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Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.022
 wR factor = 0.054
Data-to-parameter ratio = 11.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

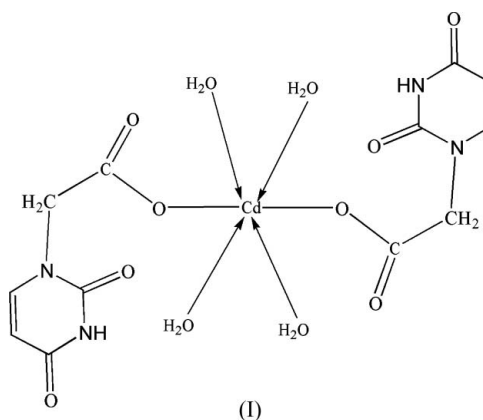
Tetraaquabis(uracil-1-acetato)cadmium(II)

In the centrosymmetric title compound, $[\text{Cd}(\text{C}_6\text{H}_5\text{N}_2\text{O}_4)_2(\text{H}_2\text{O})_4]$, the Cd^{II} cation is coordinated by two uracil-1-acetate anions *via* carboxylate O atoms, and four water molecules, forming a six-coordinate octahedral environment. $\text{O}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions link adjacent molecules into a three-dimensional network.

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Comment

The interaction of metal ions with nucleic acid bases is of great interest because of their relevance to the essential medical or toxic bioactivity of metal centres (Chruscinska *et al.*, 1998). Uracil is a component of RNA. Some of the 5-substituted uracils, *e.g.* 5-flourouracil and 5-bromouracil, exhibit significant pharmacological activity and are used as antitumour, antibacterial and antiviral drugs. These molecules may coordinate as exogenous ligands (*e.g.* inhibitors) in metalloproteins, function as cofactors in enzymatic systems or construct important cell structures, *e.g.* RNA (Lewandowski *et al.*, 2005). As a result, great efforts have been expended in the investigation of uracil derivatives and their complexes (Hueso-Ureña *et al.*, 1999, 2003; Terrón *et al.*, 2004; Hu & Wang, 2005; Hu *et al.*, 2005). Cadmium is an environmental pollutant, which inhibits RNA polymerase activity *in vivo* and reacts readily with proteins and other biological molecules (López-Garzón *et al.*, 1995). In addition, cadmium(II) has a d^{10} electron configuration which adapts to a wide variety of stereochemical environments (Sen *et al.*, 1999). Thus, we have selected Cd^{II} and 1-(carboxymethyl)uracil (Xiong *et al.*, 2005), which we synthesized previously, to extend this area of research, and we present here the crystal structure of the title uracil-1-acetate-based complex, (I).



The mononuclear complex, (I), consists of a Cd^{II} cation, four coordinated water molecules and two uracil-1-acetate

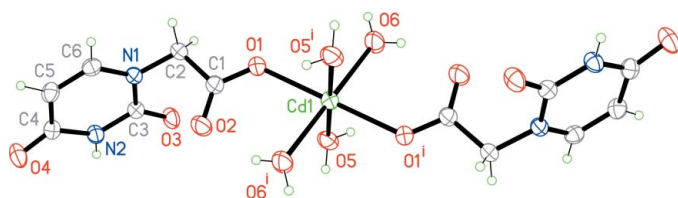


Figure 1
The coordination environment of the Cd^{II} cation in (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $-x, -y, 1 - z$.]

anions, binding through their carboxylate O atoms. The Cd^{II} cation lies on an inversion centre and the geometry around the metal centre is octahedral (Fig. 1 and Table 1). The equatorial square is formed by atoms O5, O5ⁱ, O6 and O6ⁱ [symmetry code: (i) $-x, -y, 1 - z$] and is constrained to be planar by symmetry.

In the crystal structure, N—H···O and O—H···O hydrogen bonds link the mononuclear units to form a three-dimensional network (Fig. 2 and Table 2).

Experimental

Compound (I) was synthesized in a hydrothermal process from a mixture of benzimidazole (2 mmol, 0.24 g), Cd(NO₃)₂·2H₂O (1 mmol, 0.27 g), uracil-1-acetic acid (2 mmol, 0.34 g) and water (20 ml). The reaction was carried out in a 30 ml Teflon-lined stainless-steel reactor. The reactor was heated to 423 K for 3 d and then slowly cooled to 298 K, to yield colourless crystals of (I), which were collected and washed with water.

Crystal data

[Cd(C ₆ H ₅ N ₂ O ₄) ₂ (H ₂ O) ₄]	$D_x = 1.930 \text{ Mg m}^{-3}$
$M_r = 522.70$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3064 reflections
$a = 12.6956 (9) \text{ \AA}$	$\theta = 3.0\text{--}25.2^\circ$
$b = 5.1295 (4) \text{ \AA}$	$\mu = 1.29 \text{ mm}^{-1}$
$c = 13.9659 (10) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\beta = 98.452 (1)^\circ$	Block, colourless
$V = 899.61 (11) \text{ \AA}^3$	$0.39 \times 0.22 \times 0.17 \text{ mm}$
$Z = 2$	

Data collection

Bruker APEX area-detector diffractometer	1611 independent reflections
φ and ω scans	1549 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$R_{\text{int}} = 0.019$
$T_{\text{min}} = 0.633, T_{\text{max}} = 0.811$	$\theta_{\text{max}} = 25.2^\circ$
4458 measured reflections	$h = -15 \rightarrow 11$
	$k = -6 \rightarrow 6$
	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0226P)^2 + 0.8089P]$
$R[F^2 > 2\sigma(F^2)] = 0.022$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.054$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.22 \text{ e \AA}^{-3}$
1611 reflections	$\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$
146 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997)
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.0177 (10)

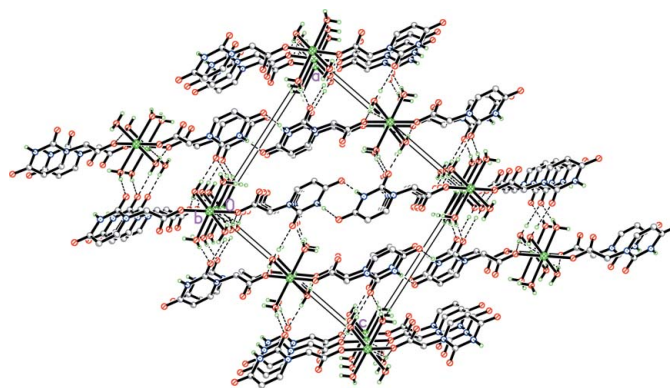


Figure 2
The three-dimensional network formed by hydrogen-bonding interactions, viewed along [010]. Hydrogen bonds are shown as dashed lines.

Table 1

Selected geometric parameters ($\text{\AA}, ^\circ$).

Cd1—O5	2.2549 (18)	N1—C6	1.369 (3)
Cd1—O1	2.2619 (15)	N1—C2	1.467 (3)
Cd1—O6	2.3240 (17)	N2—C3	1.363 (3)
O1—C1	1.270 (3)	N2—C4	1.380 (3)
O2—C1	1.233 (3)	C1—C2	1.525 (3)
O3—C3	1.225 (3)	C4—C5	1.434 (3)
O4—C4	1.233 (3)	C5—C6	1.340 (3)
N1—C3	1.368 (3)		
O5 ⁱ —Cd1—O5	180	O5—Cd1—O6 ⁱ	93.11 (7)
O5 ⁱ —Cd1—O1	90.62 (6)	O1—Cd1—O6 ⁱ	85.58 (6)
O5—Cd1—O1	89.38 (6)	O1—Cd1—O6	94.42 (6)
O5 ⁱ —Cd1—O6 ⁱ	86.89 (7)	O6 ⁱ —Cd1—O6	180

Symmetry code: (i) $-x, -y, -z + 1$.

Table 2

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
O5—H5A···O1 ⁱⁱⁱ	0.82 (2)	1.83 (2)	2.647 (2)	177 (3)
O5—H5B···O3 ⁱⁱⁱ	0.81 (2)	1.97 (2)	2.775 (2)	171 (3)
O6—H6A···O3 ^{iv}	0.82 (2)	2.05 (2)	2.863 (2)	172 (3)
O6—H6B···O2 ⁱ	0.81 (2)	1.98 (2)	2.736 (2)	156 (3)
N2—H2···O4 ^v	0.86	1.95	2.806 (2)	179

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

Water H atoms were located in difference maps and refined, with O—H and H···H distances restrained to be 0.82 (2) and 1.39 (1) \AA , respectively, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$. Other H atoms were positioned geometrically and allowed to ride on their parent atoms, with $Csp^2\text{---}H = 0.93 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$, $Csp^3\text{---}H = 0.97 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$, and $N\text{---}H = 0.86 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2002); software used to prepare material for publication: SHELXL97.

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