

Tetraaquabis(3-fluoropyridine-4-carboxylato- κ N)zinc(II) dihydrate

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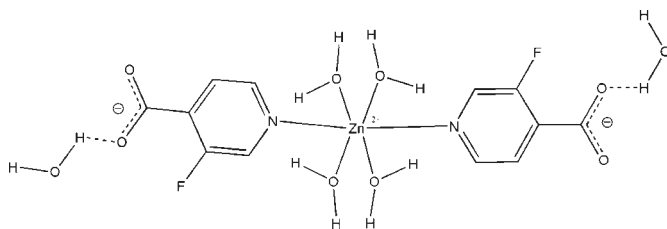
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Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.023; wR factor = 0.065; data-to-parameter ratio = 11.7.

In the title compound, $[\text{Zn}(\text{C}_6\text{H}_3\text{FNO}_2)_2(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$, the Zn^{II} atom is octahedrally coordinated in a ZnO_4N_2 environment by two 3-fluoropyridine-4-carboxylate (3-fpy4-cbx) ligands and four water molecules. The $[\text{Zn}(3\text{-fpy4-cbx})_2(\text{H}_2\text{O})_4]$ molecules form a three-dimensional network through strong $\text{O}-\text{H}\cdots\text{O}$ and weak $\text{O}-\text{H}\cdots\text{F}$ hydrogen bonds between 3-fpy4-cbx and water molecules. The crystal used for data collection was a twin, with the twin law corresponding to a 180° rotation about the real-space $[001]$ axis. The major twin fraction refined to 0.795 (1).

Related literature

For metal-organic compounds with ligands containing both pyridyl and carboxylate donor groups, see: Ellsworth *et al.* (2008); Erxleben (2003); Wang *et al.* (2006). For specific properties exhibited by related metal-organic compounds, see: Chen *et al.* (2009); Evans *et al.* (1999); Xie *et al.* (2008). For typical $\text{Zn}-\text{O}$ and $\text{Zn}-\text{N}$ bond distances in similar metal-organic compounds, see: Wang *et al.* (2006).



Experimental

Crystal data

$[\text{Zn}(\text{C}_6\text{H}_3\text{FNO}_2)_2(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$ $b = 19.1953$ (10) Å
 $M_r = 453.65$ $c = 6.8697$ (4) Å
 Monoclinic, $P2_1/n$ $\beta = 99.225$ (1) $^\circ$
 $a = 6.6042$ (4) Å $V = 859.61$ (8) Å 3

$Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.51$ mm $^{-1}$

$T = 294$ K
 $0.28 \times 0.22 \times 0.16$ mm

Data collection

Bruker SMART APEX CCD diffractometer 1734 measured reflections
 Absorption correction: multi-scan (TWINABS; Bruker, 2003) 1740 independent reflections
 $T_{\text{min}} = 0.890$, $T_{\text{max}} = 1.000$ 1605 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.023$
 $wR(F^2) = 0.065$
 $S = 1.07$
 1740 reflections
 149 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.28$ e Å $^{-3}$
 $\Delta\rho_{\text{min}} = -0.19$ e Å $^{-3}$

Table 1

Selected bond lengths (Å).

Zn1—O3	2.0953 (14)	Zn1—O4	2.1504 (13)
Zn1—N1	2.1356 (13)		

Table 2

Hydrogen-bond geometry (Å, $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O3—H3A \cdots O1 ⁱ	0.83 (3)	1.86 (3)	2.6892 (18)	174 (2)
O3—H3B \cdots O5 ⁱⁱ	0.74 (2)	2.01 (2)	2.745 (2)	176 (2)
O4—H4A \cdots O2 ⁱⁱⁱ	0.79 (3)	2.05 (3)	2.837 (2)	174 (2)
O4—H4B \cdots O5 ^{iv}	0.82 (2)	1.95 (3)	2.7643 (19)	171 (3)
O5—H5A \cdots O2	0.75 (3)	2.05 (3)	2.796 (2)	174 (3)
O5—H5B \cdots O1 ^v	0.79 (2)	1.96 (3)	2.738 (2)	167 (2)
O5—H5B \cdots F1 ^v	0.79 (2)	2.55 (2)	2.9929 (17)	117.2 (18)

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

Data collection: SMART-NT (Bruker, 2003); cell refinement: SAINT-Plus-NT (Bruker, 2003); data reduction: SAINT-Plus-NT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 2008); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2018).

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supplementary materials

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J. Fleming, J. Kelley, L. R. Peterson Jr, M. D. Smith and H.-C. zur Loye

Comment

Metal-organic compounds based on multifunctional ligands that contain both pyridyl and carboxylate donor atoms have been under study in part because of their diverse coordination modes and because they may exhibit useful properties (Ellsworth *et al.*, 2008; Erxleben, 2003). Within this context, the 3-fluoropyridine-4-carboxylate ligand (3-fpy4-cbx), has attracted our interest as a potential component for the construction of these novel materials. A further motivation is that its nonfluorinated analogue, the isonicotinate ligand (ina), has been successfully utilized to generate metal-organic frameworks having the desirable properties alluded to above (Chen *et al.*, 2009; Evans *et al.*, 1999; Wang *et al.*, 2006; Xie *et al.*, 2008). Hence, we have deemed it worthwhile to also explore the coordinating properties of the related 3-fpy4-cbx ligand. This ligand has the additional possibility of C—F \cdots H interactions, in contrast to ina. Herein, we wish to report the crystal structure of the title compound (I), which is a hydrogen bonded, three-dimensional framework.

The asymmetric unit of (I) consists of one-half of the $[\text{Zn}(\text{3-fpy4-cbx})_2(\text{H}_2\text{O})_4]$ complex and a lattice water. The Zn(II) atom is located on an inversion center through which the other half of the molecular complex and another lattice water are generated from the asymmetric unit, thus completing the formula unit of (I) (Fig. 1).

The Zn(II) atom resides in a distorted ZnO_4N_2 octahedral environment. The equatorial positions are occupied by four O atoms from water molecules and the axial positions are occupied by N atoms from two 3-fpy4-cbx ligands. The Zn—O bond distances fall within the normal range of 2.0953 (14) - 2.1504 (13) Å (Wang *et al.*, 2006), while the Zn—N distances are also normal at 2.1356 (13) Å (Wang *et al.*, 2006). The 3-fpy4-cbx ligand is noticeably noncoplanar, with a dihedral angle of 34.2 (1)° between the mean planes of its carboxylate group and its pyridyl ring.

While the carboxylate group of 3-fpy4-cbx is not coordinated to Zn(II), it does assist in the assembly of the crystal structure by acting as hydrogen bond acceptors for both coordinated and lattice waters. The lattice waters are also involved in weak C—F \cdots H₂O hydrogen bonding with the 3-fpy4-cbx ligand. These interactions create a three-dimensional, hydrogen bonded network (Table 1, Fig. 2).

Experimental

An aqueous solution of sodium 3-fluoropyridine-4-carboxylate (25 ml, 2.0 mmol) was slowly added to an aqueous solution of zinc nitrate hexahydrate (25 ml, 1.0 mmol). Colorless crystals of the title compound were obtained after slow evaporation of the resulting solution under ambient conditions.

Refinement

All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms bonded to carbon were placed in geometrically idealized positions and included as riding atoms: C—H = 0.93 Å and with $U_{\text{iso}}(\text{H}) = 1.20$

supplementary materials

2.12 $U_{\text{eq}}(\text{C})$. Oxygen-bound hydrogen atoms were located in difference Fourier maps and refined isotropically: O—H = 0.74 (2)—0.83 (3) Å and with $U_{\text{iso}}(\text{H}) = 0.94\text{--}1.69 U_{\text{eq}}(\text{O})$.

Figures

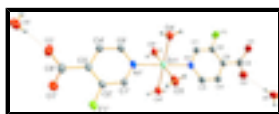


Fig. 1. The molecular complex plus lattice waters with atom-labeling scheme of (I) showing 50% probability ellipsoids for nonhydrogen atoms. All H atoms except for those of water are omitted for clarity. Hydrogen bonds are represented by dashed lines. Primed atoms are generated by the inversion symmetry operation about Zn(II), with symmetry code: 1 - x, 1 - y, 1 - z.

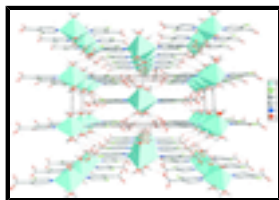


Fig. 2. Wireframe polyhedral view of the crystal packing in (I) showing the hydrogen bonding scheme. Hydrogen atoms except for those of water have been omitted for clarity. Hydrogen bonds are represented by dashed lines.

Tetraaquabis(3-fluoropyridine-4-carboxylato- κ N)zinc(II) dihydrate

Crystal data

$[\text{Zn}(\text{C}_6\text{H}_3\text{FNO}_2)_2(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$

$M_r = 453.65$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 6.6042$ (4) Å

$b = 19.1953$ (10) Å

$c = 6.8697$ (4) Å

$\beta = 99.225$ (1)°

$V = 859.61$ (8) Å³

$Z = 2$

$F(000) = 464$

$D_x = 1.753$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 7697 reflections

$\theta = 3.0\text{--}25.0^\circ$

$\mu = 1.51$ mm⁻¹

$T = 294$ K

Block, colorless

$0.28 \times 0.22 \times 0.16$ mm

Data collection

Bruker SMART APEX CCD diffractometer

Radiation source: fine-focus sealed tube graphite

ω scans

Absorption correction: multi-scan (TWINABS; Bruker, 2003)

$T_{\text{min}} = 0.890$, $T_{\text{max}} = 1.000$

1734 measured reflections

1740 independent reflections

1605 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.1^\circ$

$h = -7 \rightarrow 7$

$k = 0 \rightarrow 22$

$l = 0 \rightarrow 8$

Refinement

Refinement on F^2

Least-squares matrix: full

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$$R[F^2 > 2\sigma(F^2)] = 0.023$$

$$wR(F^2) = 0.065$$

$$S = 1.07$$

1740 reflections

149 parameters

0 restraints

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 0.0969P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\max} = 0.28 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$$

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. $R(\text{int})$ value from TWINABS output.

Cell_now output:

Rotated from first domain by 179.9 degrees about reciprocal axis -0.159 - 0.001 1.000 and real axis -0.001 0.000 1.000

Twin law to convert hkl from first to -1.000 0.000 - 0.317 this domain (*SHELXL* TWIN matrix): 0.001 - 1.000 0.000 - 0.002 0.000 1.000

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 $F^2 > \sigma(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.5000	0.5000	0.5000	0.02937 (12)
F1	0.31965 (16)	0.76809 (5)	0.48595 (19)	0.0515 (3)
C1	0.4393 (3)	0.65492 (9)	0.4885 (2)	0.0316 (4)
H1	0.3043	0.6403	0.4833	0.038*
C2	0.4808 (2)	0.72491 (9)	0.4902 (2)	0.0299 (4)
C3	0.6762 (3)	0.75042 (8)	0.4933 (2)	0.0280 (3)
C4	0.8278 (3)	0.69967 (9)	0.4946 (3)	0.0366 (4)
H4	0.9628	0.7131	0.4932	0.044*
C5	0.7798 (3)	0.63022 (9)	0.4979 (3)	0.0356 (4)
H5	0.8850	0.5978	0.5030	0.043*
C6	0.7287 (3)	0.82734 (8)	0.5010 (3)	0.0340 (4)
N1	0.5870 (2)	0.60704 (7)	0.4940 (2)	0.0297 (3)
O1	0.62449 (18)	0.86516 (6)	0.5953 (2)	0.0468 (3)
O2	0.8725 (2)	0.84601 (7)	0.4177 (2)	0.0504 (4)
O3	0.7470 (2)	0.48608 (7)	0.7293 (2)	0.0401 (3)
H3A	0.780 (4)	0.4489 (14)	0.789 (4)	0.068 (8)*

supplementary materials

H3B	0.750 (3)	0.5121 (11)	0.809 (3)	0.038 (6)*
O4	0.6983 (2)	0.47337 (8)	0.2917 (2)	0.0413 (3)
H4A	0.686 (4)	0.4385 (13)	0.230 (4)	0.061 (8)*
H4B	0.708 (4)	0.5080 (12)	0.223 (4)	0.058 (8)*
O5	1.2370 (3)	0.92014 (7)	0.5293 (2)	0.0419 (3)
H5A	1.142 (4)	0.8983 (14)	0.505 (4)	0.068 (9)*
H5B	1.340 (4)	0.8988 (11)	0.553 (3)	0.047 (7)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03564 (18)	0.01479 (16)	0.03843 (19)	-0.00133 (10)	0.00817 (12)	0.00005 (10)
F1	0.0358 (6)	0.0230 (5)	0.0947 (9)	0.0041 (4)	0.0078 (6)	-0.0037 (5)
C1	0.0308 (8)	0.0223 (9)	0.0419 (10)	-0.0026 (7)	0.0064 (7)	-0.0002 (7)
C2	0.0315 (9)	0.0201 (9)	0.0383 (9)	0.0039 (6)	0.0062 (7)	-0.0004 (6)
C3	0.0341 (9)	0.0207 (8)	0.0296 (8)	-0.0022 (6)	0.0058 (7)	0.0004 (6)
C4	0.0305 (8)	0.0261 (8)	0.0546 (11)	-0.0031 (7)	0.0114 (8)	-0.0020 (8)
C5	0.0324 (9)	0.0243 (8)	0.0511 (10)	0.0016 (7)	0.0095 (8)	-0.0011 (8)
C6	0.0363 (9)	0.0222 (9)	0.0418 (10)	-0.0036 (7)	0.0011 (8)	0.0018 (7)
N1	0.0362 (8)	0.0174 (7)	0.0364 (8)	-0.0009 (6)	0.0083 (6)	0.0001 (5)
O1	0.0422 (7)	0.0245 (6)	0.0735 (9)	-0.0040 (5)	0.0089 (7)	-0.0150 (6)
O2	0.0570 (8)	0.0287 (7)	0.0701 (9)	-0.0123 (6)	0.0238 (7)	0.0029 (6)
O3	0.0514 (8)	0.0230 (7)	0.0428 (8)	0.0047 (6)	-0.0020 (6)	0.0005 (6)
O4	0.0538 (8)	0.0267 (7)	0.0481 (8)	-0.0046 (6)	0.0220 (6)	-0.0036 (7)
O5	0.0431 (8)	0.0273 (7)	0.0546 (9)	0.0025 (7)	0.0059 (7)	-0.0002 (6)

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

Zn1—O3	2.0953 (14)	C4—C5	1.371 (2)
Zn1—O3 ⁱ	2.0953 (14)	C4—H4	0.9300
Zn1—N1 ⁱ	2.1355 (13)	C5—N1	1.345 (2)
Zn1—N1	2.1356 (13)	C5—H5	0.9300
Zn1—O4 ⁱ	2.1504 (13)	C6—O2	1.238 (2)
Zn1—O4	2.1504 (13)	C6—O1	1.250 (2)
F1—C2	1.3457 (19)	O3—H3A	0.83 (3)
C1—N1	1.336 (2)	O3—H3B	0.74 (2)
C1—C2	1.371 (2)	O4—H4A	0.79 (3)
C1—H1	0.9300	O4—H4B	0.82 (2)
C2—C3	1.377 (2)	O5—H5A	0.75 (3)
C3—C4	1.396 (2)	O5—H5B	0.79 (2)
C3—C6	1.516 (2)		
O3—Zn1—O3 ⁱ	180.0	C2—C3—C6	123.74 (15)
O3—Zn1—N1 ⁱ	92.42 (5)	C4—C3—C6	121.34 (15)
O3 ⁱ —Zn1—N1 ⁱ	87.58 (5)	C5—C4—C3	120.75 (16)
O3—Zn1—N1	87.58 (5)	C5—C4—H4	119.6
O3 ⁱ —Zn1—N1	92.42 (5)	C3—C4—H4	119.6
N1 ⁱ —Zn1—N1	180.00 (8)	N1—C5—C4	122.80 (15)

O3—Zn1—O4 ⁱ	90.79 (6)	N1—C5—H5	118.6
O3 ⁱ —Zn1—O4 ⁱ	89.21 (6)	C4—C5—H5	118.6
N1 ⁱ —Zn1—O4 ⁱ	91.25 (5)	O2—C6—O1	126.76 (16)
N1—Zn1—O4 ⁱ	88.76 (5)	O2—C6—C3	117.00 (15)
O3—Zn1—O4	89.21 (6)	O1—C6—C3	116.21 (15)
O3 ⁱ —Zn1—O4	90.79 (6)	C1—N1—C5	117.22 (15)
N1 ⁱ —Zn1—O4	88.76 (5)	C1—N1—Zn1	117.71 (11)
N1—Zn1—O4	91.24 (5)	C5—N1—Zn1	125.06 (11)
O4 ⁱ —Zn1—O4	180.0	Zn1—O3—H3A	126.1 (17)
N1—C1—C2	121.99 (16)	Zn1—O3—H3B	113.1 (17)
N1—C1—H1	119.0	H3A—O3—H3B	104 (2)
C2—C1—H1	119.0	Zn1—O4—H4A	122.5 (18)
F1—C2—C1	116.55 (14)	Zn1—O4—H4B	107.5 (18)
F1—C2—C3	121.15 (15)	H4A—O4—H4B	113 (3)
C1—C2—C3	122.29 (15)	H5A—O5—H5B	115 (3)
C2—C3—C4	114.90 (15)		
N1—C1—C2—F1	-179.40 (14)	C2—C1—N1—C5	-1.1 (2)
N1—C1—C2—C3	1.4 (3)	C2—C1—N1—Zn1	178.06 (12)
F1—C2—C3—C4	-179.08 (16)	C4—C5—N1—C1	-0.6 (3)
C1—C2—C3—C4	0.0 (2)	C4—C5—N1—Zn1	-179.72 (14)
F1—C2—C3—C6	2.6 (2)	O3—Zn1—N1—C1	-133.21 (12)
C1—C2—C3—C6	-178.23 (16)	O3 ⁱ —Zn1—N1—C1	46.79 (12)
C2—C3—C4—C5	-1.7 (2)	O4 ⁱ —Zn1—N1—C1	-42.37 (12)
C6—C3—C4—C5	176.61 (16)	O4—Zn1—N1—C1	137.63 (12)
C3—C4—C5—N1	2.1 (3)	O3—Zn1—N1—C5	45.92 (14)
C2—C3—C6—O2	-148.22 (17)	O3 ⁱ —Zn1—N1—C5	-134.08 (14)
C4—C3—C6—O2	33.6 (2)	O4 ⁱ —Zn1—N1—C5	136.77 (14)
C2—C3—C6—O1	33.4 (2)	O4—Zn1—N1—C5	-43.23 (14)
C4—C3—C6—O1	-144.78 (17)		

Symmetry codes: (i) $-x+1, -y+1, -z+1$.

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

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O3—H3A \cdots O1 ⁱⁱ	0.83 (3)	1.86 (3)	2.6892 (18)	174 (2)
O3—H3B \cdots O5 ⁱⁱⁱ	0.74 (2)	2.01 (2)	2.745 (2)	176 (2)
O4—H4A \cdots O2 ^{iv}	0.79 (3)	2.05 (3)	2.837 (2)	174 (2)
O4—H4B \cdots O5 ^v	0.82 (2)	1.95 (3)	2.7643 (19)	171 (3)
O5—H5A \cdots O2	0.75 (3)	2.05 (3)	2.796 (2)	174 (3)
O5—H5B \cdots O1 ^{vi}	0.79 (2)	1.96 (3)	2.738 (2)	167 (2)
O5—H5B \cdots F1 ^{vi}	0.79 (2)	2.55 (2)	2.9929 (17)	117.2 (18)

Symmetry codes: (ii) $-x+3/2, y-1/2, -z+3/2$; (iii) $x-1/2, -y+3/2, z+1/2$; (iv) $-x+3/2, y-1/2, -z+1/2$; (v) $x-1/2, -y+3/2, z-1/2$; (vi) $x+1, y, z$.

Fig. 1

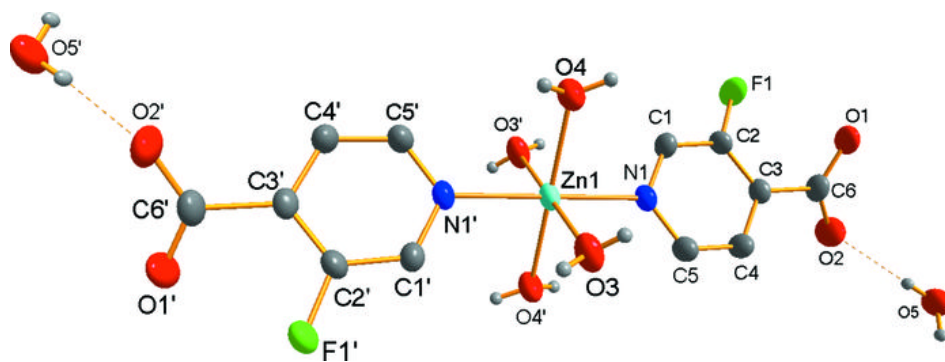


Fig. 2

