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Bis(2-aminopyridine-κN^1)bis(2-fluorobenzoato-κO)-zinc(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.042
wR factor = 0.126
Data-to-parameter ratio = 14.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $[Zn(C_7H_3FO_2)_2(C_5H_6N_2)_2]$, is a mononuclear zinc(II) compound. The Zn^{II} atom is coordinated by two N atoms from two 2-aminopyridine ligands and two O atoms from two 2-fluorobenzoate anions in a distorted tetrahedral geometry.

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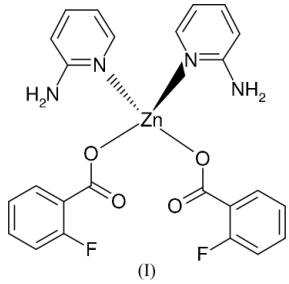
Comment

Recently, we have reported the structures of a few zinc(II) complexes (You *et al.*, 2003, 2004). As an extension of our work on the structural characterization of zinc compounds, the title compound, (I), is reported here.



(I)

Compound (I) is a mononuclear zinc(II) compound (Fig. 1). Atom Zn1 is in a tetrahedral geometry and is four-coordinated by two N atoms from two 2-aminopyridine ligands and two O atoms from two 2-fluorobenzoate anions. This ZnO_2N_2 coordination forms a distorted tetrahedral geometry, as usually observed in the structures of Zn^{II} compounds (McCleverty *et al.*, 1980), with angles subtended at atom Zn1 in the range 101.15 (10)–137.10 (10)° (Table 1). The mean Zn—O bond

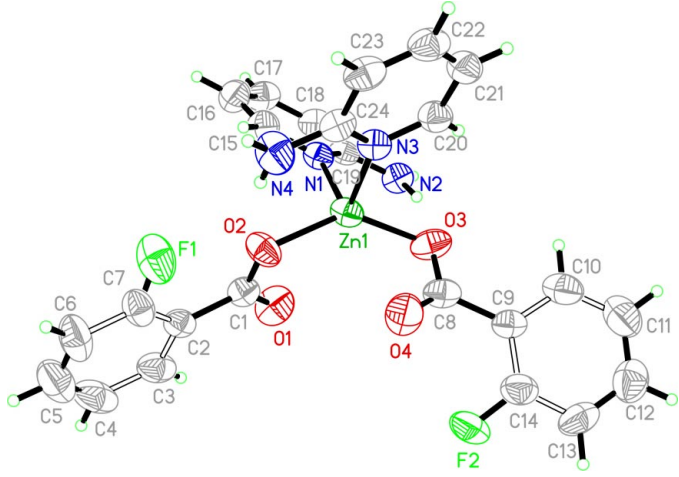


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

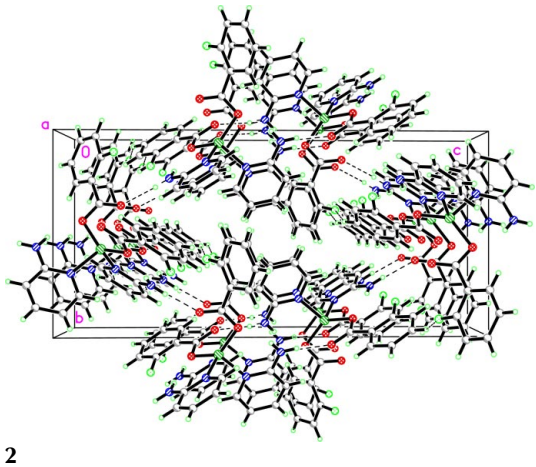


Figure 2
A packing diagram of (I), viewed along the *a* axis. Dashed lines indicate hydrogen bonds.

length [1.968 (2) Å] is shorter than the value observed in a similar Zn^{II} compound [1.987 (3) Å; Fenton *et al.*, 1998]. The mean Zn—N_{imine} bond length [2.062 (2) Å] is slightly longer than the value [2.041 (4) Å] observed in the similar compound cited above.

In the crystal structure, the molecules are linked by intermolecular N—H···O and N—H···F hydrogen bonds, forming a three-dimensional network (Table 2 and Fig. 2).

Experimental

2-Aminopyridine (0.1 mmol, 9.4 mg), 2-fluorobenzoic acid (0.1 mmol, 14.0 mg) and $Zn(CH_3COO)_2{\cdot}2H_2O$ (0.1 mmol, 22.0 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for 1 h and then filtered. The colourless filtrate was kept in air for 18 d, and colourless block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

Crystal data

$[Zn(C_7H_3FO_2)_2(C_5H_6N_2)_2]$
M_r = 531.81
Monoclinic, $P2_1/n$
a = 9.126 (2) Å
b = 11.102 (2) Å
c = 23.411 (2) Å
β = 93.707 (3)°
V = 2367.0 (7) Å^3
Z = 4
D_x = 1.492 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5568 reflections
θ = 2.5–26.7°
μ = 1.09 mm^{-1}
T = 293 (2) K
Block, colourless
0.32 × 0.22 × 0.21 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.721, T_{max} = 0.803
13 644 measured reflections
4894 independent reflections
3969 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 26.5°
$h = -11 \rightarrow 11$
$k = -12 \rightarrow 13$
$l = -19 \rightarrow 29$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.126
S = 1.02
4894 reflections
334 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0735P)^2 + 0.5892P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O2	1.962 (2)	Zn1—N3	2.056 (2)
Zn1—O3	1.975 (2)	Zn1—N1	2.069 (2)
O2—Zn1—O3	137.10 (10)	O2—Zn1—N1	101.78 (9)
O2—Zn1—N3	105.08 (9)	O3—Zn1—N1	104.43 (8)
O3—Zn1—N3	101.15 (10)	N3—Zn1—N1	103.36 (8)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O3	0.86	2.06	2.883 (3)	159
N2—H2B···O1^{i}	0.86	2.03	2.863 (3)	163
N4—H4A···F1	0.86	2.53	3.159 (4)	131
N4—H4A···O2	0.86	2.01	2.837 (3)	160
N4—H4B···O4^{ii}	0.86	2.03	2.886 (3)	175

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

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C,N). The F atoms of the 2-fluorobenzoate anions are disordered over two distinct sites, bonding to two different C atoms, *viz.* atom F1/F1′ bonded to C7/C3 and atom F2/F2′ bonded to C14/C10. The occupancies of the disordered positions F1 and F1′ (or F2 and F2′) were initially refined to 0.636 (3) and 0.364 (3) and were later fixed at 0.64 and 0.36, respectively. The unassigned maximum residual density is 1.14 Å from atom O3. The minimum residual density is 0.74 Å from atom F1.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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