

Polymeric disodium (μ -*trans*-4,4'-ethylene-dipyridyl)bis[μ -5-sulfoisophthalato(3-)]-dicadmate(II) hexahydrate

Jun Tao,^a Xin Yin,^a Rong-Bin Huang,^a Lan-Sun Zheng^a and Seik Weng Ng^{b*}

^aDepartment of Chemistry, Xiamen University, Xiamen 361005, People's Republic of China, and ^bDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

The title crystal structure, $\{Na_2[Cd_2(C_{12}H_{10}N_2)(C_8H_3O_7S)_2] \cdot 6H_2O\}_n$, contains pentagonal-bipyramidal Cd atoms and octahedral Na atoms. The Cd atom is chelated by two carboxyl groups of adjacent 5-sulfoisophthalate(3-) trianions, and it is also coordinated by the pyridyl group of the centrosymmetric heterocycle, the coordinating atoms comprising the pentagonal plane around the metal atom. In the network structure, the Na atoms occupy the voids in the network such that they exist in a six-coordinate geometry.

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Key indicators

Single-crystal X-ray study

$T = 298\text{ K}$

Mean $\sigma(C-C) = 0.003\text{ \AA}$

R factor = 0.027

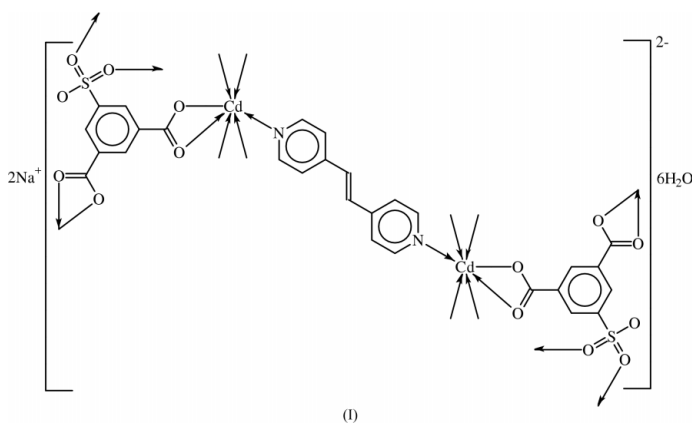
wR factor = 0.063

Data-to-parameter ratio = 15.0

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

Comment

A recent investigation of the reaction between monosodium 5-sulfoisophthalate and cadmium nitrate, in the presence of the N-donor ligand 1,4-diazobicyclo[2.2.2]octane, has reported zwitterionic aqua(5-sulfoisophthalato(1-aza-4-azoniabicyclo[2.2.2]octane)cadmate. In the crystal structure, the 5-sulfoisophthalate trianion interacts with three symmetry-related Cd atoms; the Cd atom itself is coordinated by the mono-protonated N-donor ligand [$Cd \leftarrow N = 2.437(2)\text{ \AA}$; Tao *et al.*, 2003]. The analogous reaction, which was carried out in the presence of 4,4'-*trans*-dipyridylethylene, led to the title Cd complex, (I), having two dative $Cd \leftarrow$ bonds; the bridging spacer has an inversion center at the mid-point of the central $C=C$ bond (Fig. 1 and Table 1).



In the dianion of (I), the Cd atom is chelated by the carboxyl group of one 5-sulfoisophthalate(3-) trianion [$Cd-O = 2.265(2)$ and $2.564(2)\text{ \AA}$, and $O-Cd-O = 53.4(1)^\circ$] and by that of another trianion [$Cd-O = 2.306(2)$ and $2.528(2)\text{ \AA}$, and $O-Cd-O = 53.6(1)^\circ$]. The fifth coordination site of the pentagonal plane is occupied by the N atom of the heterocycle [$Cd-N = 2.285(2)\text{ \AA}$]; the apical sites are occupied by the sulfonyl O atoms [$Cd-O = 2.342(2)$ and $2.402(2)\text{ \AA}$, and $O-Cd-O = 162.9(1)^\circ$]. The $Cd-O$ and $Cd-N$ bonds lead to the formation of a network structure; the

Na atoms occupy the voids in the network such that each exists in a six-coordinate geometry. The network structure is further consolidated by hydrogen-bonding interactions (Table 2).

Experimental

The hydrothermal synthesis was carried out with cadmium nitrate tetrahydrate (0.15 g, 0.5 mmol), the monosodium salt of 5-sulfoisophthalic acid (0.13 g, 0.5 mmol) and 4,4'-dipyridylethylene (0.09 g, 0.5 mmol) in the manner used for the preparation of a previous cadmium complex (Tao *et al.*, 2003). A volume of sodium hydroxide solution corresponding to twice the molar equivalent of Cd²⁺ was used to convert the acid to its trianion.

Crystal data

Na₂[Cd₂(C₁₂H₁₀N₂)(C₈H₃O₇S)₂]-6H₂O
M_r = 1047.42
 Monoclinic, *P*₂₁/*n*
a = 8.9936 (4) Å
b = 16.2164 (7) Å
c = 12.4217 (5) Å
 β = 101.999 (1)°
V = 1772.1 (1) Å³
Z = 2
D_x = 1.963 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 6328 reflections
 θ = 2.1–28.3°
 μ = 1.43 mm⁻¹
T = 298 (2) K
 Block, colorless
 0.30 × 0.28 × 0.22 mm

Data collection

Bruker APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.570, *T_{max}* = 0.730
 10 511 measured reflections
 4075 independent reflections
 3510 reflections with *I* > 2σ(*I*)
R_{int} = 0.022
 θ_{max} = 28.3°
h = -11 → 5
k = -19 → 20
l = -12 → 16

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.027
wR (*F*²) = 0.063
S = 0.95
 4075 reflections
 271 parameters
 H-atom parameters constrained
w = 1/[σ²(*F_o*²) + (0.0365*P*)²]
 where *P* = (*F_o*² + 2*F_c*²)/3
 (Δ/σ)_{max} = 0.001
 Δρ_{max} = 0.85 e Å⁻³
 Δρ_{min} = -0.43 e Å⁻³

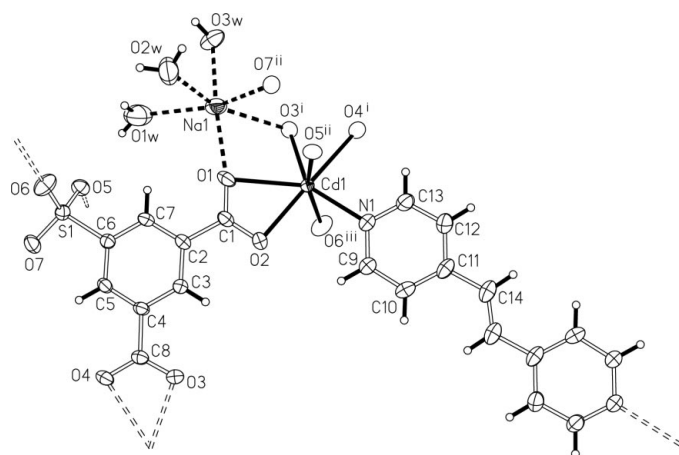


Figure 1
 ORTEPII (Johnson, 1976) plot of a segment of the title structure, with displacement ellipsoids drawn at the 50% probability level. [Symmetry codes: (i) $\frac{3}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$; (ii) $x - \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} + z$; (iii) $x - 1, y, z$.]

Table 1
 Selected geometric parameters (Å, °).

Cd1—O1	2.528 (2)	Na1—O1	2.291 (2)
Cd1—O2	2.306 (2)	Na1—O3 ⁱ	2.686 (2)
Cd1—O3 ⁱ	2.265 (2)	Na1—O7 ⁱⁱ	2.421 (2)
Cd1—O4 ⁱ	2.564 (2)	Na1—O1 _w	2.676 (3)
Cd1—O5 ⁱⁱ	2.342 (2)	Na1—O2 _w	2.384 (3)
Cd1—O6 ⁱⁱⁱ	2.402 (2)	Na1—O3 _w	2.349 (2)
Cd1—N1	2.285 (2)		
O1—Cd1—O2	53.6 (1)	O5 ⁱⁱ —Cd1—O6 ⁱⁱⁱ	162.9 (1)
O1—Cd1—O3 ⁱ	75.0 (1)	O5 ⁱⁱ —Cd1—N1	82.2 (1)
O1—Cd1—O4 ⁱ	126.6 (1)	O6 ⁱⁱⁱ —Cd1—N1	80.8 (1)
O1—Cd1—O5 ⁱⁱ	86.2 (1)	O1—Na1—O3 ⁱ	71.5 (1)
O1—Cd1—O6 ⁱⁱⁱ	109.0 (1)	O1—Na1—O7 ⁱⁱ	93.3 (1)
O1—Cd1—N1	143.3 (1)	O1—Na1—O1 _w	95.1 (1)
O2—Cd1—O3 ⁱ	122.7 (1)	O1—Na1—O2 _w	113.3 (1)
O2—Cd1—O4 ⁱ	170.1 (1)	O1—Na1—O3 _w	163.1 (1)
O2—Cd1—O5 ⁱⁱ	99.9 (1)	O3 ⁱ —Na1—O7 ⁱⁱ	75.6 (1)
O2—Cd1—O6 ⁱⁱⁱ	83.7 (1)	O3 ⁱ —Na1—O1 _w	127.9 (1)
O2—Cd1—N1	94.3 (1)	O3 ⁱ —Na1—O2 _w	155.3 (1)
O3 ⁱ —Cd1—O4 ⁱ	53.4 (1)	O3 ⁱ —Na1—O3 _w	95.9 (1)
O3 ⁱ —Cd1—O5 ⁱⁱ	100.2 (1)	O7 ⁱⁱ —Na1—O1 _w	156.6 (1)
O3 ⁱ —Cd1—O6 ⁱⁱⁱ	91.7 (1)	O7 ⁱⁱ —Na1—O2 _w	79.9 (1)
O3 ⁱ —Cd1—N1	141.3 (1)	O7 ⁱⁱ —Na1—O3 _w	94.5 (1)
O4 ⁱ —Cd1—O5 ⁱⁱ	90.0 (1)	O1 _w —Na1—O2 _w	76.6 (1)
O4 ⁱ —Cd1—O6 ⁱⁱⁱ	87.2 (1)	O1 _w —Na1—O3 _w	83.6 (1)
O4 ⁱ —Cd1—N1	88.2 (1)	O2 _w —Na1—O3 _w	82.9 (1)

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

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>
O1 _w —H1 _w 1...O5	0.86	2.26	3.094 (3)	164
O1 _w —H1 _w 2...O4 ⁱ	0.85	2.27	3.109 (4)	170
O2 _w —H2 _w 2...O4 ⁱ	0.85	2.00	2.790 (3)	156
O2 _w —H2 _w 1...O3 _w ^{iv}	0.85	2.13	2.958 (3)	164
O3 _w —H3 _w 1...O2 ^v	0.86	1.95	2.782 (3)	162
O3 _w —H3 _w 2...O7 ⁱ	0.85	2.10	2.887 (3)	153

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

The H atoms bonded to water were located and refined subject to O—H = 0.85 (1) Å and H...H = 1.39 (1) Å. The C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and were included in the refinement in the riding-model approximation. The displacement parameters of all H atoms were set to 1.2 times the equivalent isotropic displacement parameters of their parent atoms.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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