

Retraction of articles by H. Zhong *et al.*

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A series of 41 papers by H. Zhong *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 41 papers by H. Zhong *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>Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate</i>	Zhong, Zeng, Liu & Luo (2006a)	10.1107/S1600536806041122	KERQEE
<i>cis-Dichlorobis(1,10-phenanthroline)cobalt(II)</i>	Zhong, Zeng & Luo (2006)	10.1107/S1600536806047295	MEQFOE
<i>Tris(quinolin-8-olato-κ²N,O)cobalt(III) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Liu & Luo (2006b)	10.1107/S1600536806050240	MEQHEW
<i>(8-Quinololinol-κ²N,O)bis(8-quinolinolato-κ²N,O)nickel(II) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Liu & Luo (2007)	10.1107/S1600536806053232	METVUD
<i>Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate</i>	Zhong, Zeng & Luo (2007)	10.1107/S1600536806053530	METQIM
<i>(8-Quinololinol-κ²N,O)-bis(8-quinolinolato-κ²N,O)zinc(II) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
<i>(Dimethylglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')nickel(II) dinitrate dihydrate</i>	Zhong, Zeng, Yang, Luo & Li (2007a)	10.1107/S1600536807004102	YEYGOZ
<i>(Dimethylglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')zinc(II) dinitrate dihydrate</i>	Zhong, Zeng, Yang, Luo & Li (2007b)	10.1107/S1600536807004096	YEYGUF
<i>Chloridobis(1,10-phenanthroline-κN,N')copper(I) hexahydrate</i>	Zhong, Zeng, Yang, Luo & Xiao (2007)	10.1107/S160053680700791X	HEGKOU1
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)</i>	Zhong, Zeng, Yang & Luo (2007a)	10.1107/S1600536807017461	ITCPCO1
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)</i>	Zhong, Zeng, Yang & Luo (2007b)	10.1107/S160053680701879X	AVUJEG02
<i>Tetrakis(nitrato-κ²O,O')bis(4-phenylpyridine-κN)cerium(IV)</i>	Zhong, Zeng, Yang & Luo (2007c)	10.1107/S1600536807018831	CICDOI
<i>Bis(4,4'-bipyridine-κ²N,N')tetrakis(nitrato-κ²O,O')cerium(IV)</i>	Zhong, Zeng, Yang & Luo (2007d)	10.1107/S1600536807021502	YIDNEF
<i>(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)</i>	Zhong, Zeng, Yang, Luo & Xu (2007)	10.1107/S1600536807027171	EDUROL
<i>(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)</i>	Zhong, Yang, Luo & Xu (2007a)	10.1107/S1600536807028061	EDUTUT
<i>(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)</i>	Zhong, Yang, Luo & Xu (2007b)	10.1107/S1600536807028693	RIGQEE
<i>(1,10-Phenanthroline-κ²N,N')tris(phenoxyacetato)-κO;κO;κO,O'-neodymium(III)</i>	Zhong, Yang, Luo & Xu (2007c)	10.1107/S1600536807030371	UDUMEM
<i>Bis(2,2'-bipyridyl-κ²N,N')bis(thiocyanato-κN)nickel(II)</i>	Zhong, Yang, Luo & Xu (2007d)	10.1107/S1600536807031613	YEJGOJ01
<i>Bis(2,2'-bipyridyl-κ²N,N')bis(isothiocyanato-κN)copper(II)</i>	Zhong, Yang, Luo & Xu (2007e)	10.1107/S1600536807033181	UFAPOH
<i>Bis(2,2'-bipyridyl-κ²N,N')bis(thiocyanato-κN)zinc(II)</i>	Zhong, Yang, Luo & Xu (2007f)	10.1107/S1600536807035337	TIGFAR
<i>(1,10-Phenanthroline-κ²N,N')tris(3-phenylpropanoato-κO)neodymium(III)</i>	Zhong, Yang, Luo & Xu (2007g)	10.1107/S1600536807035350	TIGFEV
<i>2-Fluoro-3,5-dinitrobenzamide monohydrate</i>	Zhong, Yang, Xie & Luo (2007j)	10.1107/S1600536807038676	VIKGAY
<i>2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)</i>	Zhong, Yang, Xie & Luo (2007k)	10.1107/S1600536807039724	KILKIA
<i>1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate</i>	Zhong, Yang, Xie & Luo (2007l)	10.1107/S1600536807040779	AFETAH
<i>N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)</i>	Zhong, Yang, Xie & Luo (2007m)	10.1107/S160053680704086X	AFINAF
<i>catena-Poly[[bis(μ-anilinoacetato-κ²O:O')bis(μ-anilinoacetato-κ²O:O')bis(1,10-phenanthroline-κ²N,N')samarium(III)]-μ-anilinoacetato-κ²O:O']</i>	Zhong, Yang, Xie & Luo (2007a)	10.1107/S1600536807043528	PILDAQ
<i>2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate</i>	Zhong, Yang, Xie & Luo (2007n)	10.1107/S1600536807045199	XILWIZ
<i>catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dineodymium(III)]-di-μ-anilinoacetato]</i>	Zhong, Yang, Xie & Luo (2007b)	10.1107/S1600536807048489	WIMWEV
<i>Hexaaquacopper(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007c)	10.1107/S1600536807049525	TOLSCV01

Table 1 (continued)

Title	Reference	DOI	Refcode
<i>catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dilanthanum(III)]-di-μ-anilinoacetato]</i>	Zhong, Yang, Xie & Luo (2007d)	10.1107/S1600536807051240	GIMZEI
<i>Hexaaquachromium(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007e)	10.1107/S1600536807051227	GIMZIM
<i>Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007f)	10.1107/S1600536807052051	QUKQES01
<i>catena-Poly[(acetato-κO)(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-acetato-κ^2O:O']</i>	Zhong, Yang, Xie & Luo (2007g)	10.1107/S1600536807053494	NIQLAB
<i>Hexaaquanickel(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Zhong, Xie & Luo (2007a)	10.1107/S1600536807054372	HIPZOW
<i>catena-Poly[(acetato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-acetato-κ^2O:O']</i>	Zhong, Yang, Xie & Luo (2007h)	10.1107/S160053680705622X	XIRGOV
<i>Hexaaquazinc(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Zhong, Xie & Luo (2007b)	10.1107/S1600536807056498	XIRJEO
<i>catena-Poly[(acetato-κO)(1,10-phenanthroline-κ^2N,N')nickel(II)]-μ-acetato-κ^2O:O']</i>	Zhong, Yang, Xie & Luo (2007i)	10.1107/S1600536807058540	HIQJOH
<i>Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Xie & Luo (2007)	10.1107/S1600536807058527	HIQJUN
<i>catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dieuropium(III)]-di-μ-anilinoacetato]</i>	Zhong, Yang, Duan & Hong (2007)	10.1107/S1600536807060643	YIQMAN
<i>(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate</i>	Zhong, Yang, Luo & Li (2007)	10.1107/S1600536807061193	YIQNUI
<i>catena-Poly[(1,10-phenanthroline-κ^2N,N')praseodymium(III)]-di-μ-phenoxyacetato-κ^4O:O'-[(1,10-phenanthroline-κ^2N,N')praseodymium(III)]-di-μ-phenoxyacetato-κ^4O:O'-di-μ-phenoxyacetato-κ^3O,O':κ^3O:O,O']</i>	Zhong, Yang, Luo & Xu (2008)	10.1107/S1600536807068614	GISJIC

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2-Fluoro-3,5-dinitrobenzamide monohydrate

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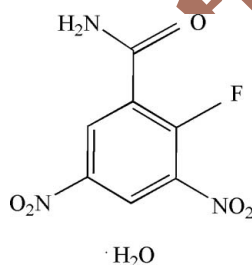
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Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.063; wR factor = 0.204; data-to-parameter ratio = 10.7.

The title complex, $\text{C}_7\text{H}_4\text{FN}_3\text{O}_5 \cdot \text{H}_2\text{O}$, contains one 2-fluoro-3,5-dinitrobenzamide molecule and one water molecule. In the crystal structure, $\text{O}-\text{H} \cdots \text{O}$, $\text{O}-\text{H} \cdots \text{F}$ and $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds result in the formation of a supramolecular network structure.

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

$\text{C}_7\text{H}_4\text{FN}_3\text{O}_5 \cdot \text{H}_2\text{O}$
 $M_r = 247.15$
Monoclinic, $C2/c$
 $a = 25.529$ (2) Å
 $b = 6.357$ (4) Å
 $c = 12.353$ (5) Å
 $\beta = 111.749$ (2)°

$V = 1862.1$ (15) Å³
 $Z = 8$
Mo $K\alpha$ radiation
 $\mu = 0.17$ mm⁻¹
 $T = 273$ (2) K
 $0.24 \times 0.15 \times 0.15$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.961$, $T_{\max} = 0.976$
5928 measured reflections
1816 independent reflections
978 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.063$
 $wR(F^2) = 0.204$
 $S = 0.99$
1816 reflections
170 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.37$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.42$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O1}-\text{H1B} \cdots \text{O4}^{\text{i}}$	0.850 (17)	2.041 (11)	2.863 (3)	162 (3)
$\text{O1}-\text{H1A} \cdots \text{O3}^{\text{ii}}$	0.85 (2)	2.54 (2)	3.273 (4)	145 (3)
$\text{O1}-\text{H1A} \cdots \text{F1}^{\text{ii}}$	0.85 (2)	2.214 (18)	2.966 (4)	147 (3)
$\text{N3}-\text{H3A} \cdots \text{O1}^{\text{iii}}$	0.81 (3)	1.820 (15)	2.629 (3)	174 (3)

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINTE* (Siemens, 1996); data reduction: *SAINTE*; 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: HK2307).

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supplementary materials

Article retracted

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2-Fluoro-3,5-dinitrobenzamide monohydrate

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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 Pr metal chains by reaction of the praseodymium(III) ion with 3,5-dinitro-2-fluoro-benzamide 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 (C₇H₄FN₃O₅) molecule and one uncoordinated water molecule.

In the crystal structure, O—H...O, O—H...F and N—H...O hydrogen bonds (Table 1) seem to be effective in the stabilization of the structure, resulting 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. Praseodymium (III) nitrate hexahydrate (217.5 mg, 0.5 mmol), 3,5-dinitro-2-fluorobenzamide (229.1 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 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

H1A, H1B (for OH₂) and H3A, H3B (for NH₂) were located in difference syntheses and refined isotropically [O—H = 0.85 (2) and 0.850 (17) Å, $U_{\text{iso}}(\text{H}) = 0.097$ (16) and 0.090 (14) Å²; N—H = 0.81 (3) and 0.83 (3) Å, $U_{\text{iso}}(\text{H}) = 0.076$ (12) and 0.09 (3) Å²]. The remaining H atoms were positioned geometrically, with C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

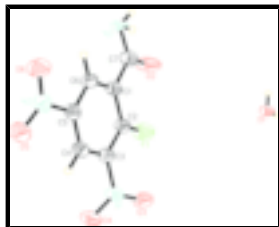


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

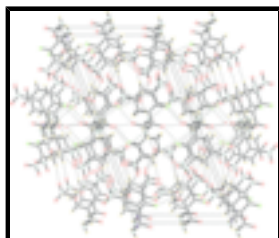


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

2-Fluoro-3,5-dinitrobenzamide monohydrate

Crystal data

$C_7H_4FN_3O_5 \cdot H_2O$

$M_r = 247.15$

Monoclinic, $C2/c$

Hall symbol: $-C 2yc$

$a = 25.529 (2) \text{ \AA}$

$b = 6.357 (4) \text{ \AA}$

$c = 12.353 (5) \text{ \AA}$

$\beta = 111.749 (2)^\circ$

$V = 1862.1 (15) \text{ \AA}^3$

$Z = 8$

$F_{000} = 1008$

$D_x = 1.763 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

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

Cell parameters from 1503 reflections

$\theta = 3.2\text{--}26.9^\circ$

$\mu = 0.17 \text{ mm}^{-1}$

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

Prism, colourless

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

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)

$T_{\min} = 0.961$, $T_{\max} = 0.976$

5928 measured reflections

1816 independent reflections

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

$R_{\text{int}} = 0.029$

$\theta_{\text{max}} = 26.2^\circ$

$\theta_{\text{min}} = 3.3^\circ$

$h = -31 \rightarrow 31$

$k = -7 \rightarrow 7$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.063$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.204$	$w = 1/[\sigma^2(F_o^2) + (0.1305P)^2 + 0.002P]$
$S = 0.99$	where $P = (F_o^2 + 2F_c^2)/3$
1816 reflections	$(\Delta/\sigma)_{\max} < 0.001$
170 parameters	$\Delta\rho_{\max} = 0.37 \text{ e } \text{\AA}^{-3}$
9 restraints	$\Delta\rho_{\min} = -0.42 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	0.40250 (9)	0.2100 (4)	0.7293 (2)	0.0892 (8)
O1	0.63158 (10)	0.2285 (4)	0.0276 (2)	0.0700 (7)
H1A	0.6362 (14)	0.212 (7)	-0.0365 (14)	0.097 (16)*
H1B	0.6666 (3)	0.230 (6)	0.069 (2)	0.090 (14)*
O2	0.50775 (11)	0.2156 (5)	0.8601 (2)	0.0965 (11)
O3	0.29274 (10)	0.1317 (4)	0.63040 (19)	0.0760 (8)
O4	0.24203 (9)	0.3063 (4)	0.7042 (2)	0.0756 (8)
O5	0.30600 (10)	0.3717 (4)	1.1127 (2)	0.0805 (8)
O6	0.39278 (12)	0.2999 (5)	1.2189 (2)	0.0907 (9)
N1	0.28703 (11)	0.2254 (4)	0.7090 (2)	0.0583 (7)
N2	0.35445 (13)	0.3192 (4)	1.1254 (2)	0.0629 (8)
N3	0.53272 (10)	0.2546 (4)	1.0473 (2)	0.0491 (7)
H3A	0.5631 (9)	0.237 (5)	1.042 (3)	0.076 (12)*
H3B	0.5194 (19)	0.140 (4)	1.056 (5)	0.09 (3)*
C1	0.43548 (12)	0.2448 (5)	0.9348 (3)	0.0523 (8)
C2	0.39099 (13)	0.2303 (5)	0.8241 (3)	0.0498 (7)

supplementary materials

C3	0.33520 (13)	0.2443 (5)	0.8193 (3)	0.0502 (8)
C4	0.32298 (13)	0.2750 (5)	0.9164 (3)	0.0520 (8)
H5	0.2859	0.2894	0.9113	0.062*
C5	0.36662 (13)	0.2839 (5)	1.0211 (3)	0.0511 (8)
C6	0.42304 (13)	0.2689 (5)	1.0327 (3)	0.0530 (8)
H7	0.4517	0.2752	1.1059	0.064*
C7	0.49530 (14)	0.2381 (5)	0.9437 (3)	0.0625 (9)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0610 (14)	0.134 (2)	0.0738 (15)	0.0015 (11)	0.0260 (12)	-0.0017 (12)
O1	0.0406 (14)	0.0910 (19)	0.0716 (17)	0.0023 (12)	0.0129 (12)	0.0041 (13)
O2	0.0419 (15)	0.195 (3)	0.0562 (16)	0.0037 (15)	0.0225 (12)	0.0020 (15)
O3	0.0557 (15)	0.112 (2)	0.0562 (14)	-0.0072 (13)	0.0161 (12)	-0.0168 (13)
O4	0.0399 (14)	0.114 (2)	0.0692 (16)	0.0105 (12)	0.0152 (12)	0.0075 (13)
O5	0.0601 (17)	0.112 (2)	0.0797 (17)	0.0049 (14)	0.0375 (14)	-0.0085 (14)
O6	0.074 (2)	0.143 (3)	0.0487 (15)	0.0138 (16)	0.0154 (14)	-0.0041 (14)
N1	0.0373 (15)	0.0792 (19)	0.0563 (17)	-0.0029 (12)	0.0148 (13)	0.0075 (14)
N2	0.059 (2)	0.0713 (18)	0.0636 (18)	-0.0019 (14)	0.0295 (16)	-0.0052 (13)
N3	0.0235 (13)	0.0753 (18)	0.0417 (14)	-0.0018 (12)	0.0041 (11)	-0.0009 (11)
C1	0.0354 (17)	0.0652 (19)	0.0558 (19)	0.0002 (13)	0.0162 (15)	0.0027 (14)
C2	0.0397 (17)	0.0690 (19)	0.0432 (16)	0.0009 (13)	0.0183 (14)	-0.0011 (13)
C3	0.0437 (18)	0.0575 (18)	0.0449 (16)	-0.0004 (13)	0.0112 (14)	0.0043 (13)
C4	0.0423 (18)	0.0555 (18)	0.061 (2)	-0.0003 (13)	0.0227 (16)	0.0045 (13)
C5	0.0470 (19)	0.0602 (18)	0.0486 (17)	0.0026 (13)	0.0207 (15)	0.0002 (13)
C6	0.0425 (17)	0.065 (2)	0.0455 (17)	-0.0019 (14)	0.0097 (14)	-0.0010 (13)
C7	0.0441 (19)	0.078 (2)	0.065 (2)	0.0009 (15)	0.0199 (18)	0.0076 (16)

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

F1—C2	1.315 (4)	O1—H1B	0.850 (17)
O2—C7	1.196 (4)	N3—H3A	0.81 (3)
O3—N1	1.193 (3)	N3—H3B	0.83 (3)
O4—N1	1.240 (4)	C1—C6	1.367 (4)
O5—N2	1.233 (3)	C1—C2	1.420 (4)
O6—N2	1.212 (4)	C2—C3	1.406 (4)
N1—C3	1.464 (4)	C3—C4	1.361 (4)
N2—C5	1.450 (4)	C4—C5	1.360 (4)
N3—C7	1.287 (4)	C4—H5	0.9300
C1—C7	1.491 (4)	C5—C6	1.397 (4)
O1—H1A	0.85 (2)	C6—H7	0.9300
F1—C2—C1	120.1 (3)	C2—C1—C7	120.0 (3)
F1—C2—C3	121.7 (3)	C3—C2—C1	118.2 (3)
O2—C7—C1	122.2 (3)	C4—C3—C2	122.1 (3)
O2—C7—N3	122.1 (3)	C4—C3—N1	116.4 (3)
N3—C7—C1	115.7 (3)	C2—C3—N1	121.5 (3)
O3—N1—O4	124.0 (3)	C5—C4—C3	118.0 (3)

O3—N1—C3	119.0 (3)	C5—C4—H5	121.0
O4—N1—C3	117.0 (3)	C3—C4—H5	121.0
O5—N2—O6	124.5 (3)	C4—C5—C6	123.0 (3)
O5—N2—C5	117.6 (3)	C4—C5—N2	118.8 (3)
O6—N2—C5	117.9 (3)	C6—C5—N2	118.2 (3)
H1A—O1—H1B	95 (3)	C1—C6—C5	119.1 (3)
C7—N3—H3A	107 (3)	C1—C6—H7	120.5
C7—N3—H3B	82 (4)	C5—C6—H7	120.5
H3A—N3—H3B	110 (2)	O2—C7—H3B	128.8 (19)
C6—C1—C2	119.6 (3)	C1—C7—H3B	98.3 (15)
C6—C1—C7	120.4 (3)		

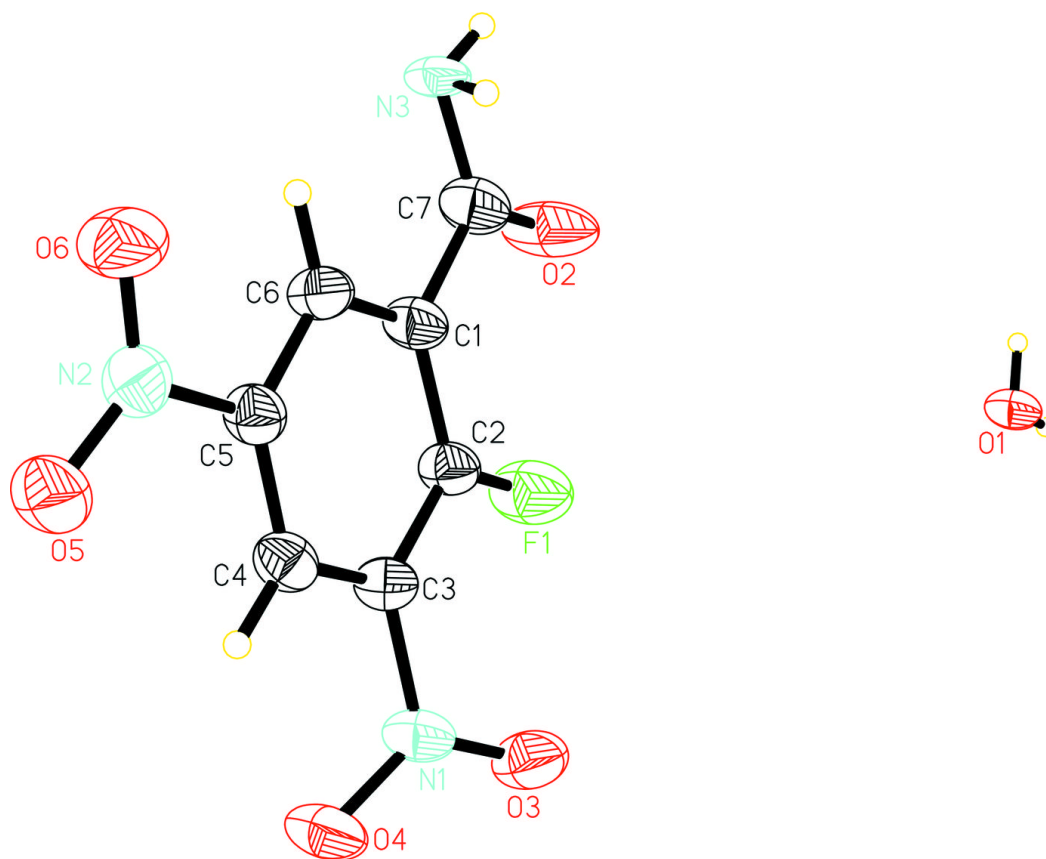
Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1B \cdots O4 ⁱ	0.850 (17)	2.041 (11)	2.863 (3)	162 (3)
O1—H1A \cdots O3 ⁱⁱ	0.85 (2)	2.54 (2)	3.273 (4)	145 (3)
O1—H1A \cdots F1 ⁱⁱ	0.85 (2)	2.214 (18)	2.966 (4)	147 (3)
N3—H3A \cdots O1 ⁱⁱⁱ	0.81 (3)	1.820 (15)	2.629 (3)	174 (3)

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

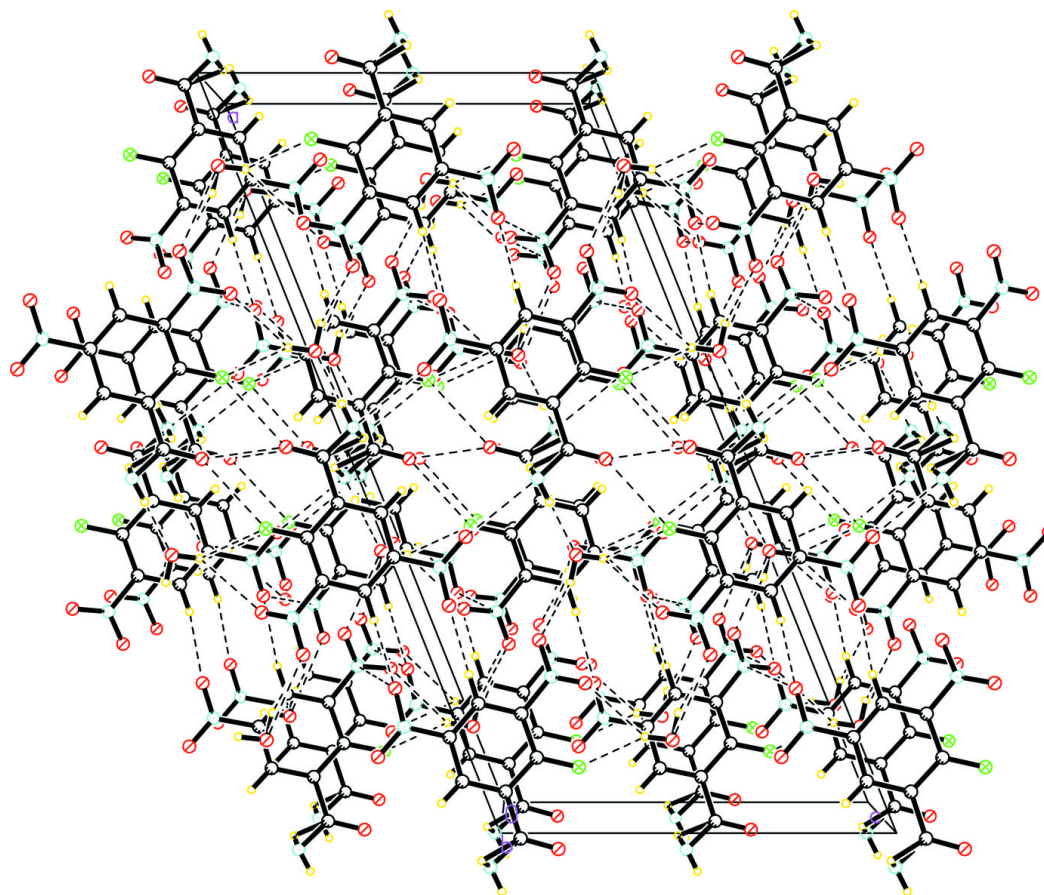
Article retracted

Fig. 1



Article

Fig. 2



Article