Acta Crystallographica Section E
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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-$\kappa^2O,O'$)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-$\kappa^2O,O'$)zinc(II)* | Chen (2006) | Journal | 10.1107/S1600536805040432 | SAZCUS |
| *Bis(2-formylphenolato-$\kappa^2O,O'$)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-$\kappa^2O,O'$)manganese(II)* | Wang & Fang (2006) | Journal | 10.1107/S1600536806021039 | IDOVED |
| *Tetraaqua(1,10-phenanthroline-$\kappa^2N,N'$)copper(II) naphthalene-1,5-disulfonate dihydrate* | Liu *et al.* (2006) | Author | 10.1107/S1600536806030637 | GENYOO |
| *Tetraaqua(1,10-phenanthroline-$\kappa^2N,N'$)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-$\kappa^2O,O'$)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-1:2$\kappa^2O$:O′-dinitrato-1$\kappa^4O,O'$-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)-$\kappa^2N^2$:$N^{2'}$]* | 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-$\kappa^2N,N'$)bis(nitrato-κO)zinc(II)* | Liu, Zeng & Chen (2007) | Author | 10.1107/S1600536807042390 | XIKYEW |
| *[N,N′-(o-Phenylene)bis(picolinamido)-$\kappa^4N,N',N'',N'''$]cobalt(II)* | Liu & Zeng (2007*a*) | Author | 10.1107/S1600536807044571 | XILFII |
| *[N,N′-(o-Phenylene)dipicolinamide-$\kappa^4N$]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-$\kappa^2N,N'$)(3,5-dinitro-2-oxidobenzoato-$\kappa^2O^1,O^2$)-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-$\kappa^2O^1,O^6$)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-1:2$\kappa^2$O:O′-dinitrato-1$\kappa^4$O,O′-samarium(III)zinc(II)* | Huang *et al.* (2009) | Journal | 10.1107/S1600536809033558 | YUCWAV |

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# *N*-(2-Fluorophenyl)carbamic acid monohydrate

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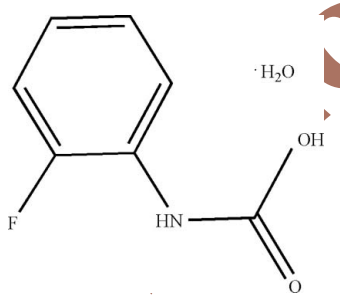
Key indicators: single-crystal X-ray study; $T$ = 273 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.055; $wR$ factor = 0.187; data-to-parameter ratio = 11.6.

In the crystal structure of the title complex, $C_7H_6FNO_2\cdot H_2O$, intramolecular O—H···O hydrogen bonds are present; intermolecular N—H···O and O—H···F hydrogen bonds result in the formation of a supramolecular network.

## Related literature

For general backgroud, see: Desiraju (1995, 1997); Braga *et al.* (1998); McCann *et al.* (1995, 1996); 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*

$C_7H_6FNO_2\cdot H_2O$
$M_r$ = 173.14
Monoclinic, $P2_1/n$
$a$ = 13.1106 (18) Å
$b$ = 4.0079 (14) Å
$c$ = 15.389 (2) Å
$\beta$ = 114.776 (7)°
$V$ = 734.2 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.14 mm$^{-1}$
$T$ = 273 (2) K
0.63 × 0.13 × 0.10 mm

### *Data collection*

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.917, $T_{max}$ = 0.987
4190 measured reflections
1368 independent reflections
831 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.050

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.187
$S$ = 1.05
1368 reflections
118 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.26 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1$A$···O2$^{i}$ | 0.82 | 2.13 | 2.928 (3) | 165 |
| N1—H1$B$···O3$^{ii}$ | 0.86 | 2.19 | 2.986 (3) | 153 |
| O3—H3$B$···F1 | 0.85 (4) | 1.88 (2) | 2.693 (3) | 158 (4) |

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

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: AT2433).

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**supplementary materials**

*Acta Cryst.* (2007). E**63**, o4453 [ **doi:10.1107/S1600536807052464** ]

# *N*-(2-Fluorophenyl)carbamic acid monohydrate

**X.-M. Yang**

## 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 La and Cu metal chains by reaction of the lanthanum(III) and copper(II) ions with *N*-(2-fluorinphenyl)carbamic 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 ($C_7H_6FNO_2$) molecule and one water molecule.

In the crystal structure, intramolecular O—H···O and intermolecular N—H···O and O—H···F 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, which was then sealed. Lanthanum (III) nitrate hexahydrate (216.4 mg, 0.5 mmol), copper nitrate hexahydrate (295.6 mg, 1 mmol), *N*-(2-fluorinphenyl)carbamic acid (310.2 mg, 2 mmol), ammonia (0.5 mol/l, 4 ml) and distilled water (8 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 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 water 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 O—H = 0.82 Å (for OH), O—H = 0.86 Å (for NH) and C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with $U_{iso}$(H) = 1.2$U_{eq}$(C,*N*) or $U_{iso}$(H) = 1.5$U_{eq}$(O).

## Figures

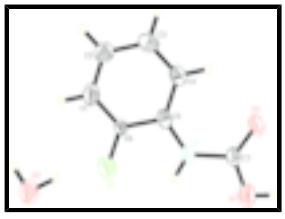

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

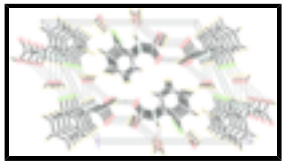

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.



## *N*-(2-Fluorophenyl)carbamic acid monohydrate

### *Crystal data*

| | |
|---|---|
| $C_7H_6FNO_2·H_2O$ | $F_{000}$ = 360 |
| $M_r$ = 173.14 | $D_x$ = 1.566 Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2yn | Cell parameters from 1874 reflections |
| $a$ = 13.1106 (18) Å | θ = 2.3–27.8° |
| $b$ = 4.0079 (14) Å | μ = 0.14 mm$^{-1}$ |
| $c$ = 15.389 (2) Å | $T$ = 273 (2) K |
| β = 114.776 (7)° | Prism, colourless |
| $V$ = 734.2 (3) Å$^3$ | 0.63 × 0.13 × 0.10 mm |
| $Z$ = 4 | |

### *Data collection*

| | |
|---|---|
| Bruker APEXII area-detector diffractometer | 1368 independent reflections |
| Radiation source: fine-focus sealed tube | 831 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.050 |
| $T$ = 273(2) K | $\theta_{max}$ = 26.0° |
| φ and ω scans | $\theta_{min}$ = 2.9° |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −16→15 |
| $T_{min}$ = 0.917, $T_{max}$ = 0.987 | $k$ = −4→4 |
| 4190 measured reflections | $l$ = −19→18 |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.055$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.187$ | $w = 1/[\sigma^2(F_o^2) + (0.1157P)^2 + 0.02P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.05$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 1368 reflections | $\Delta\rho_{max} = 0.30$ e Å$^{-3}$ |
| 118 parameters | $\Delta\rho_{min} = -0.26$ e Å$^{-3}$ |
| 3 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| F1 | 0.63168 (18) | 0.9687 (6) | 0.06633 (17) | 0.0908 (9) |
| O1 | 0.6556 (2) | 1.3947 (7) | −0.19099 (19) | 0.0786 (9) |
| H1A | 0.6746 | 1.4628 | −0.2322 | 0.118* |
| O2 | 0.82030 (18) | 1.1186 (6) | −0.13751 (14) | 0.0618 (8) |
| O3 | 0.5040 (2) | 0.5281 (7) | 0.10853 (18) | 0.0661 (8) |
| N1 | 0.71379 (19) | 1.1117 (6) | −0.05203 (16) | 0.0464 (7) |
| H1B | 0.6524 | 1.1836 | −0.0511 | 0.056* |
| C1 | 0.7882 (3) | 0.6659 (9) | 0.1629 (2) | 0.0632 (10) |
| H1 | 0.7554 | 0.6251 | 0.2049 | 0.076* |
| C2 | 0.8907 (3) | 0.5414 (8) | 0.1820 (2) | 0.0600 (9) |
| H2 | 0.9280 | 0.4131 | 0.2365 | 0.072* |
| C3 | 0.9401 (3) | 0.6046 (8) | 0.1203 (3) | 0.0591 (9) |
| H3 | 1.0110 | 0.5195 | 0.1334 | 0.071* |
| C4 | 0.8857 (2) | 0.7899 (8) | 0.0410 (2) | 0.0525 (8) |
| H4 | 0.9190 | 0.8316 | −0.0006 | 0.063* |
| C5 | 0.7794 (2) | 0.9190 (7) | 0.0214 (2) | 0.0441 (7) |
| C6 | 0.7325 (2) | 0.8493 (6) | 0.08335 (18) | 0.0359 (7) |
| C7 | 0.7358 (2) | 1.2066 (8) | −0.1298 (2) | 0.0451 (7) |
| H3A | 0.550 (4) | 0.431 (15) | 0.158 (3) | 0.10 (3)* |
| H3B | 0.554 (3) | 0.622 (9) | 0.095 (3) | 0.085 (14)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F1 | 0.0959 (16) | 0.0985 (17) | 0.1092 (18) | 0.0257 (12) | 0.0737 (14) | 0.0310 (13) |
| O1 | 0.0898 (18) | 0.094 (2) | 0.0648 (16) | −0.0135 (15) | 0.0445 (14) | 0.0057 (14) |
| O2 | 0.0600 (14) | 0.0845 (18) | 0.0570 (14) | −0.0086 (11) | 0.0403 (12) | −0.0069 (11) |
| O3 | 0.0784 (16) | 0.0705 (17) | 0.0660 (16) | 0.0091 (13) | 0.0466 (14) | 0.0077 (13) |
| N1 | 0.0484 (13) | 0.0552 (15) | 0.0470 (14) | −0.0051 (11) | 0.0313 (12) | −0.0008 (11) |
| C1 | 0.086 (2) | 0.060 (2) | 0.060 (2) | 0.0060 (18) | 0.0473 (19) | 0.0080 (16) |
| C2 | 0.064 (2) | 0.061 (2) | 0.0542 (19) | 0.0026 (16) | 0.0233 (17) | 0.0011 (16) |
| C3 | 0.0468 (17) | 0.059 (2) | 0.069 (2) | −0.0050 (15) | 0.0221 (16) | −0.0081 (17) |
| C4 | 0.0486 (16) | 0.059 (2) | 0.0568 (18) | −0.0089 (14) | 0.0293 (14) | −0.0066 (15) |
| C5 | 0.0513 (16) | 0.0434 (17) | 0.0452 (15) | −0.0114 (13) | 0.0277 (13) | −0.0094 (13) |
| C6 | 0.0408 (13) | 0.0332 (14) | 0.0435 (14) | 0.0047 (11) | 0.0275 (12) | 0.0037 (11) |
| C7 | 0.0487 (16) | 0.0534 (18) | 0.0377 (14) | −0.0125 (14) | 0.0224 (13) | −0.0056 (13) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| F1—C6 | 1.325 (3) | C1—C6 | 1.350 (4) |
| O1—C7 | 1.316 (4) | C1—H1 | 0.9300 |
| O1—H1A | 0.8200 | C2—C3 | 1.378 (5) |
| O2—C7 | 1.215 (3) | C2—H2 | 0.9300 |
| O3—H3A | 0.84 (5) | C3—C4 | 1.349 (5) |
| O3—H3B | 0.85 (4) | C3—H3 | 0.9300 |
| N1—C5 | 1.341 (4) | C4—C5 | 1.395 (4) |
| N1—C7 | 1.396 (4) | C4—H4 | 0.9300 |
| N1—H1B | 0.8600 | C5—C6 | 1.363 (4) |
| C1—C2 | 1.345 (5) | | |
| C7—O1—H1A | 109.5 | C2—C3—H3 | 120.0 |
| H3A—O3—H3B | 95 (5) | C3—C4—C5 | 120.1 (3) |
| C5—N1—C7 | 126.1 (3) | C3—C4—H4 | 119.9 |
| C5—N1—H1B | 117.0 | C5—C4—H4 | 119.9 |
| C7—N1—H1B | 117.0 | N1—C5—C6 | 112.9 (2) |
| C2—C1—C6 | 120.7 (3) | N1—C5—C4 | 128.8 (3) |
| C2—C1—H1 | 119.6 | C6—C5—C4 | 118.3 (3) |
| C6—C1—H1 | 119.6 | F1—C6—C1 | 119.4 (3) |
| C1—C2—C3 | 119.8 (3) | F1—C6—C5 | 119.5 (2) |
| C1—C2—H2 | 120.1 | C1—C6—C5 | 121.0 (3) |
| C3—C2—H2 | 120.1 | O2—C7—O1 | 125.7 (3) |
| C4—C3—C2 | 120.1 (3) | O2—C7—N1 | 122.0 (3) |
| C4—C3—H3 | 120.0 | O1—C7—N1 | 112.3 (3) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1A···O2$^{i}$ | 0.82 | 2.13 | 2.928 (3) | 165 |
| N1—H1B···O3$^{ii}$ | 0.86 | 2.19 | 2.986 (3) | 153 |

| | | | | |
|---|---|---|---|---|
| O3—H3B···F1 | 0.85 (4) | 1.88 (2) | 2.693 (3) | 158 (4) |

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

**Fig. 1**

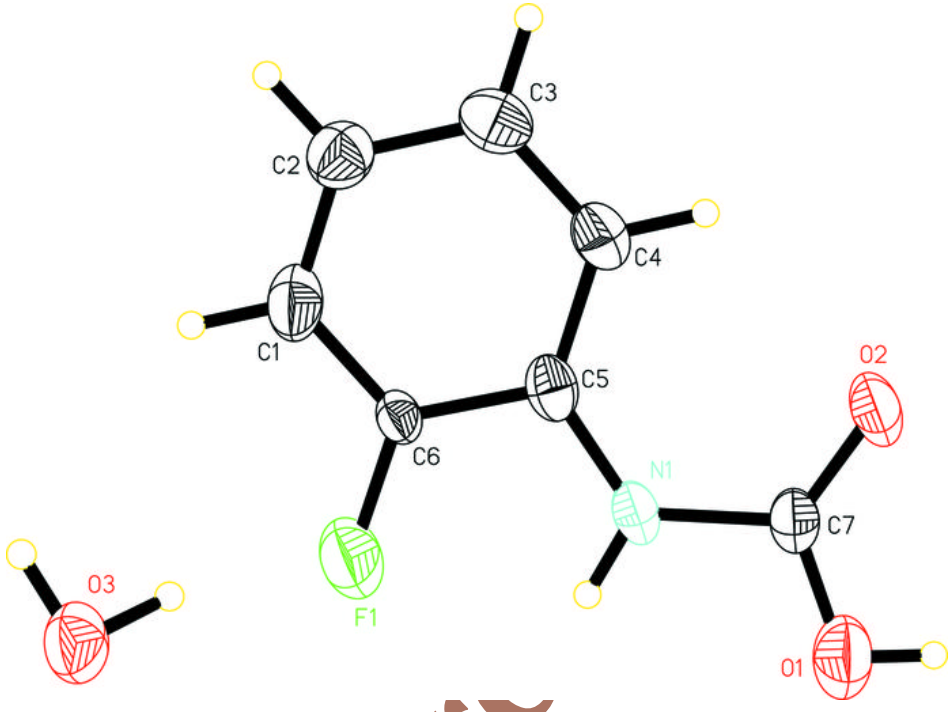

**Fig. 2**