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Crystal structure of *poly*-[diaqua-bis(μ_2 -2-((1*H*-1,2,4-triazol-5-yl)thio)acetato- κ^2 N:O)cadmium(II)], $C_8H_8CdN_6O_6S_2$

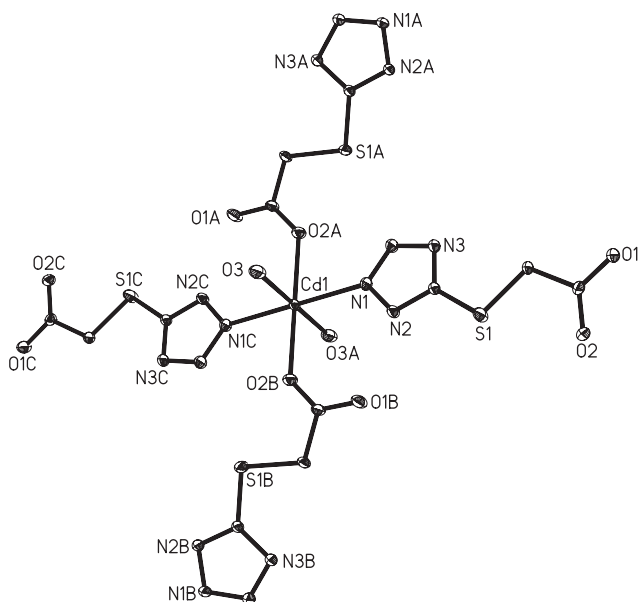


Table 1: Data collection and handling.

Crystal:	Colourless block
Wavelength:	Size $0.34 \times 0.30 \times 0.29$ mm
μ :	Mo $K\alpha$ radiation (0.71073 Å)
Diffractometer, scan mode:	17.4 cm ⁻¹
2 θ_{max} , completeness:	Bruker SMART, φ and ω
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	56.4°, >99%
Criterion for I_{obs} , $N(hkl)_{gt}$:	4288, 1400, 0.010
$N(param)_{refined}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1318
Programs:	106
	Bruker programs [6], SHELX [7]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U_{iso}^*/U_{eq}
Cd1	0.5000	1.0000	0.0000	0.02355(11)
S1	1.07241(9)	0.77499(4)	0.42157(10)	0.03988(19)
O1	1.5664(2)	0.76232(12)	0.6291(3)	0.0420(5)
O2	1.3671(2)	0.65227(12)	0.5196(2)	0.0328(4)
O3	0.3894(2)	1.04688(14)	0.2646(3)	0.0399(4)
H1W	0.3938	1.1043	0.3062	0.060*
H2W	0.2845	1.0288	0.2897	0.060*
N1	0.7707(3)	0.96176(14)	0.1586(3)	0.0275(4)
N2	0.8104(3)	0.87367(14)	0.2334(3)	0.0283(4)
H2D	0.7396	0.8242	0.2298	0.034*
N3	1.0493(2)	0.96387(15)	0.2953(3)	0.0261(4)
C1	0.9769(3)	0.87636(15)	0.3133(3)	0.0230(4)
C2	0.9173(4)	1.01295(17)	0.1997(4)	0.0285(5)
H2	0.9293	1.0774	0.1660	0.034*
C3	1.2958(3)	0.82117(16)	0.4866(3)	0.0283(5)
C4	1.4191(3)	0.73721(16)	0.5498(3)	0.0246(5)

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Abstract

$C_8H_8CdN_6O_6S_2$, monoclinic, $P2_1/c$ (no. 14), $a = 7.4175(11)$ Å, $b = 13.786(2)$ Å, $c = 7.4934(11)$ Å, $\beta = 93.835(2)^\circ$, $V = 3972.0(12)$ Å³, $Z = 2$, $R_{gt}(F) = 0.0193$, $wR_{ref}(F^2) = 0.0581$, $T = 296(2)$ K.

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A part of the title crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of [(1,2,4-triazol-3-yl)thio]acetic acid (86.7 mg, 0.30 mmol), $Cd(NO_3)_2 \cdot 4H_2O$ (46.0 mg, 0.15 mmol) and NaOH (120 mg, 0.30 mmol) was dissolved in 10 mL H_2O . Then the

solution was heated in a 25 mL Teflon-lined autoclave under autogenous pressure at 398 K for 3 days. After cooling to room temperature, colorless crystals formed (yield 43% based on Zn). Elemental analysis (C₈H₈CdN₆O₆S₂): H 1.75, C 20.86, N 18.24, O 20.84%; found: H 1.84, C 20.81, N 18.19, O 20.91%.

Experimental details

The C-bound hydrogen atoms were included in calculated positions and treated as riding atoms: d(C—H) = 0.93–0.96 Å with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5 U_{\text{eq}}(\text{C})$.

Discussion

The keen interest in the design and synthesis of coordination polymers (CPs) stems not only from their potential applications in gas storage, catalysis, drug delivery, nonlinear optics, and molecular sensing, but also because of impressive structural topologies [1, 2]. The construction of coordination architectures depends on the combination of several factors, such as the coordination geometry of metal ions, the nature of organic ligands, the use of noncovalent interactions (hydrogen bonding, halogen bonding, π – π interactions, or their combination in different ways) and sometimes the reagent ratio [3, 4]. So, understanding how these considerations affect metal coordination and influence crystal packing is at the forefront of controlling coordination frameworks. It has been documented that the geometries of organic ligands play crucial roles in determining the resulted architectures [5]. With the aim to understand the interesting chemistry of carboxylate ligand, we studied its assembly reaction of [(1,2,4-triazol-3-yl)thio]acetic acid (H₂tzta) with Cd(II) ions under hydrothermal condition.

Structure solution revealed that the asymmetric unit of title structure contain one half of a Cd(II), one deprotonated carboxylate ligand and one water ligand to construct a 2-D coordination polymer. Each Cd(II) ion, located on a crystallographic inversion center, is six-coordinated by

two carboxylate oxygens (D(Cd–O) = 2.2891(19) Å) and two thiazole nitrogen atoms (D(Cd–N) = 2.3243(19) Å) and two coordinated water molecules, forming a distorted octahedral geometry (*cf.* the figure). The bond angles of O–Cd–N are in the range of 83.21(6)°–96.79(6)°. In addition, there is a complex network of intermolecular hydrogen bonds. These interactions result in a three dimensional architecture.

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