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Key indicators

Single-crystal X-ray study  
 T = 295 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$   
 Disorder in main residue  
 R factor = 0.022  
 wR factor = 0.073  
 Data-to-parameter ratio = 13.9

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

catena-Poly[[diaqua[3-(2-pyridyl)-1H-pyrazole- $\kappa N^2$ ]-cadmium(II)]- $\mu$ -squarato- $\kappa^2 O:O'$ ]

The squarate dianion in the crystal structure of the title compound,  $[\text{Cd}(\text{C}_4\text{O}_4)(\text{C}_8\text{H}_7\text{N}_3)(\text{H}_2\text{O})_2]_n$ , links the heterocycle-chelated water-coordinated Cd atoms into a zigzag chain. The O atoms of the squarate dianions are aligned *trans* to each other in the octahedron surrounding the Cd atom. There are two independent squarate dianions and both lie on inversion centers.

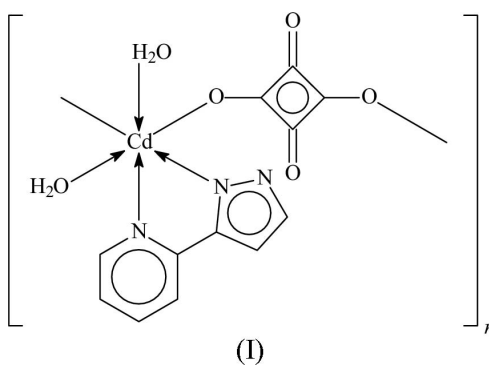
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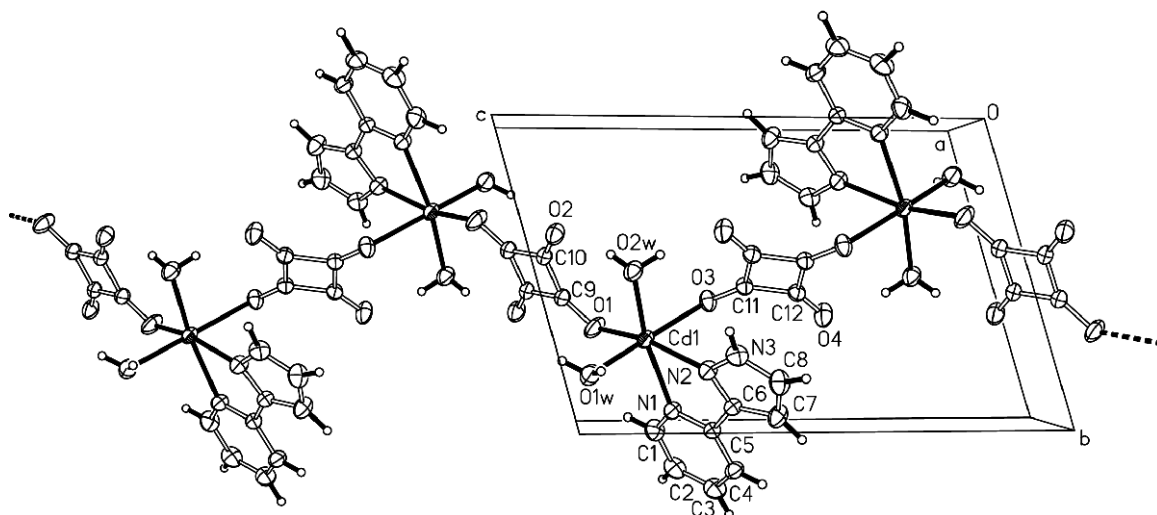
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Comment

The squarate dianion,  $\text{C}_4\text{O}_4^{2-}$ , furnishes a large number of complexes with metal cations, and because the unit carries two negative charges, it is particularly suited for complexation with divalent cations. A number of metal squarates and their complexes have been crystallographically characterized (Cambridge Structural Database, Version 5.26; Allen, 2002). The cadmium derivative exhibits an unusual cage-like channel network; the two coordinated water molecules are lost when the compound is heated but the ready rehydration implies a robust squarate–cadmium framework (Maji *et al.*, 2001). This compound,  $[\text{Cd}(\text{C}_4\text{O}_4)(\text{H}_2\text{O})_2]$ , is known to afford an adduct with 4,4'-bipyridine, but the adduct is sensitive to the loss of the three water molecules (Wang *et al.*, 2004). The present adduct with 2-pyridylpyrazole, (I) (Fig. 1), is an air-stable compound.



The aromatic amine functions in a chelating mode and two of its N atoms occupy *cis* sites of the octahedral coordination geometry around the Cd atom. The two water molecules are also aligned *cis* to each other. The mode of bonding of the squarate dianion gives rise to the formation of a zigzag chain structure. A similar reaction between  $[\text{Cd}(\text{C}_4\text{O}_4)(\text{H}_2\text{O})_2]$  and triethanolamine gave instead the bis-triethanolamine complex in which the squarate anion exists in the outer coordination sphere (Uçar *et al.*, 2004).



**Figure 1**  
ORTEP plot (Johnson, 1976) of a fragment of the polymeric chain of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii. Only one disorder component is shown.

## Experimental

Cadmium nitrate tetrahydrate (0.62 g, 2 mmol) and 2-pyridylpyrazole (0.29 g, 2 mmol) were added to a hot aqueous solution of squaric acid (0.23 g, 2 mmol). The pH was adjusted to 6 with drops of 0.2 M sodium hydroxide. The solution was allowed to evaporate at room temperature and pale-yellow prismatic crystals were obtained after one week. Analysis calculated for  $C_{12}H_{11}CdN_3O_6$ : C 35.53, H 2.73, N 10.36%; found: C 35.57, H 2.70; N 10.34%.

### Crystal data

$[Cd(C_4O_4)(C_8H_7N_3)(H_2O)_2]$   
 $M_r = 405.64$   
 Triclinic,  $P\bar{1}$   
 $a = 6.066$  (1) Å  
 $b = 8.643$  (2) Å  
 $c = 13.272$  (3) Å  
 $\alpha = 104.87$  (3)°  
 $\beta = 97.27$  (3)°  
 $\gamma = 93.29$  (3)°  
 $V = 664.2$  (2) Å<sup>3</sup>

$Z = 2$   
 $D_x = 2.028$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 6304 reflections  
 $\theta = 3.2$ – $27.5$ °  
 $\mu = 1.68$  mm<sup>-1</sup>  
 $T = 295$  (2) K  
 Prism, yellow  
 $0.38 \times 0.25 \times 0.18$  mm

### Data collection

Rigaku R-Axis RAPID IP diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  
 $T_{min} = 0.504$ ,  $T_{max} = 0.737$   
 6388 measured reflections

2938 independent reflections  
 2774 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.013$   
 $\theta_{max} = 27.5$ °  
 $h = -7 \rightarrow 6$   
 $k = -11 \rightarrow 11$   
 $l = -17 \rightarrow 17$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.022$   
 $wR(F^2) = 0.073$   
 $S = 1.34$   
 2938 reflections  
 212 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0287P)^2 + 0.7719P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.001$   
 $\Delta\rho_{max} = 0.45$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.41$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Cd1—O1	2.240 (2)	Cd1—O2 <sub>w</sub>	2.233 (2)
Cd1—O3	2.378 (2)	Cd1—N1	2.315 (3)
Cd1—O1 <sub>w</sub>	2.371 (6)	Cd1—N2	2.339 (3)
O1—Cd1—O3	91.4 (1)	O3—Cd1—N2	86.1 (1)
O1—Cd1—O1 <sub>w</sub>	98.9 (3)	O1 <sub>w</sub> —Cd1—O2 <sub>w</sub>	83.3 (3)
O1—Cd1—O2 <sub>w</sub>	100.9 (1)	O1 <sub>w</sub> —Cd1—N1	96.8 (2)
O1—Cd1—N1	92.1 (1)	O1 <sub>w</sub> —Cd1—N2	85.1 (3)
O1—Cd1—N2	164.2 (1)	O2 <sub>w</sub> —Cd1—N1	166.8 (1)
O3—Cd1—O1 <sub>w</sub>	168.8 (4)	O2 <sub>w</sub> —Cd1—N2	94.7 (1)
O3—Cd1—O2 <sub>w</sub>	90.5 (1)	N1—Cd1—N2	72.3 (1)
O3—Cd1—N1	87.1 (1)		

**Table 2**

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1 <sub>w</sub> —H1 <sub>w</sub> 1 $\cdots$ O1 <sup>i</sup>	0.85	2.26	3.04 (2)	152
O1 <sub>w</sub> —H1 <sub>w</sub> 2 $\cdots$ O2 <sup>ii</sup>	0.85	1.90	2.661 (6)	148
O1 <sub>w</sub> '—H1 <sub>w</sub> 3 $\cdots$ O2 <sup>ii</sup>	0.85	1.94	2.692 (9)	146
O2 <sub>w</sub> —H2 <sub>w</sub> 2 $\cdots$ O2	0.85	1.84	2.668 (3)	165
O2 <sub>w</sub> —H2 <sub>w</sub> 1 $\cdots$ O4 <sup>iii</sup>	0.85	1.84	2.679 (3)	168
N3—H3 <sub>n</sub> $\cdots$ O3 <sup>i</sup>	0.85	2.05	2.809 (3)	149

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

The aromatic H atoms were placed at calculated positions ( $C-H = 0.93$  Å and  $N-H = 0.85$  Å) and were included in the refinement in the riding-model approximation, with  $U_{iso}(H)$  values set at 1.2 times  $U_{eq}(C, N)$ . The water O—H bonds were rotated around the Cd—O<sub>water</sub> axes to fit the electron density [ $O-H = 0.85$  Å and  $U_{iso}(H) = 1.2U_{eq}(O)$ ]. One of the water molecules is disordered over two sites [occupancy factors are 0.59 (3) and 0.41 (3)]; bond dimensions involving the minor component are not listed in Table 1. The minor component water molecule forms only one hydrogen bond.

Data collection: RAPID-AUTO (Rigaku, 1998); cell refinement: RAPID-AUTO; data reduction: CrystalStructure (Rigaku/MS, 2002); program(s) used to solve structure: SHELXS97 (Sheldrick,

1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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