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Key indicators

Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
 R factor = 0.027
 wR factor = 0.064
Data-to-parameter ratio = 13.3

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

Bis(2-aminopyridine)bis(4-fluorobenzoato)-cadmium(II)

In the title compound, $[\text{Cd}(\text{C}_7\text{H}_4\text{F}_2\text{O}_2)_2(\text{C}_5\text{H}_6\text{N}_2)_2]$, the Cd^{II} atom is six-coordinated by four O atoms from two 2-fluorobenzoate anions, and two pyridine N atoms from the two 2-aminopyridine ligands, giving a severely distorted octahedral geometry. All of the O atoms and both the amine groups of the ligands contribute to form a network consisting of intra- and intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds.

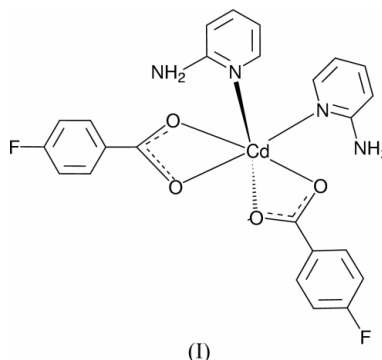
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Comment

Recently, we reported an Ni^{II} -benzoate complex with 2-aminopyridine (Xia *et al.*, 2003). As a subsequent investigation, we prepared a Cd^{II} -2-fluorobenzoate complex, (I), with 2-aminopyridine and its crystal structure is reported here.



As shown in Fig. 1, complex (I) is an electronically neutral compound which is similar to our recently reported Ni^{II} complex (Xia *et al.*, 2003). The Cd^{II} atom in the complex, six-coordinated by two imine N atoms from two 2-aminopyridine ligands and by four O atoms from two benzoate anions, exhibits an octahedral configuration. In the CdO_4N_2 polyhedron, three O atoms (O2, O3 and O4) and an N atom (N1) constitute the basal plane, with an r.m.s deviation of $0.165(1)\text{ \AA}$; the Cd atom is $0.248(1)\text{ \AA}$ above the plane towards atom N3. Atoms N3 and O1 are located at the two axial positions of the octahedron. The three *trans* angles for the Cd^{II} polyhedron are $156.71(8)$, $151.80(7)$ and $145.97(8)^\circ$, and all the other angles around the central Cd^{II} atom deviate significantly from 90° , indicating a severely distorted octahedral geometry (Table 1).

The average Cd–N bond length is $2.287(2)\text{ \AA}$, which is comparable with the Cd–N(imine) bond distances [$2.279(18)$ and $2.309(14)\text{ \AA}$] in the Cd^{II} complex with a Schiff base (Zhu *et al.*, 2003). The mean Cd–O distance of $2.366(2)\text{ \AA}$ lies in the normal Cd–O range in cadmium carboxylate complexes. The $\text{O1}-\text{Cd1}-\text{O2}$ [$55.54(7)^\circ$] and $\text{O3}-\text{Cd1}-\text{O4}$

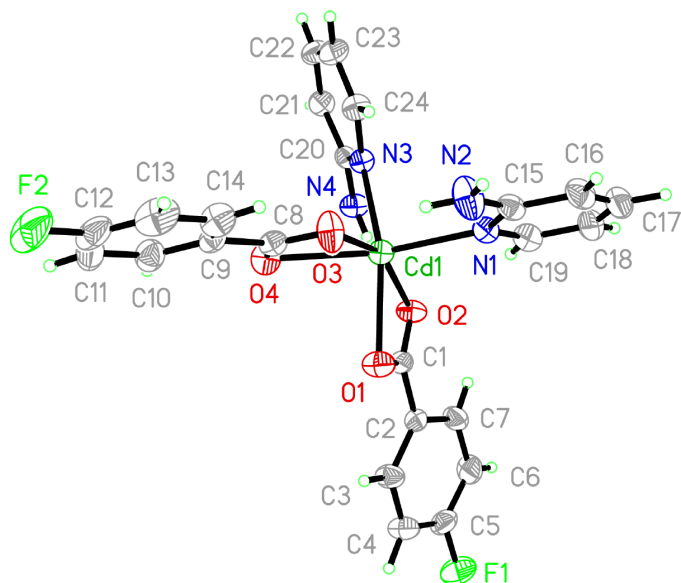


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

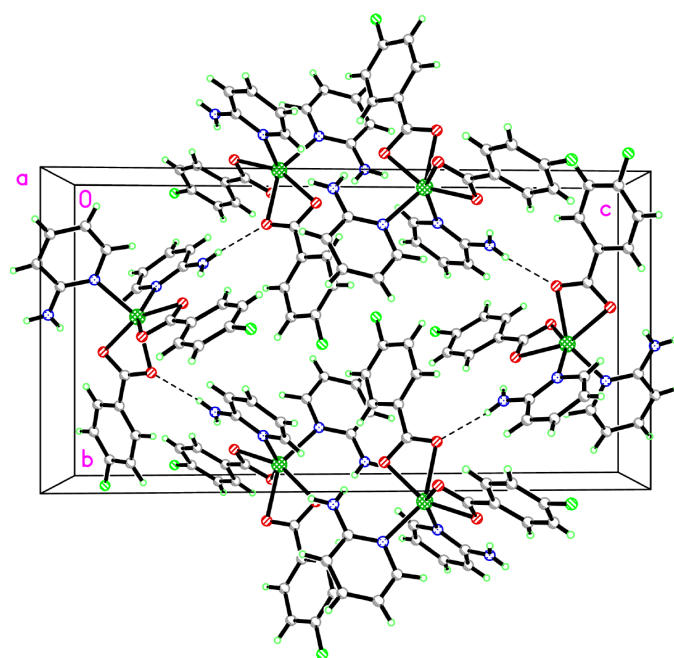


Figure 2
The crystal packing for (I), showing intermolecular N—H...O hydrogen bonds as dashed lines.

[54.33 (7)°] angles are significantly narrower than the corresponding O—Ni—O angles [62.02 (4) and 61.79 (4)°] in the Ni^{II}-benzoate complex (Xia *et al.*, 2003).

All the O atoms and the primary N atoms contribute to the formation of N—H...O hydrogen bonds (Fig. 2 and Table 2). The N—H...O hydrogen bonds link symmetry-related molecules to form a network.

Experimental

Cadmium 4-fluorobenzoate (1 mmol, 391 mg) and 2-aminopyridine (2.0 mmol, 188 mg) were suspended in a mixed solvent of acetonitrile

and water (*v/v* = 1:1, 10 ml). The suspension was stirred for *ca* 0.5 h and filtered. After keeping the filtrate in air for one week, large blue prismatic crystals were formed. They were filtered and washed three times with the same solvent mixture, and dried in a vacuum desiccator using anhydrous CaCl₂ (yield 65%). Elemental analysis found: C 50.01, H 3.60, N 9.49%; calculated for C₂₄H₂₀CdF₂N₄O₄: C 49.80, H 3.48, N 9.68%.

Crystal data

[Cd(C₇H₄F₂O₂)₂(C₅H₆N₂)₂]
M_r = 578.84
 Monoclinic, *P*2₁/*n*
a = 9.185 (4) Å
b = 11.737 (5) Å
c = 22.328 (8) Å
 β = 95.167 (6)°
V = 2397.3 (16) Å³
Z = 4

D_x = 1.604 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 5153 reflections
 θ = 2.5–26.2°
 μ = 0.96 mm⁻¹
T = 298 (2) K
 Prism, blue
 0.37 × 0.32 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.717, *T_{max}* = 0.838
 12 213 measured reflections

4208 independent reflections
 3292 reflections with *I* > 2σ(*I*)
R_{int} = 0.027
 θ_{\max} = 25.0°
h = -10 → 10
k = -13 → 13
l = -22 → 26

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.027
wR(*F*²) = 0.064
S = 1.01
 4208 reflections
 316 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0299P)^2 + 0.2894P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.51 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.43 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cd1—N1	2.285 (2)	Cd1—O1	2.339 (2)
Cd1—N3	2.288 (2)	Cd1—O2	2.369 (2)
Cd1—O3	2.333 (2)	Cd1—O4	2.421 (2)
N1—Cd1—N3	97.23 (8)	O3—Cd1—O2	156.71 (8)
N1—Cd1—O3	97.53 (8)	O1—Cd1—O2	55.54 (7)
N3—Cd1—O3	102.12 (9)	N1—Cd1—O4	151.80 (7)
N1—Cd1—O1	103.34 (8)	N3—Cd1—O4	88.23 (8)
N3—Cd1—O1	145.97 (8)	O3—Cd1—O4	54.33 (7)
O3—Cd1—O1	101.71 (8)	O1—Cd1—O4	86.26 (8)
N1—Cd1—O2	93.26 (8)	O2—Cd1—O4	113.61 (7)
N3—Cd1—O2	96.89 (8)		

Table 2

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2—H2A...O3	0.86	2.02	2.870 (4)	172
N2—H2B...O1 ⁱ	0.86	2.11	2.958 (3)	169
N4—H4A...O2	0.86	2.12	2.969 (3)	169
N4—H4B...O4 ⁱⁱ	0.86	2.10	2.914 (3)	157

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

H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms with N—H and C—H distances of 0.83 and 0.96 Å, respectively. The *U*_{iso}(H) values were set equal to 1.2*U*_{eq}(C or N).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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References

- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997a). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997b). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Xia, D.-S., Wang, Y.-F., Liu, W.-J., Zeng, Q.-F., Wang, D.-Q. & Zhu, H.-L. (2003). *Z. Kristallogr. New Cryst. Struct.* **218**, 311–312.
- Zhu, H.-L., Shao, S.-C., Ma, J.-L., Qiu, X.-Y., Sun, L. & Yang, S. (2003). *Acta Cryst.* **E59**, m843–m844.