

Dong-Kui Tian, Song-Lin Li* and
 Jian-Feng Hou

Department of Chemistry, Tianjin University,
 Tianjin 300072, People's Republic of China

Correspondence e-mail: slli@tju.edu.cn

Key indicators

Single-crystal X-ray study
 T = 294 K
 Mean $\sigma(C-C)$ = 0.005 Å
 R factor = 0.056
 wR factor = 0.144
 Data-to-parameter ratio = 15.7

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

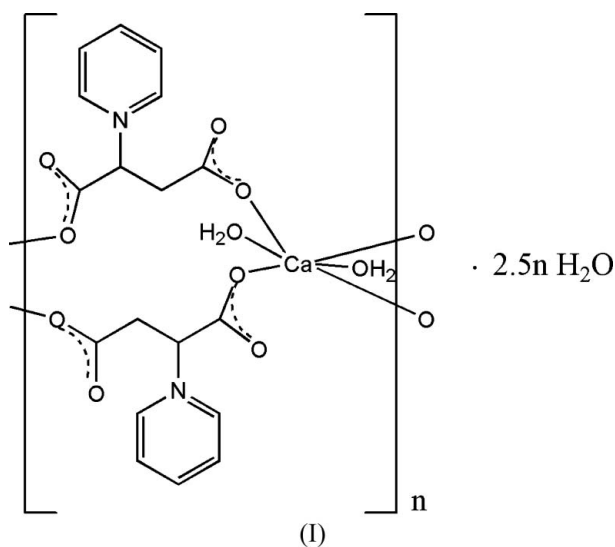
catena-Poly[[[diaquacalcium(II)]bis[μ -2-(pyridinium-1-yl)butanedioato- $\kappa O^1:O^4$]] 2.5-hydrate]

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In the title calcium carboxylate, $\{[Ca(C_9H_8NO_4)_2(H_2O)_2] \cdot 2.5H_2O\}_n$, prepared by the interaction of sodium 2-(pyridinium-1-yl)butanedioate with $CaCl_2 \cdot 6H_2O$ in water, adjacent Ca^{2+} ions are joined by a pair of racemic 2-(pyridinium-1-yl)butanedioate anions, forming coordination polymer strands which are further extended into a three-dimensional structure by hydrogen bonds between pendant O atoms of the carboxylate groups and water molecules.

Comment

As depicted in Fig. 1, the Ca^{2+} cation in the title compound, (I), is in a distorted octahedral environment with four O atoms from the carboxylate groups of four different 2-(pyridinium-1-yl)butanedioate (*L*) ligands lying in the equatorial plane, and the two aqua ligands occupying the axial positions. Although the Ca–O bond lengths [2.320–2.420 (3) Å] are normal, the angles O1W–Ca1–O2W of 157.27 (11)° and O5–Ca1–O7ⁱ of 162.23 (10)° (symmetry code as in Table 1) deviate drastically from linearity. In addition, it should be noted that the carboxylate groups of *L* act in different coordination modes: one is in a mono-*syn* mode and the other in a mono-*anti-skew* mode with the Ca^{2+} ion 0.6903 Å above the plane of the carboxylate group. With adjacent Ca^{2+} ions bridged by a pair of racemic *L* anions, compound (I) displays a one-dimensional strand structure, as shown in Fig. 2.



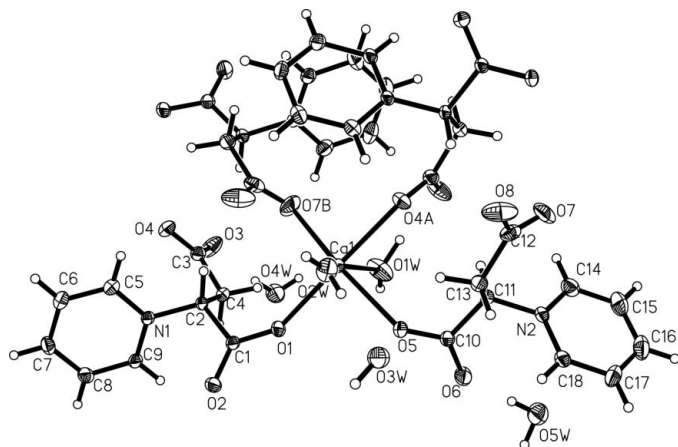


Figure 1
The coordination environment of Ca^{II} in (I). Displacement ellipsoids are drawn at the 35% probability level. [Symmetry codes: (A) $x, 2 - y, \frac{1}{2} + z$; (B) $x, 2 - y, -\frac{1}{2} + z$.]

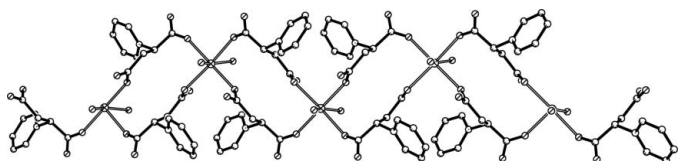


Figure 2
The one-dimensional polymer strand of compound (I). H atoms have been omitted for clarity.

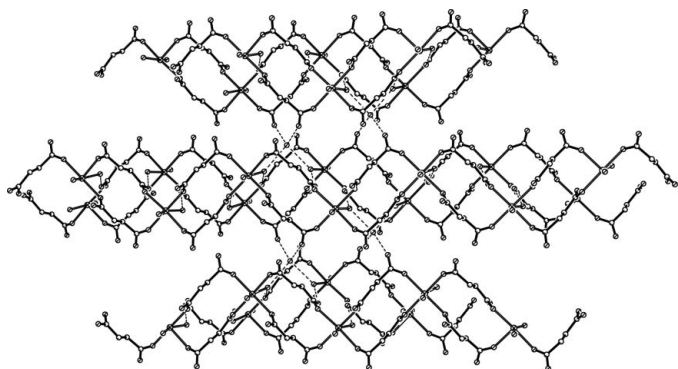


Figure 3
The hydrogen-bonded layer structure of (I). Pyridyl rings and H atoms have been omitted for clarity.

molecules (Fig. 3). In constructing the layer, atom O3W, which is located on an inversion center, acts as hydrogen-bond donor to two pendant O atoms of two carboxylate groups from two strands [$\text{O3W} \cdots \text{O2}^{\text{v}}$ and $= \text{O3W} \cdots \text{O2}^{\text{viii}}$ 2.936 (3) Å; symmetry code (v) as in Table 2; (viii) $-x, 1 - y, z + \frac{1}{2}$] and hydrogen-bond acceptor to an aqua ligand of the third strand [$\text{O3W} \cdots \text{O2W} = 2.951$ (3) Å]. Different layers are connected into a three-dimensional structure through various intermolecular hydrogen-bond interactions between pendant O atoms [$\text{O5W} \cdots \text{O6} = 2.762$ (3) Å and $\text{O4W} \cdots \text{O3} = 2.672$ (3) Å] and aqua ligands [$\text{O4W} \cdots \text{O1W}^{\text{iii}} = 2.730$ (3) Å].

Experimental

N-Succinopyridine was prepared according to the procedures of Kostyanovsky *et al.* (2003) and Kotov *et al.* (2001). The sodium salt NaL was obtained by neutralization of HL with NaOH in aqueous solution and recrystallization in water. Compound (I) was prepared by reaction of NaL (0.217 mg, 1 mmol) and $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$ in distilled water (5 ml). Crystals of (I) suitable for X-ray structure analysis were obtained by standing the reaction mixture for several days at ambient temperature.

Crystal data

$[\text{Ca}(\text{C}_9\text{H}_8\text{NO}_4)_2(\text{H}_2\text{O})_2] \cdot 2.5\text{H}_2\text{O}$
 $M_r = 509.48$
 Monoclinic, $C2/c$
 $a = 31.766$ (14) Å
 $b = 9.8281$ (13) Å
 $c = 14.2746$ (16) Å
 $\beta = 103.018$ (16)°
 $V = 4342$ (2) Å³
 $Z = 8$

$D_x = 1.559$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 40 reflections
 $\theta = 9.3$ – 25.8°
 $\mu = 0.36$ mm⁻¹
 $T = 294$ (2) K
 Block, colorless
 $0.28 \times 0.22 \times 0.20$ mm

Data collection

Siemens P4 diffractometer
 ω scans
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 $T_{\text{min}} = 0.909$, $T_{\text{max}} = 0.930$
 5549 measured reflections
 4744 independent reflections
 3569 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$
 $\theta_{\text{max}} = 27.0^\circ$
 $h = -1 \rightarrow 40$
 $k = -1 \rightarrow 12$
 $l = -18 \rightarrow 17$
 3 standard reflections
 every 120 reflections
 intensity decay: 8%

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.056$
 $wR(F^2) = 0.144$
 $S = 1.13$
 4744 reflections
 303 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2 + 15.5672P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.44$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.32$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ca1—O1	2.320 (2)	O2—C1	1.240 (4)
Ca1—O5	2.335 (2)	O3—C3	1.244 (4)
Ca1—O7 ⁱ	2.348 (3)	O4—C3	1.245 (4)
Ca1—O1W	2.352 (3)	O5—C10	1.259 (4)
Ca1—O4 ⁱⁱ	2.357 (2)	O6—C10	1.235 (4)
Ca1—O2W	2.421 (3)	O7—C12	1.248 (5)
O1—C1	1.263 (3)	O8—C12	1.245 (4)
O1—Ca1—O5	90.03 (8)	O7 ⁱ —Ca1—O2W	117.15 (10)
O1—Ca1—O7 ⁱ	91.38 (10)	O1W—Ca1—O2W	157.27 (11)
O5—Ca1—O7 ⁱ	162.23 (10)	O4 ⁱⁱ —Ca1—O2W	87.40 (9)
O1—Ca1—O1W	97.24 (10)	C1—O1—Ca1	151.0 (2)
O5—Ca1—O1W	80.08 (11)	O2—C1—O1	125.8 (3)
O7 ⁱ —Ca1—O1W	82.14 (12)	C3—O4—Ca1 ⁱ	135.4 (2)
O1—Ca1—O4 ⁱⁱ	178.11 (9)	O3—C3—O4	125.0 (3)
O5—Ca1—O4 ⁱⁱ	89.36 (8)	O3—C3—C4	117.1 (3)
O7 ⁱ —Ca1—O4 ⁱⁱ	88.66 (10)	C10—O5—Ca1	139.1 (2)
O1W—Ca1—O4 ⁱⁱ	80.89 (9)	O6—C10—O5	126.0 (3)
O1—Ca1—O2W	94.27 (9)	O8—C12—O7	123.1 (4)
O5—Ca1—O2W	80.38 (9)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H10A \cdots O4W ⁱⁱⁱ	0.89	1.84	2.730 (4)	179
O1W—H10B \cdots O3 ⁱⁱ	0.98	1.80	2.715 (4)	154
O2W—H20A \cdots O3W	0.81	2.14	2.951 (4)	178
O2W—H20B \cdots O8 ^{iv}	0.87	1.92	2.771 (4)	166
O3W—H30A \cdots O2 ^v	0.90	2.05	2.935 (3)	167
O4W—H40A \cdots O3	0.87	1.81	2.672 (4)	170
O4W—H40B \cdots O5W ^{vi}	0.83	1.99	2.798 (4)	165
O5W—H50A \cdots O6	0.93	1.84	2.761 (4)	174
O5W—H50B \cdots O4W ^{vii}	0.92	1.96	2.845 (4)	162

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

All H atoms were located in a difference Fourier map and allowed to ride on their respective parent atoms. For the CH and CH₂ groups, $U_{\text{iso}}(\text{H})$ values were set equal to $1.2U_{\text{eq}}(\text{carrier atom})$ and for the water molecules, they were set equal to $1.5U_{\text{eq}}(\text{carrier atom})$.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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