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Hexakis[μ-9-methyl-3-(1*H*-tetrazol-5-io)-4*H*-pyrido[1,2-*a*]pyrimidin-4-onato(2–)]-tricadmium(II)

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Key indicators

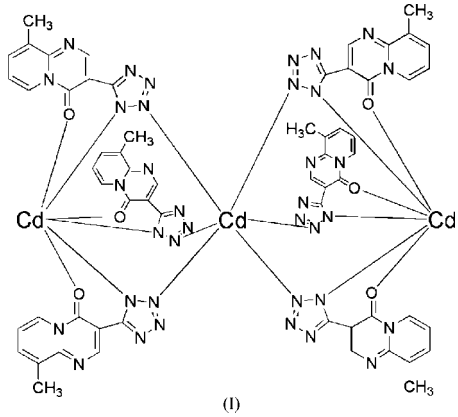
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.032
wR factor = 0.079
Data-to-parameter ratio = 15.4

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

The centrosymmetric molecule of the title Cd^{II} complex, $[Cd_3(C_{10}H_7N_6O)_6]$, is located on a threefold axis. The pyridopyrimidine ligands bridge neighbouring Cd atoms, forming a trinuclear complex. π–π Stacking is observed between neighbouring complex molecules.

Comment

Recent developments in polynuclear cadmium complexes concern their interesting topologies and properties (Zheng *et al.*, 2003; Bu *et al.*, 2005; Chandrasekhar *et al.*, 2005; Liu, 2005; Yong *et al.*, 2005). We present here the structure of the title trinuclear Cd^{II} complex incorporating a tetrazole ligand, $[Cd_3(pemirolast)_6]$ [pemirolast = 9-methyl-3-(1*H*-tetrazol-5-io)-4*H*-pyrido[1,2-*a*]pyrimidin-4-one, which is an anti-allergic drug], (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The trinuclear molecule has a threefold axis of symmetry with three Cd atoms located on the threefold axis. The central Cd1 atom is also located on an inversion centre and coordinated by six N atoms from six pemirolast ligands, with the Cd1—N bond length of 2.335 (2) Å; the bond angles around the Cd1 centre are close to 90°, showing an almost ideal octahedral geometry. The terminal Cd2 atom is coordinated by three N atoms and three O atoms from three pemirolast ligands, with the Cd2—N and Cd2—O bond lengths of 2.294 (2) and 2.351 (2) Å, respectively. Atom Cd2 has a slightly distorted octahedral coordination geometry (Table 1). In the trinuclear units, all of the pemirolast ligands adopt an *O*,*N*,*N*-tridentate chelating-bridging coordination mode, using the tetrazole groups to bridge adjacent Cd atoms, giving rise to the trinuclear complex.

The C2-containing pyridopyrimidine is nearly parallel with the C2^{i}-containing one [symmetry code: (i) $2-x, 1-x+y, \frac{1}{2}-$

z], the dihedral angle being 4.89 (11)° (Fig. 2). The distances of atoms on the C2-pyridoperimidine from the mean plane of the C2^{i}-pyridoperimidine are 3.294 (3) (C5), 3.409 (3) (C6), 3.392 (3) (C8) and 3.272 (3) Å (N6). These clearly suggest the existence of π–π stacking in the crystal structure of (I).

Experimental

A mixture of $Cd(ClO_4)_2\cdot 6H_2O$ (0.05 mmol) and the potassium salt of 9-methyl-3-(1*H*-tetrazol-5-yl)-4*H*-pyrido[1,2-*a*]pyrimidin-4-one (0.10 mmol) was placed in a heavy-walled Pyrex tube containing pyridine (0.05 ml), ethanol (0.30 ml) and H_2O (0.10 ml). The tube was frozen in liquid N_2, sealed under vacuum, and then heated at 393 K for 2 d. **Caution:** $Cd(ClO_4)_2\cdot 6H_2O$ is potentially explosive and should be used with care. Colourless crystals suitable for X-ray diffraction analysis were collected, washed with ethanol, and dried in air.

Crystal data

$[Cd_3(C_{10}H_7N_6O)_6]$	Mo $K\alpha$ radiation
M_r = 1700.53	Cell parameters from 15120 reflections
Trigonal, $R\bar{3}c$	θ = 1.8–28.3°
a = 18.302 (3) Å	μ = 1.14 mm^{-1}
c = 31.099 (6) Å	T = 293 (2) K
V = 9021 (3) Å^3	Block, colourless
Z = 6	0.44 × 0.39 × 0.30 mm
D_x = 1.878 Mg m^{-3}	

Data collection

Siemens SMART CCD diffractometer	1874 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.043
Absorption correction: none	θ_{max} = 28.3°
15306 measured reflections	$h = -24 \rightarrow 18$
2466 independent reflections	$k = -10 \rightarrow 24$
	$l = -40 \rightarrow 40$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.032	$w = 1/[\sigma^2(F_o^2) + (0.0385P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.079	$(\Delta/\sigma)_{max}$ = 0.002
S = 0.99	$\Delta\rho_{max}$ = 0.88 e Å^{-3}
2466 reflections	$\Delta\rho_{min}$ = −0.66 e Å^{-3}
160 parameters	

Table 1
Selected bond lengths (Å).

Cd1—N2	2.335 (2)	Cd2—O1	2.3514 (19)
Cd2—N1	2.294 (2)		

Aromatic H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined in the riding mode, with U_{iso}(H) = 1.2U_{eq}(C). The methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, the torsion angles refined, and U_{iso}(H) = 1.5U_{eq}(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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, 1998); software used to prepare material for publication: *SHELXTL*.

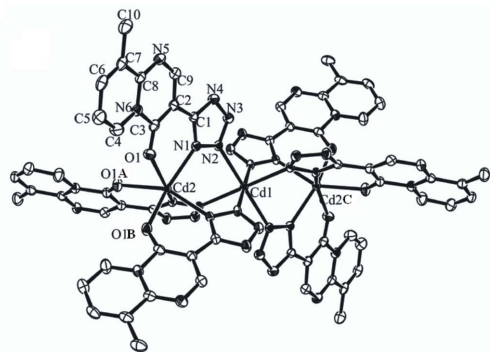


Figure 1
The molecular structure of (I) with 50% probability displacement ellipsoids [symmetry codes: (A) $-y, x-y, z$; (B) $-x+y, -x, z$; (C) $-x, -y, -z$]. H atoms have been omitted for clarity.

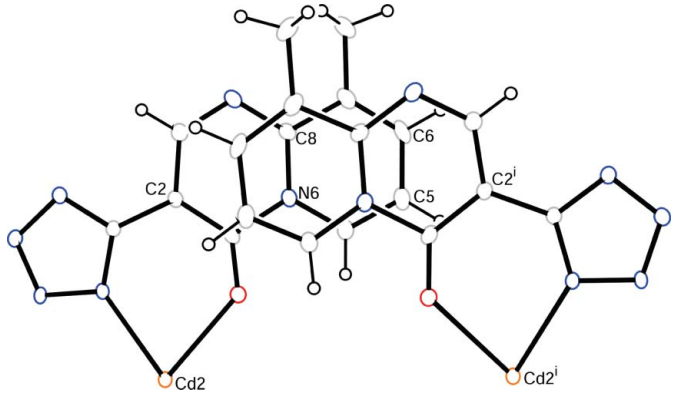


Figure 2
A diagram showing the π–π stacking [symmetry code: (i) $2-x, 1-x+y, \frac{1}{2}-z$].

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References

Bruker (1998). *SMART*, *SAINT* and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Bu, X.-H., Tong, M.-L., Li, J.-R., Chang, H.-C., Li, L.-J. & Kitagawa, S. (2005). *CrystEngComm*, **7**, 411–416.
Chandrasekhar, V., Azhakar, R., Zacchini, S., Bickley, J. F. & Steiner, A. (2005). *Inorg. Chem.* **44**, 4608–4615.
Liu, X.-W. (2005). *Acta Cryst.* E**61**, m1777–m1778.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Yong, G.-P., Qiao, S., Wang, Z.-Y. & Cui, Y. (2005). *Inorg. Chim. Acta*, **358**, 3905–3913.
Zheng, S.-L., Zhang, J.-P., Chen, X.-M., Huang, Z.-L., Lin, Z.-Y. & Wong, W.-T. (2003). *Chem. Eur. J.* **9**, 3888–3896.