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Key indicators

Single-crystal X-ray study
 $T = 295\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.008\text{ \AA}$
 R factor = 0.044
 wR factor = 0.128
Data-to-parameter ratio = 15.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Di- μ -pyridine-2,5-dicarboxylato- $1\kappa^2\text{N},\text{O}^2:2\kappa\text{O}^5;-$
 $1\kappa\text{O}^5:2\kappa^2\text{N},\text{O}^2$ -bis[aqua(2,2'-bipyridine- $\kappa^2\text{N},\text{N}'$)-
cadmium(II)] dihydrateIn the crystal structure of the title cadmium(II) complex, $[\text{Cd}_2(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{C}_{10}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2]\cdot 2\text{H}_2\text{O}$, the pyridine-2,5-dicarboxylate (pydc) dianions bridge the Cd^{II} ions to form a centrosymmetric dimeric complex. Each Cd^{II} ion has a distorted octahedral coordination geometry.Received 3 October 2005
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Comment

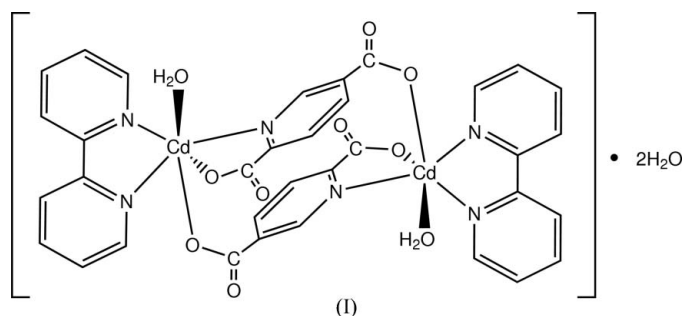
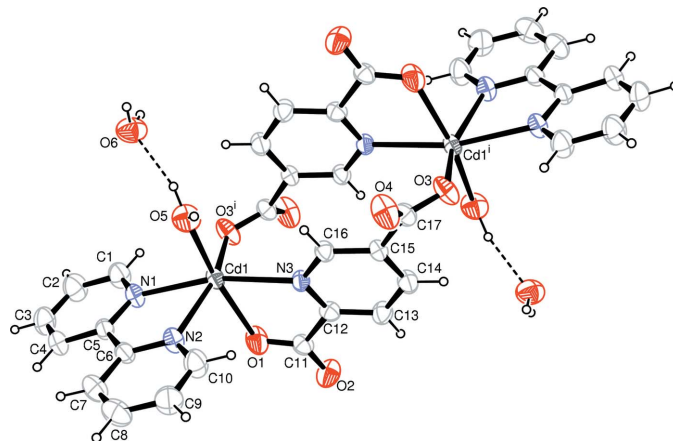
As a multidentate ligand, pyridinedicarboxylate (pydc) has been widely used to prepare multinuclear metal complexes (Gao *et al.*, 2005). We recently prepared the title Cd^{II} complex, (I), and the present X-ray structure determination shows this to be a dimeric complex.The molecular structure of (I) is shown in Fig. 1. Each Cd^{II} ion is surrounded by one coordinated water molecule, one 2,2'-bipyridine ligand and two pydc dianions, to give a distorted octahedral geometry. Two pydc dianions bridge two

Figure 1

The molecular structure of (I), with 50% probability displacement ellipsoids (arbitrary spheres for H atoms) [symmetry code: (i) $1 - x, 1 - y, 2 - z$]. Dashed lines represent hydrogen bonds.

Cd^{II} ions to form a centrosymmetric dimeric complex. The Cd—O distances are comparable with the values of 2.297 (3) Å in [Cd(Hpydc)₂(H₂O)₂] and 2.330 (2) Å in [Cd(Hpydc)₂(H₂O)₂] (Gao *et al.*, 2005).

Extensive hydrogen bonding occurs in (I) (Table 2), which consolidates the crystal structure.

Experimental

An ethanol solution (10 ml) of 2,2'-bipyridine (0.031 g, 0.2 mmol) was mixed with an aqueous solution (5 ml) containing CdCl₂·2.5H₂O (0.046 g, 0.2 mmol) and H₂pydc (0.067 g, 0.4 mmol). The mixture was refluxed for 5 h and then filtered. After three weeks, colourless single crystals of (I) were obtained from the filtrate.

Crystal data

[Cd ₂ (C ₇ H ₃ NO ₄) ₂ (C ₁₀ H ₈ N ₂) ₂ ·(H ₂ O) ₂ ·2H ₂ O]	Z = 1
<i>M_r</i> = 939.44	<i>D_x</i> = 1.824 Mg m ⁻³
Triclinic, <i>P</i> $\bar{1}$	Mo <i>K</i> α radiation
<i>a</i> = 7.4046 (9) Å	Cell parameters from 6217 reflections
<i>b</i> = 9.6272 (11) Å	<i>θ</i> = 2.5–27.4°
<i>c</i> = 12.5769 (17) Å	<i>μ</i> = 1.32 mm ⁻¹
<i>α</i> = 81.988 (5)°	<i>T</i> = 295 (1) K
<i>β</i> = 74.517 (4)°	Block, colourless
<i>γ</i> = 89.581 (7)°	0.24 × 0.12 × 0.09 mm
<i>V</i> = 855.16 (18) Å ³	

Data collection

Rigaku R-AXIS RAPID diffractometer	3816 independent reflections
<i>ω</i> scans	3605 reflections with <i>I</i> > 2σ(<i>I</i>)
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	<i>R_{int}</i> = 0.051
<i>T_{min}</i> = 0.820, <i>T_{max}</i> = 0.890	<i>θ_{max}</i> = 27.5°
7511 measured reflections	<i>h</i> = -9 → 9
	<i>k</i> = -12 → 12
	<i>l</i> = -16 → 15

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0374P)^2 + 3.5499P]$
$R[F^2 > 2\sigma(F^2)] = 0.044$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.128$	(Δ/σ) _{max} < 0.001
<i>S</i> = 1.21	$\Delta\rho_{max} = 1.97 \text{ e } \text{Å}^{-3}$
3816 reflections	$\Delta\rho_{min} = -0.83 \text{ e } \text{Å}^{-3}$
244 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å).

Cd1—O1	2.258 (4)	Cd1—N1	2.331 (4)
Cd1—O3 ⁱ	2.289 (4)	Cd1—N2	2.367 (5)
Cd1—O5	2.227 (4)	Cd1—N3	2.392 (4)

Symmetry code: (i) $-x + 1, -y + 1, -z + 2$.

Table 2

Hydrogen-bond 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>
O5—H51···O1 ⁱⁱ	0.90	2.48	3.149 (6)	131
O5—H51···O2 ⁱⁱ	0.90	1.82	2.649 (6)	152
O5—H52···O6	0.92	1.85	2.741 (7)	165
O6—H61···O3 ⁱⁱⁱ	0.86	2.26	3.118 (6)	171
O6—H62···O4 ^{iv}	0.86	2.18	2.784 (7)	127

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

Water H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions, with $U_{iso}(\text{H}) = 1.2U_{eq}(\text{O})$. Aromatic H atoms were placed in calculated positions, with C—H = 0.93 Å, and were included in the final cycles of refinement in riding mode, with $U_{iso}(\text{H}) = 1.2U_{eq}(\text{C})$. The highest peak in the final difference Fourier map is 1.1 Å from atom Cd1.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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