

Diaquabis(1*H*-1,2,4-triazole-3-carboxylato)cadmium(II)

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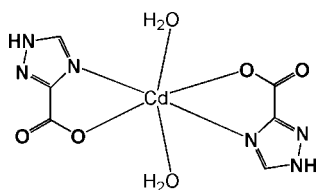
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.027; wR factor = 0.077; data-to-parameter ratio = 11.4.

In the title complex, $[\text{Cd}(\text{C}_3\text{H}_2\text{N}_3\text{O}_2)_2(\text{H}_2\text{O})_2]$, the Cd^{II} atom is coordinated by two N and two O atoms from two deprotonated 1*H*-1,2,4-triazole-3-carboxylic acid ligands (TRIA) and two water molecules. The Cd atom is located on an inversion centre. In the crystal structure, molecules are linked together *via* O—H...O and N—H...O hydrogen bonds, forming a three-dimensional network.

Related literature

For related literature, see: Guo & Wang (2005), Zhu *et al.* (2007*a,b*).



Experimental

Crystal data

$[\text{Cd}(\text{C}_3\text{H}_2\text{N}_3\text{O}_2)_2(\text{H}_2\text{O})_2]$

$M_r = 372.58$

Monoclinic, $P2_1/c$

$a = 9.2722$ (16) Å

$b = 8.8318$ (14) Å

$c = 6.9714$ (17) Å

$\beta = 92.230$ (1)°

$V = 570.46$ (19) Å³

$Z = 2$

Mo $K\alpha$ radiation

$\mu = 1.95$ mm⁻¹

$T = 298$ (1) K

$0.32 \times 0.23 \times 0.11$ mm

Data collection

Bruker SMART CCD

diffractometer

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.574$, $T_{\max} = 0.814$

2791 measured reflections

1002 independent reflections

843 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.077$

$S = 1.09$

1002 reflections

88 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 1.21$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.60$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O3}-\text{H3C}\cdots\text{O2}^{\text{i}}$	0.85	1.90	2.715 (3)	159
$\text{O3}-\text{H3B}\cdots\text{O1}^{\text{ii}}$	0.85	1.91	2.736 (3)	162
$\text{N3}-\text{H3}\cdots\text{O2}^{\text{iii}}$	0.86	1.89	2.728 (4)	164

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINTE* (Siemens, 1996); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2190).

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supporting information

Acta Cryst. (2008). E64, m119 [https://doi.org/10.1107/S1600536807063994]

Diaquabis(1*H*-1,2,4-triazole-3-carboxylato)cadmium(II)

Jie Zhu, Xian-Hong Yin, Yu Feng, Fei-Long Hu, Yue Zhuang and Cui-Wu Lin

S1. Comment

Recently, although the crystal structure of methyl 1*H*-1,2,4-triazole-3-carboxylate has been reported (Guo & Wang, 2005), metal complexes with triazole ligands have been rarely of interest for decades despite the biological importance of the triazole group. We have reported the crystal structures of two new copper(II) complexes diaquobis(1*H*-1,2,4-triazole-3-carboxylato)copper(II) and (1*H*-1,2,4-triazole-3-carboxylato)(1,10-phen)copper(II)chloride (Zhu, *et al.*, 2007, 2008). As a further investigation, we report in this paper the crystal structure of a new cadmium(II) complex, diaquobis(1*H*-1,2,4-triazole-3-carboxylato)cadmium(II).

As shown in Fig. 1, the title compound consists of a centrosymmetric mononuclear cadmium(II) complex cation. In the cation the Cd atom is six-coordinated by two N and two O atoms from two TRIA ligands and two O atoms from two water molecules. The Cd^{II} atom is in a slightly distorted octahedral environment. The Cd—O distances range from 2.315 (2) to 2.321 (3) Å, and the Cd—N bond length is 2.293 (3) Å, *i.e.* normal values. The C1—C2 bond length is 1.495 (5) Å, being in the normal C—C ranges in cadmium carboxylate complexes. The angles around Cd^{II} atom are from 73.57 (9) to linear. The TRIA molecule acts as a bidentate ligand.

In the title compound, the water molecules contribute to the formation of intermolecular hydrogen bonds involving carboxylate O atoms. Additional hydrogen bonds exist between the N—H groups of the triazole and carboxylate O atoms.

S2. Experimental

1*H*-1,2,4-triazole-3-carboxylic acid and CdCl₂·2.5H₂O were available commercially and were used without further purification. 1*H*-1,2,4-triazole-3-carboxylic acid (1 mmol, 113 mg) was dissolved in distilled water (15 ml) and CdCl₂·2.5H₂O (0.5 mmol, 114.2 mg) was added in distilled water (5 ml) with stirring at 323 K. The resulting colorless solution was allowed to react for 5 h and was then filtered. Colorless crystals suitable for X-ray analysis were obtained by slow evaporation of a water solution over a period of one month (yield 75%). Anal. Calcd (%) for C₆H₃CdN₃O₆ (Mr = 372.58): C, 19.34; H, 2.16; N, 22.56. Found (%): C, 19.28; H, 2.22; N, 22.49.

S3. Refinement

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with O—H, N—H and C—H distances of 0.85 Å, 0.86 Å and 0.93 Å, respectively, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$, $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

H atoms of the water molecules were located in a difference Fourier map and refined using a riding method. The highest peak in the difference map is 1.21 (1) Å from Cd1 and the largest hole is 0.60 (2) Å from Cd1.

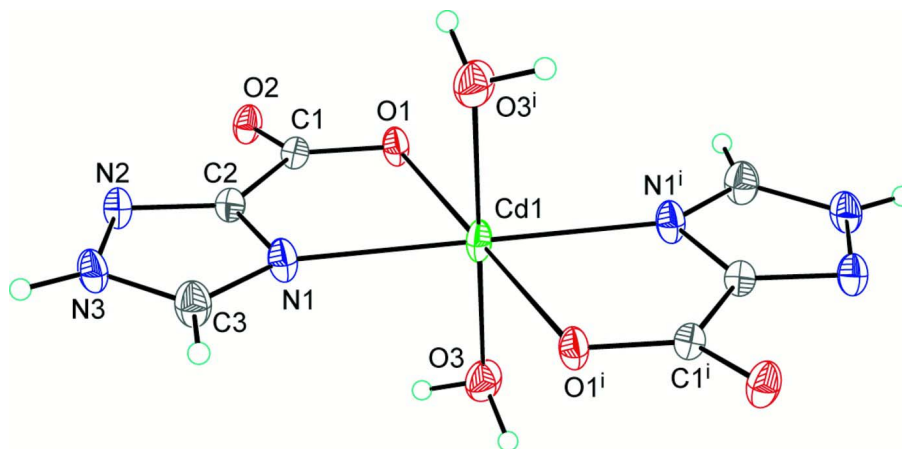


Figure 1

The structure of the title compound showing 50% probability displacement ellipsoids and the atom-numbering scheme. Symmetry code: (i) $-x, -y, -z$.

Diaquabis(1*H*-1,2,4-triazole-3-carboxylato)cadmium(II)

Crystal data

$[\text{Cd}(\text{C}_3\text{H}_2\text{N}_3\text{O}_2)_2(\text{H}_2\text{O})_2]$

$M_r = 372.58$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 9.2722$ (16) Å

$b = 8.8318$ (14) Å

$c = 6.9714$ (17) Å

$\beta = 92.230$ (1)°

$V = 570.46$ (19) Å³

$Z = 2$

$F(000) = 364$

$D_x = 2.169$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2042 reflections

$\theta = 2.2$ – 28.2 °

$\mu = 1.95$ mm⁻¹

$T = 298$ K

Prism, colorless

$0.32 \times 0.23 \times 0.11$ mm

Data collection

Bruker SMART CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.574$, $T_{\max} = 0.814$

2791 measured reflections

1002 independent reflections

843 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.023$

$\theta_{\max} = 25.0$ °, $\theta_{\min} = 2.2$ °

$h = -9 \rightarrow 11$

$k = -10 \rightarrow 10$

$l = -8 \rightarrow 7$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.077$

$S = 1.09$

1002 reflections

88 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

$w = 1/[\sigma^2(F_o^2) + (0.0445P)^2 + 0.5043P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 1.21$ e Å⁻³

$\Delta\rho_{\min} = -0.60$ e Å⁻³

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.0000	0.0000	0.0000	0.02817 (18)
N1	0.2289 (4)	-0.0228 (3)	0.1335 (5)	0.0311 (8)
N2	0.4348 (3)	0.1039 (3)	0.2024 (4)	0.0311 (7)
N3	0.4480 (3)	-0.0451 (4)	0.2456 (5)	0.0323 (7)
H3	0.5255	-0.0865	0.2927	0.039*
O1	0.1027 (2)	0.2387 (2)	-0.0103 (3)	0.0293 (6)
O2	0.2867 (2)	0.3785 (2)	0.1013 (4)	0.0313 (6)
O3	-0.0921 (3)	0.0865 (3)	0.2849 (4)	0.0409 (7)
H3B	-0.0262	0.1228	0.3596	0.049*
H3C	-0.1369	0.0171	0.3426	0.049*
C1	0.2259 (3)	0.2549 (4)	0.0702 (5)	0.0242 (7)
C2	0.2995 (4)	0.1123 (4)	0.1356 (5)	0.0253 (7)
C3	0.3259 (4)	-0.1186 (4)	0.2057 (6)	0.0364 (9)
H3A	0.3110	-0.2215	0.2255	0.044*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0187 (2)	0.0234 (2)	0.0416 (3)	-0.00318 (12)	-0.00840 (16)	-0.00195 (14)
N1	0.0245 (18)	0.0259 (16)	0.042 (2)	0.0022 (12)	-0.0097 (14)	-0.0001 (13)
N2	0.0212 (15)	0.0333 (16)	0.0384 (17)	0.0024 (13)	-0.0050 (13)	-0.0017 (14)
N3	0.0253 (17)	0.0296 (15)	0.0415 (19)	0.0079 (14)	-0.0077 (14)	0.0029 (14)
O1	0.0226 (12)	0.0230 (12)	0.0414 (15)	-0.0009 (9)	-0.0103 (10)	0.0046 (10)
O2	0.0237 (13)	0.0225 (12)	0.0474 (15)	-0.0025 (10)	-0.0034 (11)	0.0009 (10)
O3	0.0377 (15)	0.0390 (15)	0.0458 (16)	-0.0120 (12)	-0.0014 (12)	-0.0053 (12)
C1	0.0204 (17)	0.0246 (17)	0.0275 (18)	-0.0005 (14)	0.0001 (13)	-0.0012 (14)
C2	0.0225 (18)	0.0259 (17)	0.0274 (18)	-0.0006 (14)	-0.0006 (13)	-0.0017 (14)
C3	0.032 (2)	0.0286 (19)	0.048 (2)	0.0017 (17)	-0.0058 (17)	0.0011 (17)

Geometric parameters (\AA , $^\circ$)

Cd1—N1	2.293 (3)	N2—N3	1.355 (4)
Cd1—N1 ⁱ	2.293 (3)	N3—C3	1.325 (5)
Cd1—O1 ⁱ	2.315 (2)	N3—H3	0.8600
Cd1—O1	2.315 (2)	O1—C1	1.261 (4)
Cd1—O3 ⁱ	2.321 (3)	O2—C1	1.244 (4)

Cd1—O3	2.321 (3)	O3—H3B	0.8500
N1—C3	1.321 (5)	O3—H3C	0.8500
N1—C2	1.361 (4)	C1—C2	1.495 (5)
N2—C2	1.323 (4)	C3—H3A	0.9300
N1—Cd1—N1 ⁱ	180.00 (17)	C2—N2—N3	102.0 (3)
N1—Cd1—O1 ⁱ	106.43 (9)	C3—N3—N2	111.2 (3)
N1 ⁱ —Cd1—O1 ⁱ	73.57 (9)	C3—N3—H3	124.4
N1—Cd1—O1	73.57 (9)	N2—N3—H3	124.4
N1 ⁱ —Cd1—O1	106.43 (9)	C1—O1—Cd1	117.1 (2)
O1 ⁱ —Cd1—O1	180.0	Cd1—O3—H3B	111.7
N1—Cd1—O3 ⁱ	87.30 (11)	Cd1—O3—H3C	111.8
N1 ⁱ —Cd1—O3 ⁱ	92.70 (11)	H3B—O3—H3C	109.5
O1 ⁱ —Cd1—O3 ⁱ	83.82 (9)	O2—C1—O1	125.0 (3)
O1—Cd1—O3 ⁱ	96.18 (9)	O2—C1—C2	119.2 (3)
N1—Cd1—O3	92.70 (11)	O1—C1—C2	115.8 (3)
N1 ⁱ —Cd1—O3	87.30 (11)	N2—C2—N1	113.8 (3)
O1 ⁱ —Cd1—O3	96.18 (9)	N2—C2—C1	124.7 (3)
O1—Cd1—O3	83.82 (9)	N1—C2—C1	121.4 (3)
O3 ⁱ —Cd1—O3	180.00 (12)	N1—C3—N3	109.2 (3)
C3—N1—C2	103.7 (3)	N1—C3—H3A	125.4
C3—N1—Cd1	144.8 (3)	N3—C3—H3A	125.4
C2—N1—Cd1	111.4 (2)		
O1 ⁱ —Cd1—N1—C3	4.2 (5)	Cd1—O1—C1—C2	9.1 (4)
O1—Cd1—N1—C3	-175.8 (5)	N3—N2—C2—N1	-0.5 (4)
O3 ⁱ —Cd1—N1—C3	-78.6 (5)	N3—N2—C2—C1	178.4 (3)
O3—Cd1—N1—C3	101.4 (5)	C3—N1—C2—N2	0.9 (5)
O1 ⁱ —Cd1—N1—C2	-179.7 (2)	Cd1—N1—C2—N2	-176.8 (2)
O1—Cd1—N1—C2	0.3 (2)	C3—N1—C2—C1	-178.1 (3)
O3 ⁱ —Cd1—N1—C2	97.5 (3)	Cd1—N1—C2—C1	4.2 (4)
O3—Cd1—N1—C2	-82.5 (3)	O2—C1—C2—N2	-9.7 (5)
C2—N2—N3—C3	-0.1 (4)	O1—C1—C2—N2	171.8 (3)
N1—Cd1—O1—C1	-5.4 (2)	O2—C1—C2—N1	169.2 (3)
N1 ⁱ —Cd1—O1—C1	174.6 (2)	O1—C1—C2—N1	-9.3 (5)
O3 ⁱ —Cd1—O1—C1	-90.8 (2)	C2—N1—C3—N3	-0.9 (5)
O3—Cd1—O1—C1	89.2 (2)	Cd1—N1—C3—N3	175.3 (3)
Cd1—O1—C1—O2	-169.3 (3)	N2—N3—C3—N1	0.7 (5)

Symmetry code: (i) $-x, -y, -z$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3C \cdots O2 ⁱⁱ	0.85	1.90	2.715 (3)	159
O3—H3B \cdots O1 ⁱⁱⁱ	0.85	1.91	2.736 (3)	162
N3—H3 \cdots O2 ^{iv}	0.86	1.89	2.728 (4)	164

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