016 (12)
C6	0.0426 (16)	0.072 (2)	0.0509 (16)	-0.0012 (13)	0.0137 (13)	-0.0012 (13)
C7	0.0405 (17)	0.093 (2)	0.0538 (18)	-0.0022 (14)	0.0150 (15)	0.0039 (14)

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

O1—C7	1.261 (3)	N4—H4C	0.799 (16)
O1—H1	0.8200	N4—H4B	0.82 (4)
O2—C7	1.171 (4)	N4—H4A	0.778 (16)
O3—N1	1.190 (3)	C1—C6	1.331 (4)
O4—N1	1.200 (3)	C1—C2	1.385 (4)
O5—N2	1.197 (3)	C1—C7	1.447 (4)
O6—N2	1.191 (3)	C2—C3	1.371 (4)
N1—C3	1.424 (4)	C3—C4	1.336 (4)
N2—C5	1.415 (4)	C4—C5	1.346 (4)
N3—C2	1.281 (4)	C4—H4	0.9300
N3—H3A	0.8600	C5—C6	1.343 (4)
N3—H3B	0.8600	C6—H6	0.9300
C7—O1—H1	109.5	C2—C1—C7	120.3 (3)
O3—N1—O4	123.9 (3)	N3—C2—C3	120.9 (3)

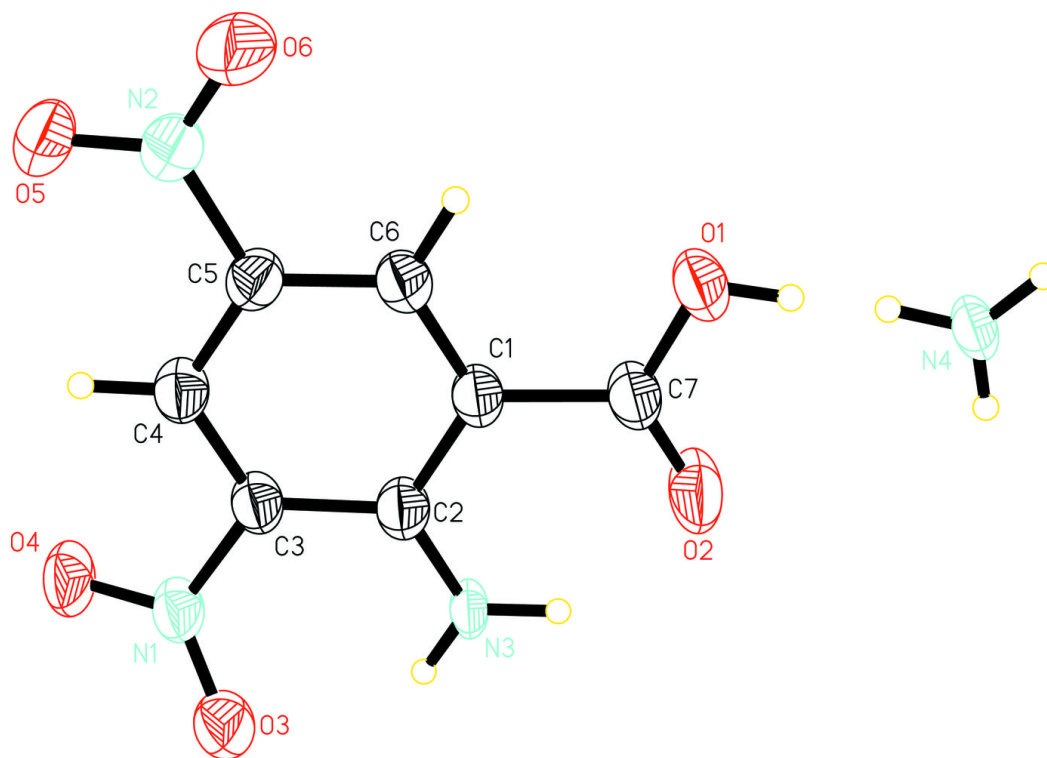
O3—N1—C3	118.3 (3)	N3—C2—C1	120.5 (3)
O4—N1—C3	117.8 (3)	C3—C2—C1	118.5 (3)
O6—N2—O5	124.9 (3)	C4—C3—C2	121.3 (3)
O6—N2—C5	117.3 (3)	C4—C3—N1	116.3 (3)
O5—N2—C5	117.8 (3)	C2—C3—N1	122.4 (3)
C2—N3—H3A	120.0	C3—C4—C5	118.1 (3)
C2—N3—H3B	120.0	C3—C4—H4	120.9
H3A—N3—H3B	120.0	C5—C4—H4	120.9
H4C—N4—H4B	114 (3)	C6—C5—C4	122.6 (3)
H4C—N4—H4A	122 (3)	C6—C5—N2	119.0 (3)
H4B—N4—H4A	124 (3)	C4—C5—N2	118.3 (3)
H4B—N4—H4C	114 (3)	C1—C6—C5	119.6 (3)
H4A—N4—H4C	122 (3)	C1—C6—H6	120.2
H4C—N4—H4B	114 (3)	C5—C6—H6	120.2
H4A—N4—H4B	124 (3)	O2—C7—O1	122.1 (3)
H4C—N4—H4B	114 (3)	O2—C7—C1	121.2 (3)
C6—C1—C2	119.7 (3)	O1—C7—C1	116.7 (3)
C6—C1—C7	120.0 (3)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N4—H4C...O3 ⁱ	0.799 (16)	2.62 (3)	3.201 (4)	130 (3)
N4—H4C...N3 ⁱ	0.799 (16)	2.141 (19)	2.910 (4)	161 (3)
N4—H4A...O4 ⁱⁱ	0.778 (16)	2.048 (18)	2.822 (4)	173 (3)
N3—H3B...O2 ⁱ	0.86	2.07	2.820 (4)	145
N3—H3A...N4 ⁱ	0.86	2.23	2.910 (4)	135
N4—H4B...O2	0.82 (4)	2.52 (4)	3.012 (4)	120 (3)
N4—H4B...O1	0.82 (4)	1.737 (18)	2.554 (3)	175 (6)
N3—H3A...O3	0.86	2.00	2.602 (3)	126
N3—H3B...O2	0.86	1.84	2.501 (3)	133

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

Fig. 1



Article re

Fig. 2

