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Poly[bis(μ_2-pyrazine-2-carboxylato)-$\kappa^3N^1,O:O';\kappa^3N^1,O:O$-cadmium(II)]

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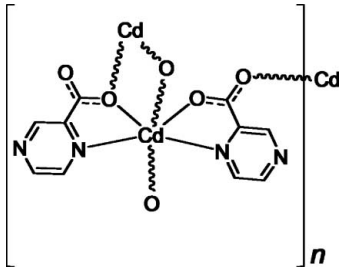
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.048; wR factor = 0.065; data-to-parameter ratio = 14.8.

In the structure of the title compound, $[Cd(C_5H_3N_2O_2)_2]_n$, the Cd^{II} ion is six-coordinated by two N atoms and four O atoms from three different pyrazine-2-carboxylate ligands. One N atom and one O atom of the carboxylate group in the ligand coordinate to the metal center, forming a five-membered chelate ring. The carboxylate anion adopts two types of bridging modes, *viz*. μ_2-O and *syn–anti*. Two Cd^{II} ions form a centrosymmetric dimer *via* a μ_2-O bridge, and the dimers are linked through the *syn–anti* carboxylate functional group, forming a two-dimensional polymeric structure extending along (100).

Related literature

The title compound is isostructural with the Mn(II) complex, see: Cai *et al.* (2002); Devereux *et al.* (2002); Liang *et al.* (2002). For a homologous Cd(II) complex with a picolinate ligand, see: Deloume & Loiseleur (1974).



Experimental

Crystal data

$[Cd(C_5H_3N_2O_2)_2]$
M_r = 358.59
Monoclinic, $P2_1/c$
a = 10.304 (2) Å
b = 11.044 (2) Å
c = 10.274 (2) Å
β = 107.89 (3)°
V = 1112.7 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.98 mm^{-1}
T = 293 K
0.18 × 0.13 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
11295 measured reflections
2550 independent reflections
1943 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.065
S = 1.16
2550 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2262).

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supporting information

Acta Cryst. (2010). E**66**, m93 [doi:10.1107/S1600536809053525]

Poly[bis(μ_2-pyrazine-2-carboxylato)-$\kappa^3N^1,O:O';\kappa^3N^1,O:O$-cadmium(II)]

Ge Liu

S1. Comment

Pyrazine-2-carboxylate is a suitable multidentate bridging ligand to build coordination polymers and several novel structural coordination polymers containing derivatives of pyrazinecarboxylate have been obtained. Here, we report the reaction of pyrazine-2-carboxylate with a Cd^{II} salt, which afforded a two-dimensional Cd^{II} coordination polymer. The compound is isostructural with the Mn^{II} complex (Cai *et al.*, 2002; Devereux *et al.*, 2002; Liang *et al.*, 2002). An isostructural Cd(II) complex including picolinate in place of pyrazine-2-carboxylate has also been X-ray characterized (Deloume & Loiseleur, 1974).

In the structure of the title compound, each Cd^{II} ion is six-coordinated by two N atoms and four O atoms from three different pyrazine-2-carboxylate ligands (Fig. 1). One N atom and one O atom of the neighboring carboxylate of the ligand coordinate to the center Cd^{II} ion forming a five-member chelate ring. The carboxylate of the ligand adopts two types of bridging mode: μ_2-O and *syn–anti*. The second N atom is not involved in bonding, so the complex is also isostructural with the Cd(II) complex with picolinate (Deloume & Loiseleur, 1974). Cd^{II} ion form a dimer *via* an μ_2-O bridge, and these dimers are linked through *syn–anti* carboxy O atoms, to form a two-dimensional structure.

S2. Experimental

A mixture of cadmium(II) nitrate (1 mmol), pyrazine-2-carboxylate (0.5 mmol), NaOH (1 mmol), tetrazolate (0.5 mmol) and water (10 ml) was sealed in a 23 ml Teflon-lined reactor, heated to 433 K at 10.8 K/h and kept at this temperature for three days, finally cooled to 303 K at 5.4 K/h (yield 20%).

S3. Refinement

Hydrogen atoms were included in calculated positions and treated as riding on their parent C atoms with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

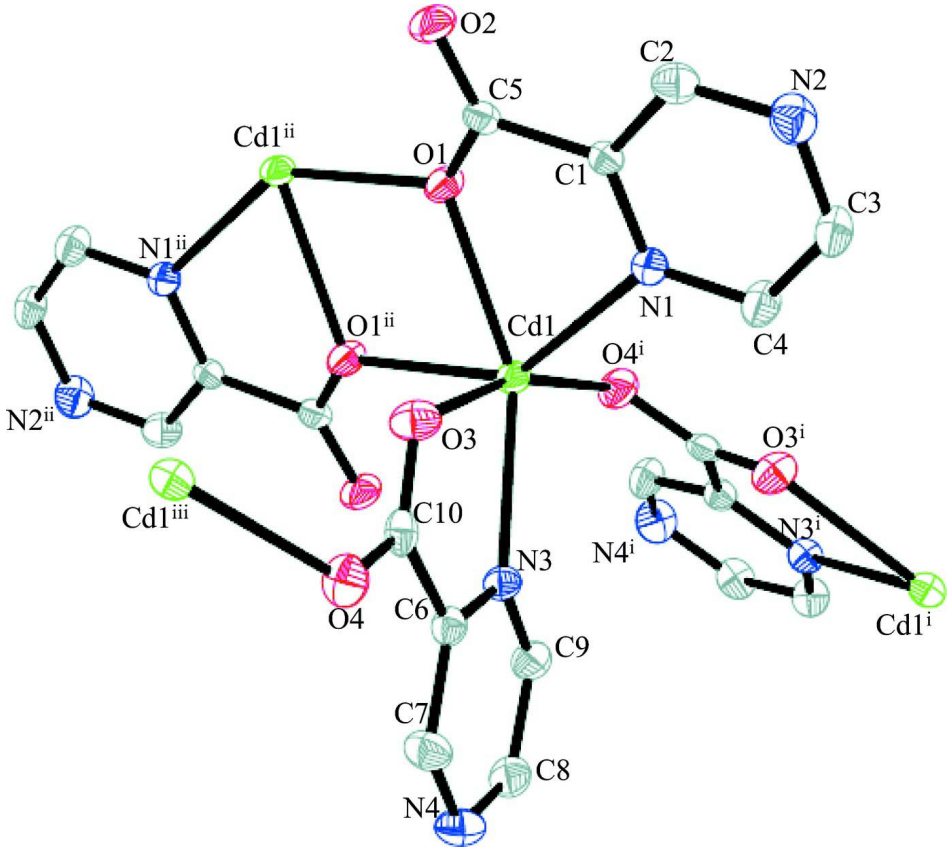

Figure 1

A view of the title compound showing the coordination of Cd atom with the atom-labelling scheme. Ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) *x*, -*y* + 3/2, *z* + 1/2; (ii) -*x*, -*y* + 1, -*z*; (iii) *x*, -*y* + 3/2, *z*

Poly[bis(μ_2-pyrazine-2-carboxylato)- $\kappa^3N^1,O:O';\kappa^3N^1,O:O$- cadmium(II)]

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c = 10.274 (2) Å
β = 107.89 (3)°
V = 1112.7 (4) Å^3
Z = 4
$F(000)$ = 696
D_x = 2.141 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9922 reflections
θ = 3.1–27.5°
μ = 1.98 mm^{-1}
T = 293 K
Block, colourless
0.18 × 0.13 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
11295 measured reflections
2550 independent reflections
1943 reflections with $I > 2\sigma(I)$
R_{int} = 0.069
θ_{max} = 27.5°, θ_{min} = 3.1°

$h = -13 \rightarrow 13$
$k = -14 \rightarrow 14$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.065$
$S = 1.16$
2550 reflections
172 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0199P)^2 + 0.0187P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.80$ e Å^{-3}
$\Delta\rho_{min} = -0.64$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3232 (4)	0.6168 (3)	0.1469 (4)	0.0246 (9)
C2	0.4605 (4)	0.6443 (4)	0.1809 (4)	0.0373 (10)
H2	0.5148	0.6004	0.1402	0.045*
C3	0.4363 (5)	0.7903 (4)	0.3276 (4)	0.0398 (12)
H3	0.4728	0.8507	0.3915	0.048*
C4	0.2983 (5)	0.7643 (4)	0.2953 (4)	0.0377 (11)
H4	0.2446	0.8077	0.3370	0.045*
C5	0.2594 (4)	0.5175 (4)	0.0442 (4)	0.0283 (10)
C6	−0.1395 (4)	0.8772 (4)	−0.0343 (4)	0.0294 (10)
C7	−0.2299 (5)	0.9723 (4)	−0.0745 (5)	0.0415 (12)
H7	−0.2229	1.0226	−0.1446	0.050*
C8	−0.3322 (5)	0.9200 (4)	0.0826 (5)	0.0412 (12)
H8	−0.3991	0.9315	0.1250	0.049*
C9	−0.2419 (4)	0.8262 (4)	0.1254 (4)	0.0376 (12)
H9	−0.2484	0.7770	0.1967	0.045*
C10	−0.0370 (4)	0.8481 (4)	−0.1094 (4)	0.0303 (10)
Cd1	0.00719 (3)	0.63837 (3)	0.10693 (3)	0.02760 (11)
N1	0.2415 (3)	0.6773 (3)	0.2048 (3)	0.0294 (8)
N2	0.5188 (4)	0.7323 (4)	0.2710 (4)	0.0438 (10)
N3	−0.1448 (3)	0.8035 (3)	0.0671 (3)	0.0298 (8)
N4	−0.3279 (4)	0.9948 (4)	−0.0163 (4)	0.0473 (11)
O1	0.1363 (3)	0.4919 (2)	0.0364 (3)	0.0345 (7)
O2	0.3285 (3)	0.4700 (3)	−0.0196 (3)	0.0416 (8)
O3	0.0344 (3)	0.7562 (3)	−0.0752 (3)	0.0396 (8)
O4	−0.0375 (3)	0.9214 (3)	−0.2042 (3)	0.0411 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.023 (2)	0.027 (2)	0.024 (2)	0.0016 (18)	0.0073 (17)	0.0029 (18)
C2	0.032 (2)	0.039 (3)	0.044 (3)	0.001 (2)	0.016 (2)	0.001 (2)
C3	0.042 (3)	0.044 (3)	0.033 (3)	−0.009 (2)	0.010 (2)	−0.011 (2)

C4	0.036 (3)	0.042 (3)	0.038 (3)	−0.008 (2)	0.015 (2)	−0.011 (2)
C5	0.026 (2)	0.027 (2)	0.030 (3)	0.005 (2)	0.006 (2)	0.003 (2)
C6	0.028 (2)	0.032 (3)	0.028 (2)	−0.003 (2)	0.0085 (18)	−0.003 (2)
C7	0.043 (3)	0.040 (3)	0.042 (3)	0.008 (2)	0.013 (2)	0.011 (2)
C8	0.034 (3)	0.053 (3)	0.040 (3)	0.005 (2)	0.017 (2)	−0.007 (3)
C9	0.039 (3)	0.042 (3)	0.035 (3)	0.004 (2)	0.017 (2)	−0.003 (2)
C10	0.026 (2)	0.039 (3)	0.025 (2)	−0.013 (2)	0.0066 (19)	−0.006 (2)
Cd1	0.02236 (16)	0.02999 (17)	0.03203 (18)	0.00188 (16)	0.01067 (12)	−0.00474 (17)
N1	0.029 (2)	0.029 (2)	0.029 (2)	0.0000 (16)	0.0077 (17)	−0.0018 (16)
N2	0.035 (2)	0.052 (2)	0.045 (2)	−0.008 (2)	0.013 (2)	−0.004 (2)
N3	0.026 (2)	0.034 (2)	0.032 (2)	0.0025 (16)	0.0122 (17)	−0.0026 (17)
N4	0.039 (2)	0.048 (3)	0.057 (3)	0.015 (2)	0.016 (2)	0.000 (2)
O1	0.0240 (16)	0.0357 (17)	0.045 (2)	−0.0046 (14)	0.0130 (14)	−0.0159 (15)
O2	0.0314 (18)	0.049 (2)	0.049 (2)	0.0041 (15)	0.0189 (16)	−0.0136 (16)
O3	0.0391 (19)	0.040 (2)	0.0485 (19)	0.0050 (15)	0.0268 (16)	0.0049 (16)
O4	0.048 (2)	0.0451 (19)	0.0348 (18)	−0.0053 (16)	0.0193 (16)	0.0032 (16)

Geometric parameters (Å, º)

C1—N1	1.348 (5)	C7—H7	0.9300
C1—C2	1.383 (5)	C8—N4	1.321 (6)
C1—C5	1.523 (5)	C8—C9	1.372 (6)
C2—N2	1.350 (5)	C8—H8	0.9300
C2—H2	0.9300	C9—N3	1.339 (5)
C3—N2	1.332 (5)	C9—H9	0.9300
C3—C4	1.388 (6)	C10—O3	1.240 (5)
C3—H3	0.9300	C10—O4	1.265 (5)
C4—N1	1.341 (5)	Cd1—O4^{i}	2.227 (3)
C4—H4	0.9300	Cd1—O1^{ii}	2.256 (3)
C5—O2	1.224 (4)	Cd1—O1	2.346 (3)
C5—O1	1.277 (4)	Cd1—N1	2.352 (3)
C6—N3	1.336 (5)	Cd1—N3	2.356 (3)
C6—C7	1.380 (5)	Cd1—O3	2.366 (3)
C6—C10	1.522 (5)	O1—Cd1^{ii}	2.256 (3)
C7—N4	1.346 (5)	O4—Cd1^{iii}	2.227 (3)
N1—C1—C2	120.6 (4)	O4—C10—C6	114.6 (4)
N1—C1—C5	117.8 (3)	O4^{i}—Cd1—O1^{ii}	96.34 (11)
C2—C1—C5	121.6 (4)	O4^{i}—Cd1—O1	110.68 (11)
N2—C2—C1	122.5 (4)	O1^{ii}—Cd1—O1	71.28 (11)
N2—C2—H2	118.8	O4^{i}—Cd1—N1	98.14 (11)
C1—C2—H2	118.8	O1^{ii}—Cd1—N1	140.96 (11)
N2—C3—C4	122.7 (4)	O1—Cd1—N1	69.70 (10)
N2—C3—H3	118.6	O4^{i}—Cd1—N3	94.39 (11)
C4—C3—H3	118.6	O1^{ii}—Cd1—N3	96.46 (11)
N1—C4—C3	120.7 (4)	O1—Cd1—N3	152.84 (11)
N1—C4—H4	119.6	N1—Cd1—N3	118.22 (11)
C3—C4—H4	119.6	O4^{i}—Cd1—O3	163.44 (10)

O2—C5—O1	126.9 (4)	O1^{ii}—Cd1—O3	92.72 (11)
O2—C5—C1	118.7 (4)	O1—Cd1—O3	85.35 (10)
O1—C5—C1	114.3 (4)	N1—Cd1—O3	83.22 (11)
N3—C6—C7	120.8 (4)	N3—Cd1—O3	70.77 (11)
N3—C6—C10	117.8 (4)	C4—N1—C1	117.6 (4)
C7—C6—C10	121.2 (4)	C4—N1—Cd1	126.8 (3)
N4—C7—C6	122.5 (4)	C1—N1—Cd1	114.8 (2)
N4—C7—H7	118.8	C3—N2—C2	115.9 (4)
C6—C7—H7	118.8	C6—N3—C9	116.7 (4)
N4—C8—C9	122.7 (4)	C6—N3—Cd1	115.1 (3)
N4—C8—H8	118.7	C9—N3—Cd1	128.0 (3)
C9—C8—H8	118.7	C8—N4—C7	115.7 (4)
N3—C9—C8	121.6 (4)	C5—O1—Cd1^{ii}	128.4 (3)
N3—C9—H9	119.2	C5—O1—Cd1	118.3 (3)
C8—C9—H9	119.2	Cd1^{ii}—O1—Cd1	108.72 (11)
O3—C10—O4	127.1 (4)	C10—O3—Cd1	118.1 (3)
O3—C10—C6	118.2 (4)	C10—O4—Cd1^{iii}	121.9 (3)

N1—C1—C2—N2	−0.7 (6)	C8—C9—N3—Cd1	−173.5 (3)
C5—C1—C2—N2	179.6 (4)	O4^{i}—Cd1—N3—C6	172.6 (3)
N2—C3—C4—N1	0.6 (7)	O1^{ii}—Cd1—N3—C6	−90.5 (3)
N1—C1—C5—O2	172.7 (4)	O1—Cd1—N3—C6	−29.6 (4)
C2—C1—C5—O2	−7.6 (6)	N1—Cd1—N3—C6	70.9 (3)
N1—C1—C5—O1	−8.3 (5)	O3—Cd1—N3—C6	0.2 (3)
C2—C1—C5—O1	171.4 (4)	O4^{i}—Cd1—N3—C9	−13.4 (3)
N3—C6—C7—N4	−0.9 (7)	O1^{ii}—Cd1—N3—C9	83.5 (3)
C10—C6—C7—N4	175.2 (4)	O1—Cd1—N3—C9	144.4 (3)
N4—C8—C9—N3	−1.2 (7)	N1—Cd1—N3—C9	−115.0 (3)
N3—C6—C10—O3	1.6 (6)	O3—Cd1—N3—C9	174.2 (4)
C7—C6—C10—O3	−174.6 (4)	C9—C8—N4—C7	0.9 (7)
N3—C6—C10—O4	179.9 (3)	C6—C7—N4—C8	0.1 (7)
C7—C6—C10—O4	3.7 (6)	O2—C5—O1—Cd1^{ii}	−5.3 (6)
C3—C4—N1—C1	0.0 (6)	C1—C5—O1—Cd1^{ii}	175.9 (2)
C3—C4—N1—Cd1	−169.2 (3)	O2—C5—O1—Cd1	−158.4 (3)
C2—C1—N1—C4	0.1 (6)	C1—C5—O1—Cd1	22.8 (4)
C5—C1—N1—C4	179.8 (3)	O4^{i}—Cd1—O1—C5	−112.2 (3)
C2—C1—N1—Cd1	170.6 (3)	O1^{ii}—Cd1—O1—C5	158.0 (4)
C5—C1—N1—Cd1	−9.7 (4)	N1—Cd1—O1—C5	−20.9 (3)
O4^{i}—Cd1—N1—C4	−66.6 (3)	N3—Cd1—O1—C5	91.6 (3)
O1^{ii}—Cd1—N1—C4	−177.3 (3)	O3—Cd1—O1—C5	63.6 (3)
O1—Cd1—N1—C4	−175.7 (4)	O4^{i}—Cd1—O1—Cd1^{ii}	89.81 (14)
N3—Cd1—N1—C4	32.9 (4)	O1^{ii}—Cd1—O1—Cd1^{ii}	0.0
O3—Cd1—N1—C4	96.7 (3)	N1—Cd1—O1—Cd1^{ii}	−178.94 (15)
O4^{i}—Cd1—N1—C1	124.0 (3)	N3—Cd1—O1—Cd1^{ii}	−66.4 (3)
O1^{ii}—Cd1—N1—C1	13.3 (4)	O3—Cd1—O1—Cd1^{ii}	−94.46 (13)
O1—Cd1—N1—C1	14.9 (3)	O4—C10—O3—Cd1	−179.5 (3)
N3—Cd1—N1—C1	−136.6 (3)	C6—C10—O3—Cd1	−1.5 (5)
O3—Cd1—N1—C1	−72.7 (3)	O4^{i}—Cd1—O3—C10	−26.6 (5)

C4—C3—N2—C2	−1.1 (7)	O1^{ii}—Cd1—O3—C10	96.6 (3)
C1—C2—N2—C3	1.2 (6)	O1—Cd1—O3—C10	167.6 (3)
C7—C6—N3—C9	0.6 (6)	N1—Cd1—O3—C10	−122.3 (3)
C10—C6—N3—C9	−175.6 (3)	N3—Cd1—O3—C10	0.7 (3)
C7—C6—N3—Cd1	175.3 (3)	O3—C10—O4—Cd1^{iii}	31.3 (5)
C10—C6—N3—Cd1	−0.9 (4)	C6—C10—O4—Cd1^{iii}	−146.8 (3)
C8—C9—N3—C6	0.4 (6)		

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