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Hexakis(μ_2-4-amino-4*H*-1,2,4-triazole)hexachlorotricadmium(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(N–C) = 0.007 Å
R factor = 0.032
wR factor = 0.090
Data-to-parameter ratio = 14.7

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

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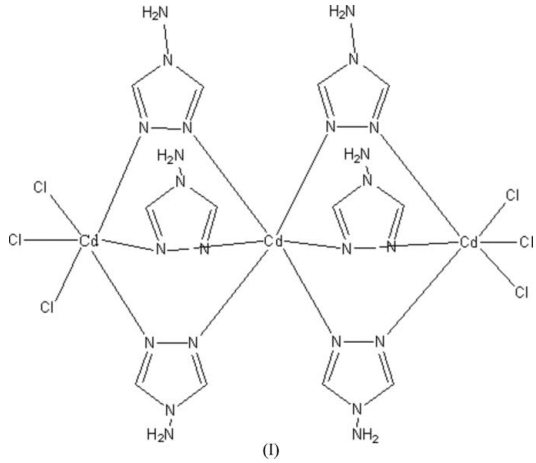
The molecule of the title trinuclear cadmium(II) complex, $[Cd_3Cl_6(atrz)_6]$ (atrz = 4-amino-1,2,4-triazole, $C_2H_4N_4$), has a threefold axis of symmetry with three Cd atoms located on the threefold axis. The atrz ligands bridge neighbouring Cd atoms to form the trinuclear complex.

Comment

A large number of metal complexes with 1,2,4-triazole derivatives have been prepared and characterized, as a result of their interesting magnetic properties and novel topologies. We present here the structure of the title trinuclear Cd^{II} complex incorporating the triazole ligand, $[Cd_3(atrz)_6Cl_6]$ (atrz = 4-amino-1,2,4-triazole), (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 Cd2 atom is also located on an inversion centre and coordinated by six N atoms from six atrz ligands, while the terminal Cd1 atom is coordinated by three Cl atoms and three N atoms from three atrz ligands. Each Cd atom has a distorted octahedral coordination geometry (Table 1). The atrz ligands bridge neighbouring Cd atoms to form the trinuclear complex.

Neighbouring trinuclear complexes are linked by N—H···Cl hydrogen bonds (Fig. 2 and Table 2).

Experimental

The atrz ligand was synthesized according to the literature method of Herbst & Garrison (1953). An aqueous solution (10 ml) of $CdCl_2$ (0.2 mmol, 36.6 mg) and atrz (0.6 mmol, 50.4 mg) was stirred for 5 h at room temperature and filtered. Colourless crystals of (I) were obtained from the filtrate.

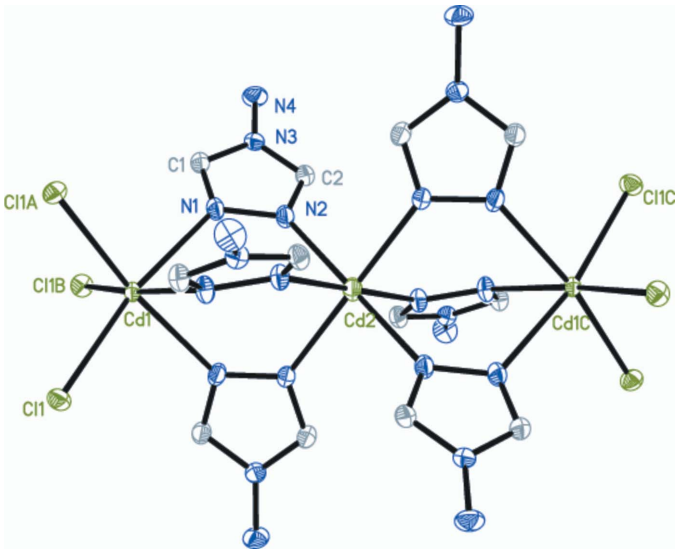


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted. [Symmetry codes: (A) $-y+1, x-y+2, z$; (B) $-x+y-1, -x+1, z$; (C) $-x, -y+2, -z$.]

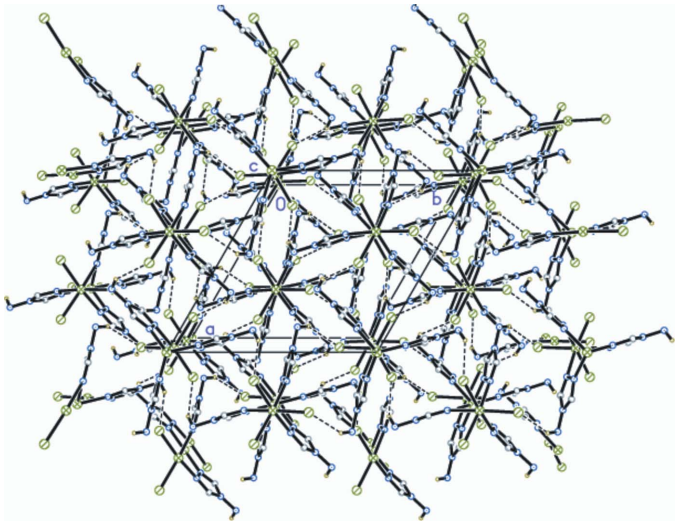


Figure 2
A unit-cell packing diagram for (I), showing the hydrogen bonding (dashed lines).

Crystal data

$[Cd_3Cl_6(C_2H_4N_4)_6]$
$M_r = 1054.48$
Trigonal, $R\overline{3}$
$a = 13.032\ (4)$ Å
$c = 17.558\ (7)$ Å
$V = 2582.4\ (15)$ Å^3
$Z = 3$
$D_x = 2.034$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 908 reflections
$\theta = 2.2$–$25.0°$
$\mu = 2.35$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
0.24 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.568$, $T_{max} = 0.720$
4399 measured reflections
1015 independent reflections
886 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 25.0°$
$h = -15 \rightarrow 13$
$k = -8 \rightarrow 15$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.090$
$S = 1.10$
1015 reflections
69 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0302P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.68$ e Å^{-3}
$\Delta\rho_{min} = -2.08$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1^{i}	2.469 (4)	Cd2—N2^{i}	2.294 (4)
Cd1—Cl1	2.6148 (14)		
N1^{i}—Cd1—N1^{ii}	84.33 (15)	N1^{ii}—Cd1—Cl1^{i}	91.40 (11)
N1^{i}—Cd1—N1	84.32 (15)	Cl1—Cd1—Cl1^{i}	97.32 (4)
N1^{i}—Cd1—Cl1	91.40 (11)	N2^{i}—Cd2—N2	90.65 (15)
N1^{ii}—Cd1—Cl1	86.29 (11)	N2^{i}—Cd2—N2	89.35 (15)
N1—Cd1—Cl1	170.03 (11)	N2—Cd2—N2	179.999 (1)
Cl1—Cd1—Cl1^{ii}	97.32 (4)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···Cl1^{iii}	0.89	2.76	3.546 (7)	147

Symmetry code: (iii) $y-\frac{4}{3}, -x+y-\frac{2}{3}, -z+\frac{1}{3}$.

H atoms on C atoms were placed in calculated positions and allowed to ride on their parent atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. Amino H atoms were located in a difference Fourier map and refined as riding in their as-found positions relative to the parent N atom, with N—H = 0.89 Å and $U_{iso}(H) = 1.2U_{eq}(N)$. The deepest hole in the electron-density map is 0.53 Å away from atom Cl1.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); 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*.

References

Bruker (1998). *SMART*, *SAINT* and *SHELXTL* (Version 5.10). Bruker AXS, Madison, Wisconsin, USA.
Herbst, R. M. & Garrison, J. A. (1953). *J. Org. Chem.* **18**, 872–877.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.