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Tetraaquabis(hydrogen maleato)cadmium(II)

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Key indicators

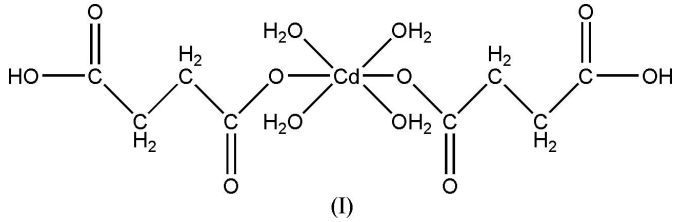
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.019
wR factor = 0.049
Data-to-parameter ratio = 11.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $[Cd(C_4H_3O_4)_2(H_2O)_4]$, crystallizes in the centrosymmetric space group $P\overline{1}$ with the Cd atom occupying an inversion centre and the monodentate hydrogen maleate anions arranged in a *trans* configuration. A network of intra- and intermolecular O—H···O bonds helps to stabilize the crystal packing.

Comment

Recently, salts of dicarboxylic acids, including those of fumaric acid, have been found to display porous metal–organic network structures (Li *et al.*, 1999). By contrast, the title compound, (I) (Fig. 1), consists of isolated molecules. The bond length and angles in (I) (Table 1) are similar to those of the analogous compound tetraaquabis(hydrogen maleato)-iron(II) (Barman *et al.*, 2002).



(I)

The Cd atoms in (I) occupy inversion centres and the monodentate hydrogen maleate ($HO_2CCH{=}CHCO_2^-$) ligands are in a *trans* configuration. The distorted octahedral cadmium coordination is completed by four water molecules. There are some intra- and intermolecular hydrogen bonds in (I) (Fig. 1, Table 2). The O2···O3 distance of the intramolecular hydrogen bond of 2.425 (2) Å is particularly short. Hydrogen bonds involving the water molecules help to link the molecules into a three-dimensional network (Fig. 2).

Experimental

Cadmium chloride (0.2 g) was stirred with a solution of maleic acid (0.25 g) in water at room temperature for 20 min. The resulting solution was filtered and the filtrate was evaporated at room temperature. Colourless crystals of (I) were obtained.

Crystal data

$[Cd(C_4H_3O_4)_2(H_2O)_4]$
M_r = 414.59
Triclinic, $P\overline{1}$
a = 5.4094 (5) Å
b = 7.4222 (8) Å
c = 9.4238 (14) Å
α = 110.151 (8)°
β = 105.133 (11)°
γ = 92.302 (7)°
V = 339.33 (8) Å^3
Z = 1
D_x = 2.029 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 36 reflections
θ = 2.3–10.3°
μ = 1.67 mm^{-1}
T = 293 (2) K
Plate, colourless
0.40 × 0.30 × 0.08 mm

Data collection

Bruker *P*4 diffractometer	R_{int} = 0.021
ω scans	θ_{max} = 26.0°
Absorption correction: ψ scan (*XSCANS*; Bruker, 1996)	$h = -6 \rightarrow 1$
	$k = -8 \rightarrow 8$
T_{min} = 0.593, T_{max} = 0.877	$l = -11 \rightarrow 11$
1723 measured reflections	3 standard reflections
1296 independent reflections	every 97 reflections
1292 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0361P)^2 + 0.0305P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.019	
$wR(F^2)$ = 0.049	
S = 1.11	$(\Delta/\sigma)_{max} < 0.001$
1296 reflections	$\Delta\rho_{max}$ = 0.53 e Å^{-3}
114 parameters	$\Delta\rho_{min}$ = −0.45 e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	Extinction correction: *SHELXL*97
	Extinction coefficient: 0.231 (9)

Table 1
Selected geometric parameters (Å, °).

Cd1—O4	2.3090 (15)	Cd1—O6	2.3027 (16)
Cd1—O5	2.2405 (17)		
O4—C4—C3	116.59 (18)	O5—Cd1—O4	80.95 (6)
O5—Cd1—O6	86.76 (7)	O6—Cd1—O4	92.75 (6)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H1O5···O1^{i}	0.86 (5)	1.93 (5)	2.777 (3)	170 (4)
O5—H2O5···O2^{ii}	0.71 (4)	2.22 (4)	2.872 (2)	154 (5)
O6—H1O6···O1^{iii}	0.80 (4)	2.06 (4)	2.846 (3)	164 (3)
O6—H2O6···O4^{iv}	0.68 (3)	2.13 (4)	2.811 (2)	178 (4)
O2—H2*B*···O3	0.82	1.61	2.425 (2)	179

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

The water H atoms were positioned geometrically (Nardelli, 1999) and refined freely. Other H atoms were placed in idealized positions (C—H = 0.93 Å and O—H = 0.82 Å) and refined as riding with the constraint U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O).

Data collection: *XSCANS* (Bruker, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXTL* (Bruker, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The author thanks Shandong Normal University for help with the X-ray structure determination.

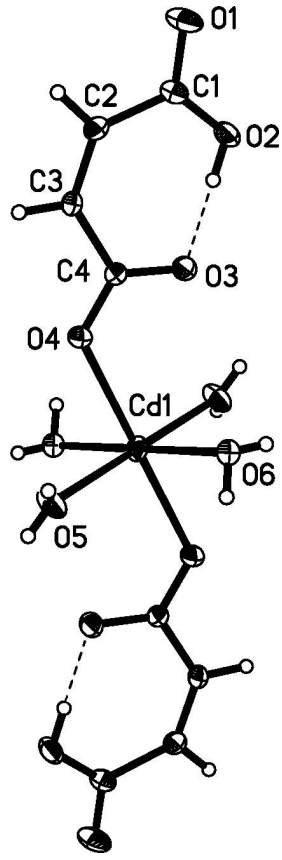


Figure 1
View of (I) with 30% displacement ellipsoids (arbitrary spheres for the H atoms). The intramolecular hydrogen bonds are indicated by dashed lines and the unlabelled atoms are generated by the symmetry code ($-x$, $-y$, $-z$).

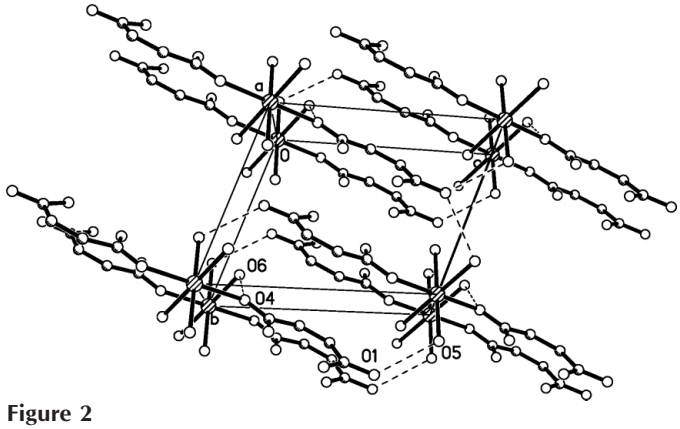


Figure 2
A packing diagram of (I) with the H atoms omitted. The dashed lines denote the short O···O separations associated with the hydrogen bonds made by the water molecules.

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