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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
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate	Zhong, Zeng, Liu & Luo (2006*a*)	10.1107/S1600536806041122	KERQEE
cis-Dichlorobis(1,10-phenanthroline)cobalt(II)	Zhong, Zeng & Luo (2006)	10.1107/S1600536806047295	MEQFOE
Tris(quinolin-8-olato-κ^2N,O)cobalt(III) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2006*b*)	10.1107/S1600536806050240	MEQHEW
(8-Quinolinol-κ^2N,O)bis(8-quinolinolato-κ^2N,O)nickel(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2007)	10.1107/S1600536806053232	METVUD
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate	Zhong, Zeng & Luo (2007)	10.1107/S1600536806053530	METQIM
(8-Quinolinol-κ^2N,O)-bis(8-quinolinolato-κ^2N,O)zinc(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')nickel(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*a*)	10.1107/S1600536807004102	YEYGOZ
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')zinc(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*b*)	10.1107/S1600536807004096	YEYGUF
Chloridobis(1,10-phenanthroline-$\kappa N,N'$)copper(I) hexahydrate	Zhong, Zeng, Yang, Luo & Xiao (2007)	10.1107/S160053680700791X	HEGKOU01
Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)	Zhong, Zeng, Yang & Luo (2007*a*)	10.1107/S1600536807017461	ITCPCO01
Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)	Zhong, Zeng, Yang & Luo (2007*b*)	10.1107/S160053680701879X	AVUJEG02
Tetrakis(nitrato-κ^2O,O')bis(4-phenylpyridine-κN)cerium(IV)	Zhong, Zeng, Yang & Luo (2007*c*)	10.1107/S1600536807018831	CICDOI
Bis(4,4′-bipyridine-κ^2N,N')tetrakis(nitrato-κ^2O,O')cerium(IV)	Zhong, Zeng, Yang & Luo (2007*d*)	10.1107/S1600536807021502	YIDNEF
(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)	Zhong, Zeng, Yang, Luo & Xu (2007)	10.1107/S1600536807027171	EDUROL
(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)	Zhong, Yang, Luo & Xu (2007*a*)	10.1107/S1600536807028061	EDUTUT
(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)	Zhong, Yang, Luo & Xu (2007*b*)	10.1107/S1600536807028693	RIGQEE
(1,10-Phenanthroline-κ^2N,N')tris(phenoxyacetato)-$\kappa O;\kappa O;\kappa O,O'$-neodymium(III)	Zhong, Yang, Luo & Xu (2007*c*)	10.1107/S1600536807030371	UDUMEM
Bis(2,2′-bipyridyl-κ^2N,N')bis(thiocyanato-κN)nickel(II)	Zhong, Yang, Luo & Xu (2007*d*)	10.1107/S1600536807031613	YEJGOJ01
Bis(2,2′-bipyridyl-κ^2N,N')bis(isothiocyanato-κN)copper(II)	Zhong, Yang, Luo & Xu (2007*e*)	10.1107/S1600536807033181	UFAPOH
Bis(2,2′-bipyridyl-κ^2N,N')bis(thiocyanato-κN)zinc(II)	Zhong, Yang, Luo & Xu (2007*f*)	10.1107/S1600536807035337	TIGFAR
(1,10-Phenanthroline-κ^2N,N')tris(3-phenylpropanoato-κO)neodymium(III)	Zhong, Yang, Luo & Xu (2007*g*)	10.1107/S1600536807035350	TIGFEV
2-Fluoro-3,5-dinitrobenzamide monohydrate	Zhong, Yang, Xie & Luo (2007*j*)	10.1107/S1600536807038676	VIKGAY
2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)	Zhong, Yang, Xie & Luo (2007*k*)	10.1107/S1600536807039724	KILKIA
1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate	Zhong, Yang, Xie & Luo (2007*l*)	10.1107/S1600536807040779	AFETAH
N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)	Zhong, Yang, Xie & Luo (2007*m*)	10.1107/S160053680704086X	AFINAF
catena-Poly[[bis(μ-anilinoacetato-$\kappa^2O:O'$)bis(μ-anilinoacetato-$\kappa^3O,O':O$)bis[(1,10-phenanthroline-κ^2N,N')samarium(III)]-μ-anilinoacetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*a*)	10.1107/S1600536807043528	PILDAQ
2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate	Zhong, Yang, Xie & Luo (2007*n*)	10.1107/S1600536807045199	XILWIZ
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dineodymium(III)]-di-μ-anilinoacetato]	Zhong, Yang, Xie & Luo (2007*b*)	10.1107/S1600536807048489	WIMWEV
Hexaaquacopper(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*c*)	10.1107/S1600536807049525	TOLSCV01

Table 1 (continued)

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

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

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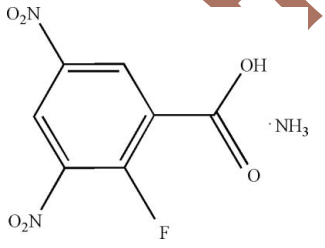
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.171; data-to-parameter ratio = 11.0.

In the crystal structure of the title complex, $C_7H_3FN_2O_6\cdot NH_3$, the uncoordinated ammonia molecule interacts with nearby nitro and carboxyl groups and the F atom of the 3,5-dinitro-2-fluorobenzoic acid by way of N—H···O, N—H···F and O—H···N hydrogen bonds. These hydrogen bonds lead to a supramolecular network structure.

Related literature

For related literature, see: Allen *et al.* (1987); Braga *et al.* (1998); Desiraju (1995, 1997); Maira *et al.* (2001); McCann *et al.* (1995, 1996); Min & Lee (2002); Wai *et al.* (1990); Yaghi *et al.* (1996).



Experimental

Crystal data

$C_7H_3FN_2O_6\cdot NH_3$
M_r = 247.15
Monoclinic, $C2/c$
a = 25.08 (2) Å
b = 6.214 (3) Å
c = 12.237 (4) Å
β = 112.004 (1)°
V = 1768.0 (19) 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 APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.959, T_{max} = 0.975
6068 measured reflections
1876 independent reflections
977 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.172
S = 1.01
1876 reflections
171 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···O4^{i}	0.830 (18)	1.996 (18)	2.813 (4)	168 (3)
N3—H3A···F1^{ii}	0.739 (15)	2.228 (17)	2.940 (4)	162 (2)
O1—H1···N3^{iii}	0.82 (3)	1.76 (4)	2.579 (4)	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: *APEX2* (Bruker, 2005); 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: AT2369).

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supplementary materials

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

H. Zhong, X.-M. Yang, H.-L. Xie and C.-J. Luo

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 structure (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 Pr metal chains by reaction of the praseodymium(III) ion with 3,5-dinitro-2-fluorobenzoic acid ligand. Unfortunately, we obtained only the title compound, (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). In the title complex (I), contains one 3,5-dinitro-2-fluorobenzoic acid molecule and one uncoordinated ammonia molecule. The uncoordinated ammonia molecule interacts with nearby nitro and carboxyl groups and F atom of the 3,5-dinitro-2-fluorobenzoic acid ligands by way of N—H···O, N—H···F and O—H···N hydrogen bonds, with the N···O, N···F and O···N distances of 2.813 (4), 2.940 (4) and 2.579 (4) Å, respectively (Fig. 2 and Table 1). These hydrogen bonds lead to a supramolecular network structure.

Experimental

Crystals of the title compound (I) were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb, which was then sealed. Praseodymium (III) nitrate hexahydrate (217.5 mg, 0.5 mmol), 3,5-dinitro-2-fluorobenzoic acid (230.1 mg, 1 mmol), ammonia (0.5 mol/l, 2 ml) 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 colourless solution was decanted from small colourless crystals. These crystals were washed with distilled water, followed by ethanol, and allowed to air-dry at room temperature.

Refinement

H atoms of ammonia and hydroxyl group were located from difference Fourier syntheses and refined with restraints to the O—H distances and the H—O—H angles. 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_{iso}(H) = 1.2U_{eq}(C).

Figures

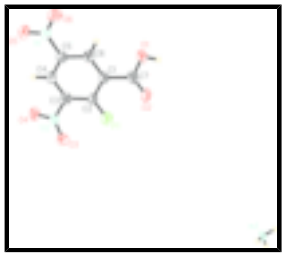

Fig. 1. The structure of the title molecule (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

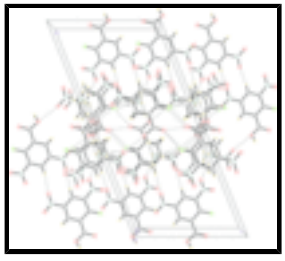

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

3,5-Dinitro-2-fluorobenzoic acid–ammonia (1/1)

Crystal data

$C_7H_3FN_2O_6·NH_3$	F_{000} = 1008
M_r = 247.15	D_x = 1.857 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 1499 reflections
a = 25.08 (2) Å	θ = 3.0–26.9º
b = 6.214 (3) Å	μ = 0.18 mm^{-1}
c = 12.237 (4) Å	*T* = 273 (2) K
β = 112.004 (1)º	Prism, colourless
V = 1768.0 (19) Å^3	0.24 × 0.15 × 0.14 mm
Z = 8	

Data collection

Bruker APEXII area-detector diffractometer	1876 independent reflections
Radiation source: fine-focus sealed tube	977 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.032
T = 273(2) K	θ_{max} = 27.0º
φ and ω scans	θ_{min} = 3.4º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −31→31
T_{min} = 0.959, T_{max} = 0.975	*k* = −7→7
6068 measured reflections	*l* = −15→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.172$	$w = 1/[\sigma^2(F_o^2) + (0.1059P)^2 + 0.02P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
1876 reflections	$\Delta\rho_{max} = 0.27$ e Å^{-3}
171 parameters	$\Delta\rho_{min} = -0.30$ e Å^{-3}
6 restraints	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.014 (3)

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}
F1	0.40241 (8)	0.2109 (4)	0.72936 (17)	0.0874 (7)
O1	0.53280 (10)	0.2528 (3)	1.04732 (19)	0.0660 (7)
O2	0.50766 (10)	0.2179 (5)	0.85991 (19)	0.0934 (9)
O3	0.29277 (9)	0.1317 (4)	0.63059 (17)	0.0747 (7)
O4	0.24215 (9)	0.3061 (4)	0.70445 (19)	0.0743 (7)
O5	0.30610 (9)	0.3713 (4)	1.11276 (19)	0.0799 (7)
O6	0.39272 (12)	0.3013 (4)	1.2183 (2)	0.0915 (9)
N3	0.63157 (10)	0.2284 (4)	0.0279 (2)	0.0512 (6)
N1	0.35425 (12)	0.3194 (4)	1.1251 (2)	0.0618 (7)
N2	0.28703 (10)	0.2260 (4)	0.7096 (2)	0.0571 (7)
C1	0.43546 (11)	0.2452 (4)	0.9348 (2)	0.0510 (7)
C2	0.39091 (11)	0.2306 (4)	0.8240 (2)	0.0495 (7)
C3	0.33530 (12)	0.2445 (4)	0.8196 (2)	0.0505 (7)
C4	0.32304 (12)	0.2745 (4)	0.9169 (2)	0.0521 (7)
H4	0.2852	0.2882	0.9114	0.063*

C5	0.36643 (12)	0.2841 (4)	1.0208 (2)	0.0506 (7)
C6	0.42307 (12)	0.2693 (4)	1.0325 (2)	0.0531 (7)
H6	0.4524	0.2758	1.1066	0.064*
C7	0.49529 (12)	0.2386 (5)	0.9436 (3)	0.0606 (8)
H1	0.5630 (14)	0.246 (4)	1.036 (2)	0.064 (9)*
H3A	0.6302 (10)	0.217 (4)	−0.0331 (15)	0.050 (7)*
H3B	0.6656 (9)	0.231 (5)	0.074 (2)	0.085 (12)*
H3C	0.620 (3)	0.110 (9)	0.048 (4)	0.060 (2)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0594 (13)	0.1295 (18)	0.0730 (13)	−0.0004 (10)	0.0243 (10)	−0.0022 (10)
O1	0.0385 (13)	0.0933 (17)	0.0601 (14)	−0.0008 (10)	0.0113 (11)	−0.0013 (10)
O2	0.0407 (13)	0.188 (3)	0.0543 (14)	0.0040 (13)	0.0208 (11)	0.0013 (13)
O3	0.0542 (13)	0.1070 (18)	0.0586 (13)	−0.0069 (12)	0.0162 (11)	−0.0154 (12)
O4	0.0406 (13)	0.1082 (18)	0.0699 (14)	0.0103 (11)	0.0159 (10)	0.0071 (11)
O5	0.0591 (15)	0.1091 (18)	0.0814 (15)	0.0028 (12)	0.0376 (12)	−0.0094 (13)
O6	0.0797 (19)	0.140 (2)	0.0500 (14)	0.0146 (14)	0.0186 (13)	−0.0040 (13)
N3	0.0286 (12)	0.0725 (16)	0.0467 (15)	0.0015 (10)	0.0074 (11)	0.0027 (12)
N1	0.0571 (17)	0.0696 (16)	0.0631 (16)	0.0001 (12)	0.0274 (14)	−0.0040 (12)
N2	0.0371 (14)	0.0770 (17)	0.0542 (15)	−0.0022 (11)	0.0137 (11)	0.0071 (12)
C1	0.0377 (15)	0.0616 (17)	0.0546 (17)	0.0004 (12)	0.0181 (13)	0.0025 (12)
C2	0.0387 (15)	0.0663 (17)	0.0455 (15)	0.0006 (12)	0.0180 (13)	−0.0012 (11)
C3	0.0434 (16)	0.0561 (16)	0.0477 (15)	−0.0001 (11)	0.0119 (13)	0.0041 (11)
C4	0.0424 (16)	0.0555 (16)	0.0608 (17)	0.0006 (11)	0.0222 (14)	0.0044 (12)
C5	0.0468 (17)	0.0589 (16)	0.0470 (15)	0.0031 (12)	0.0185 (13)	0.0011 (11)
C6	0.0439 (16)	0.0623 (17)	0.0486 (16)	−0.0009 (12)	0.0119 (13)	−0.0004 (12)
C7	0.0413 (16)	0.076 (2)	0.0585 (18)	−0.0003 (13)	0.0123 (15)	0.0044 (14)

Geometric parameters (Å, °)

F1—C2	1.300 (3)	N3—H3C	0.86 (6)
O1—C7	1.268 (4)	C1—C6	1.352 (4)
O2—C7	1.183 (4)	C1—C2	1.400 (4)
O3—N2	1.184 (3)	C1—C7	1.464 (4)
O4—N2	1.211 (3)	C2—C3	1.378 (4)
O5—N1	1.203 (3)	C3—C4	1.350 (4)
O6—N1	1.191 (3)	C4—C5	1.330 (4)
N1—C5	1.436 (4)	C4—H4	0.9300
N2—C3	1.438 (4)	C5—C6	1.376 (4)
N3—H3A	0.739 (15)	C6—H6	0.9300
N3—H3B	0.830 (18)	O1—H1	0.82 (3)
F1—C2—C1	120.4 (2)	C6—C1—C2	120.0 (3)
F1—C2—C3	122.0 (3)	C6—C1—C7	120.4 (3)
O1—C7—O2	122.5 (3)	C2—C1—C7	119.6 (3)
O1—C7—C1	115.3 (3)	C3—C2—C1	117.6 (2)
O2—C7—C1	122.2 (3)	C4—C3—C2	122.4 (3)

O3—N2—O4	123.8 (3)	C4—C3—N2	116.5 (3)
O3—N2—C3	119.1 (2)	C2—C3—N2	121.1 (3)
O4—N2—C3	117.1 (3)	C5—C4—C3	118.3 (3)
O5—N1—O6	124.1 (3)	C5—C4—H4	120.8
O5—N1—C5	117.8 (3)	C3—C4—H4	120.8
O6—N1—C5	118.1 (3)	C4—C5—C6	122.7 (3)
C7—O1—H1	102 (2)	C4—C5—N1	119.1 (3)
H3C—N3—H3A	108 (4)	C6—C5—N1	118.2 (2)
H3C—N3—H3B	101 (3)	C1—C6—C5	119.1 (3)
H3A—N3—H3B	110 (2)	C1—C6—H6	120.5
H3A—N3—H3C	108 (4)	C5—C6—H6	120.5
H3B—N3—H3C	101 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3B···O4^{i}	0.830 (18)	1.996 (18)	2.813 (4)	168 (3)
N3—H3A···F1^{ii}	0.739 (15)	2.228 (17)	2.940 (4)	162 (2)
O1—H1···N3^{iii}	0.82 (3)	1.76 (4)	2.579 (4)	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.

Fig. 1

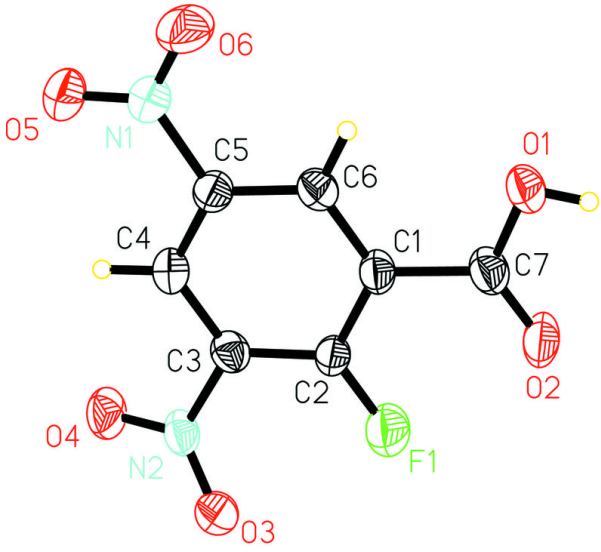

Fig. 2