catena-Poly[[zinc-bis(*μ*-2-sulfido-1*H*-benzimidazol-3-ium-5-carboxylato)-*κ²O:S;κ²S:O*] trihydrate]

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In the title compound, $\{[Zn(C_8H_5N_2O_2S)_2]\cdot3H_2O\}_n$, the Zn^{II} atom, lying on a twofold rotation axis, is four-coordinated by two S atoms and two O atoms from four 2-sulfido-1*H*-benzimidazol-3-ium-5-carboxylate (H_2mbidc) ligands in a distorted tetrahedral geometry. Two H_2mbidc ligands bridge two Zn^{II} atoms, generating a double-chain along [$\bar{1}$01]. Adjacent chains are linked by N—H···O and O—H···O hydrogen bonds, forming a three-dimensional supramolecular network. One of the two water molecules also lies on a twofold rotation axis.

Related literature

For coordination polymers with helical chain structures, see: Chen & Liu (2002); Cui *et al.* (2003); Hu *et al.* (2008); Ngo & Lin (2002); Xiao *et al.* (2007); Yan *et al.* (2005).
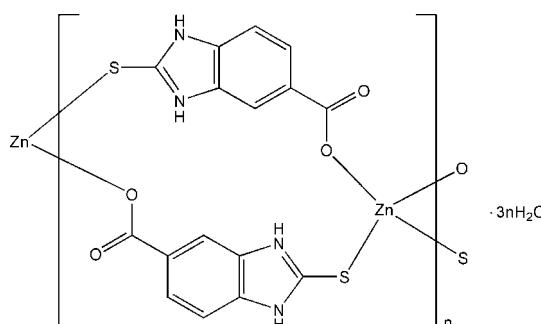
Experimental

Crystal data

$[Zn(C_8H_5N_2O_2S)_2]\cdot3H_2O$	$V = 965.6$ (6) Å³
$M_r = 505.86$	$Z = 2$
Monoclinic, $P2/n$	Mo $K\alpha$ radiation
$a = 8.031$ (1) Å	$\mu = 1.54$ mm⁻¹
$b = 9.732$ (3) Å	$T = 293$ K
$c = 12.436$ (7) Å	$0.20 \times 0.18 \times 0.15$ mm
$\beta = 96.584$ (9)°	

Data collection

Bruker APEXII CCD diffractometer	4749 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	1710 independent reflections
	1267 reflections with $I > 2\sigma(I)$
$T_{min} = 0.749$, $T_{max} = 0.802$	$R_{int} = 0.049$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$	137 parameters
$wR(F^2) = 0.099$	H-atom parameters constrained
$S = 0.98$	$\Delta\rho_{max} = 0.42$ e Å⁻³
1710 reflections	$\Delta\rho_{min} = -0.28$ e Å⁻³

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1W	0.86	1.88	2.738 (5)	174
N2—H2···O1^i	0.86	1.98	2.812 (4)	163
O1W—H1A···O2^{ii}	0.84	2.21	2.907 (4)	140
O2W—H2A···O1	0.82	2.02	2.837 (4)	177

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL*.

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supporting information

catena-Poly[[zinc-bis(*μ*-2-sulfido-1*H*-benzimidazol-3-ium-5-carboxylato)-*κ²O:S;κ²S:O*] trihydrate]

Ya-Ping Li, Da-Jun Sun, Hu Zang, Li-Ying Han and Guan-Fang Su

S1. Comment

In recent years, the synthesis of novel coordination polymers with helical structures has attracted much attention owing to the fundamental role of helicity in biology and their potential utilization in advanced materials (Cui *et al.*, 2003; Ngo & Lin, 2002; Yan *et al.*, 2005). In general, the V-shaped organic ligands have already been proven to be efficient for the generation of helical complexes (Chen & Liu, 2002; Hu *et al.*, 2008; Xiao *et al.*, 2007). 2-Mercapto-1*H*-benzo[*d*]imidazole-5-carboxylic acid (H₃mbidc) is a rigid V-shaped ligand, in which the S atom can coordinate to a variety of metal ions and the carboxylate group can adopt rich coordination modes, meeting the requirements of the coordination geometries of metal ions in assembly process. We selected H₃mbidc as a bridging ligand and Zn^{II} ion as a metal center, generating a new double-chain coordination polymer, whose structure is reported here.

In the title compound (Fig. 1), the Zn^{II} atom is four-coordinated by two S atoms and two carboxylate O atoms from four individual H₂mbidc ligands in a distorted tetrahedral coordination geometry. The Cd—O and Cd—S bond lengths are 1.987 (3) and 2.3159 (12) Å. Each H₂mbidc ligand bridges two neighboring Zn^{II} atoms, generating a double-chain (Fig. 2). Furthermore, N—H···O and O—H···O hydrogen bonds (Table 1) link the chains together, resulting in a supramolecular structure.

S2. Experimental

A mixture of H₃mbidc (0.971 g, 5 mmol), NaOH (0.4 g, 10 mmol) and ZnCl₂ (1.36 g, 10 mmol) in water (50 ml) was boiled for 20 min with stirring. Then the mixture was cooled to room temperature. The resulting solution was filtered and allowed to stand. After a week, colorless crystals of the title compound were obtained.

S3. Refinement

H atoms on C and N were positioned geometrically and refined as riding atoms, with C—H = 0.93 and N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(C,N). H atoms of water molecules were located in a difference Fourier map and refined as riding atoms, with U_{iso}(H) = 1.5U_{eq}(O).
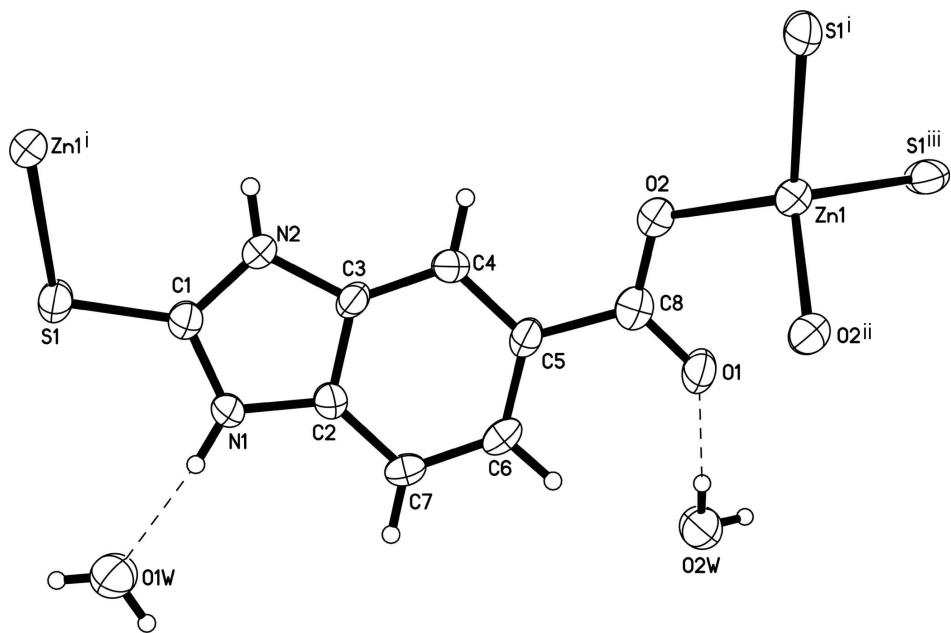
Figure 1

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. Dashed lines denote hydrogen bonds. [Symmetry codes: (i) 1 - *x*, 1 - *y*, 2 - *z*; (ii) 3/2 - *x*, *y*, 3/2 - *z*; (iii) 1/2 + *x*, 1 - *y*, -1/2 + *z*.]
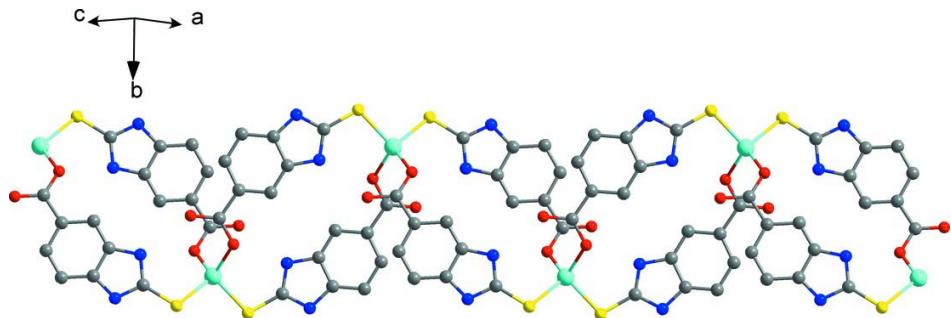
Figure 2

A view of the double-chain structure in the title compound.

***catena*-Poly[[zinc-bis(*µ*-2-sulfido-1*H*-benzimidazol-3-ium-5-carboxylato)-*κ²O*:*S*;*κ²S*:*O*] trihydrate]**

Crystal data
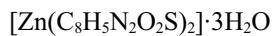
[Zn(C$_8$H$_5$N$_2$O$_2$S)$_2$]·3H$_2$O	$F(000) = 516$
$M_r = 505.86$	$D_x = 1.740$ Mg m^{-3}
Monoclinic, $P2/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yac	Cell parameters from 4749 reflections
$a = 8.031$ (1) Å	$\theta = 1.3–26.0°$
$b = 9.732$ (3) Å	$\mu = 1.54$ mm^{-1}
$c = 12.436$ (7) Å	$T = 293$ K
$\beta = 96.584$ (9)°	Block, colorless
$V = 965.6$ (6) Å^3	$0.20 \times 0.18 \times 0.15$ mm
$Z = 2$	

Data collection

Bruker APEXII CCD diffractometer	4749 measured reflections
Radiation source: fine-focus sealed tube	1710 independent reflections
Graphite monochromator	1267 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.049$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
	$h = -9 \rightarrow 8$
$T_{min} = 0.749$, $T_{max} = 0.802$	$k = -9 \rightarrow 11$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.042$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.099$	
$S = 0.98$	H-atom parameters constrained
1710 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 0.5228P]$ where $P = (F_o^2 + 2F_c^2)/3$
137 parameters	
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.42$ e Å^{-3}
	$\Delta\rho_{min} = -0.28$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.7500	0.20862 (7)	0.7500	0.0295 (2)
S1	0.46579 (13)	0.94066 (11)	1.22275 (9)	0.0366 (3)
O1	0.9750 (3)	0.4579 (3)	0.7829 (2)	0.0360 (7)
O2	0.8006 (3)	0.3368 (3)	0.8738 (2)	0.0323 (7)
N1	0.6753 (4)	0.9126 (3)	1.0706 (2)	0.0283 (8)
H1	0.6905	0.9997	1.0655	0.034*
N2	0.5899 (4)	0.7152 (3)	1.1261 (2)	0.0298 (8)
H2	0.5423	0.6551	1.1630	0.036*
C1	0.5795 (4)	0.8514 (4)	1.1382 (3)	0.0266 (9)
C2	0.7452 (4)	0.8136 (4)	1.0112 (3)	0.0258 (9)
C3	0.6897 (4)	0.6859 (4)	1.0445 (3)	0.0249 (9)
C4	0.7307 (4)	0.5650 (4)	0.9970 (3)	0.0269 (9)
H4	0.6920	0.4807	1.0191	0.032*
C5	0.8334 (4)	0.5746 (4)	0.9136 (3)	0.0261 (9)
C6	0.8901 (5)	0.7016 (4)	0.8817 (3)	0.0325 (10)
H6	0.9578	0.7048	0.8259	0.039*
C7	0.8494 (5)	0.8233 (4)	0.9299 (3)	0.0348 (10)
H7	0.8900	0.9075	0.9089	0.042*
C8	0.8752 (5)	0.4488 (4)	0.8531 (3)	0.0280 (9)
O1W	0.7018 (4)	1.1927 (3)	1.0612 (2)	0.0472 (8)
H1A	0.7766	1.2210	1.0243	0.071*
H1B	0.6896	1.2530	1.1073	0.071*
O2W	1.2500	0.6297 (5)	0.7500	0.0456 (11)
H2A	1.1720	0.5777	0.7590	0.068*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0350 (4)	0.0257 (4)	0.0303 (4)	0.000	0.0144 (3)	0.000
S1	0.0409 (7)	0.0283 (7)	0.0448 (6)	−0.0041 (5)	0.0230 (5)	−0.0092 (5)
O1	0.0392 (16)	0.0356 (18)	0.0363 (16)	−0.0035 (14)	0.0184 (13)	−0.0098 (14)
O2	0.0401 (16)	0.0301 (18)	0.0289 (15)	−0.0035 (13)	0.0129 (12)	−0.0031 (12)
N1	0.0341 (19)	0.0180 (18)	0.0353 (18)	−0.0021 (15)	0.0148 (15)	−0.0016 (15)
N2	0.0358 (19)	0.025 (2)	0.0323 (18)	−0.0004 (16)	0.0181 (15)	0.0008 (16)
C1	0.026 (2)	0.026 (2)	0.029 (2)	0.0005 (18)	0.0077 (17)	−0.0018 (17)
C2	0.026 (2)	0.022 (2)	0.030 (2)	0.0017 (17)	0.0081 (16)	−0.0006 (17)
C3	0.026 (2)	0.030 (2)	0.0206 (18)	0.0023 (17)	0.0088 (16)	0.0013 (17)
C4	0.029 (2)	0.023 (2)	0.030 (2)	0.0004 (17)	0.0091 (17)	0.0042 (17)
C5	0.028 (2)	0.031 (2)	0.0209 (19)	0.0029 (18)	0.0067 (16)	−0.0017 (17)
C6	0.033 (2)	0.038 (3)	0.029 (2)	−0.003 (2)	0.0162 (17)	0.003 (2)
C7	0.042 (2)	0.028 (3)	0.039 (2)	−0.0067 (19)	0.021 (2)	0.0044 (19)
C8	0.025 (2)	0.035 (3)	0.024 (2)	0.0016 (19)	−0.0012 (17)	−0.0022 (18)
O1W	0.064 (2)	0.0356 (19)	0.0453 (18)	−0.0104 (16)	0.0178 (15)	−0.0048 (15)
O2W	0.046 (3)	0.037 (3)	0.058 (3)	0.000	0.023 (2)	0.000

Geometric parameters (Å, º)

Zn1—O2	1.987 (3)	C2—C3	1.400 (5)
Zn1—S1^i	2.3159 (12)	C3—C4	1.374 (5)
S1—C1	1.707 (4)	C4—C5	1.400 (5)
O1—C8	1.254 (4)	C4—H4	0.9300
O2—C8	1.284 (5)	C5—C6	1.391 (5)
N1—C1	1.342 (4)	C5—C8	1.494 (5)
N1—C2	1.373 (5)	C6—C7	1.384 (6)
N1—H1	0.8600	C6—H6	0.9300
N2—C1	1.338 (5)	C7—H7	0.9300
N2—C3	1.392 (4)	O1W—H1A	0.84
N2—H2	0.8600	O1W—H1B	0.83
C2—C7	1.388 (5)	O2W—H2A	0.82
O2—Zn1—O2^{ii}	102.22 (17)	C4—C3—N2	132.5 (4)
O2—Zn1—S1^i	111.74 (8)	C4—C3—C2	122.2 (3)
O2^{ii}—Zn1—S1^i	114.66 (8)	N2—C3—C2	105.3 (3)
O2—Zn1—S1^{iii}	114.66 (8)	C3—C4—C5	116.9 (4)
O2^{ii}—Zn1—S1^{iii}	111.74 (8)	C3—C4—H4	121.5
S1^i—Zn1—S1^{iii}	102.30 (6)	C5—C4—H4	121.5
C1—S1—Zn1^i	103.48 (14)	C6—C5—C4	120.7 (4)
C8—O2—Zn1	115.9 (2)	C6—C5—C8	119.0 (3)
C1—N1—C2	109.0 (3)	C4—C5—C8	120.2 (4)
C1—N1—H1	125.5	C7—C6—C5	122.4 (3)
C2—N1—H1	125.5	C7—C6—H6	118.8
C1—N2—C3	109.5 (3)	C5—C6—H6	118.8
C1—N2—H2	125.3	C6—C7—C2	116.7 (4)

C3—N2—H2	125.3	C6—C7—H7	121.6
N2—C1—N1	108.8 (3)	C2—C7—H7	121.6
N2—C1—S1	128.2 (3)	O1—C8—O2	123.3 (4)
N1—C1—S1	123.1 (3)	O1—C8—C5	119.4 (4)
N1—C2—C7	131.5 (4)	O2—C8—C5	117.2 (3)
N1—C2—C3	107.4 (3)	H1A—O1W—H1B	107.0
C7—C2—C3	121.0 (4)		

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

Hydrogen-bond geometry (Å, º)

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N1—H1⋯O1*W*	0.86	1.88	2.738 (5)	174
N2—H2⋯O1[iv]	0.86	1.98	2.812 (4)	163
O1*W*—H1*A*⋯O2[v]	0.84	2.21	2.907 (4)	140
O2*W*—H2*A*⋯O1	0.82	2.02	2.837 (4)	177

Symmetry codes: (iv) *x*−1/2, −*y*+1, *z*+1/2; (v) *x*, *y*+1, *z*.