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Crystallographic report

Polymeric {bis[5-(2-aminobenzyl)tetrazolato] cadmium(II)}$_n$

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In polymeric {bis[5-(2-aminobenzyl)tetrazolato]cadmium(II)}$_n$, the N_6 coordination geometry around cadmium, is a distorted octahedron. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; tetrazole; hydrothermal synthesis; cadmium complex

COMMENT

In a continuation of research into new materials prepared under hydrothermal conditions,[1,2] the reaction of 2-aminobenzonitrile with $Cd(ClO_4)_2{\cdot}6H_2O$ and NaN_3 under hydrothermal conditions gave the title compound. In the structure, the coordination environment around the cadmium centre is best described as a slightly distorted N_6 octahedron (Fig. 1). Each tetrazole ligand chelates the cadmium atom, forming a six-membered ring. At the same time, each ligand bridges a different symmetry-related cadmium atom, leading to the formation of a linear chain.

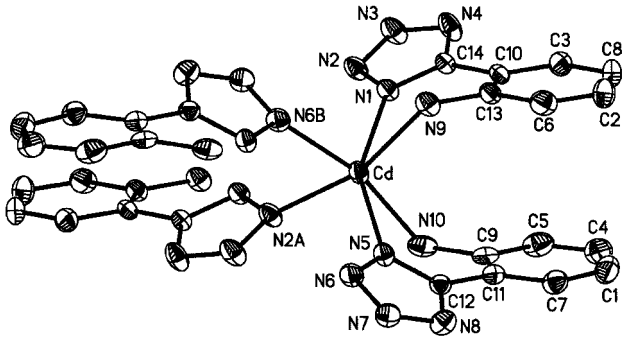

Figure 1. Molecular structure of {bis[5-(2-aminobenzyl)tetrazolato]cadmium(II)}$_n$; hydrogen atoms are omitted for clarity. Key geometric parameters: Cd–N2A 2.321(4), Cd–N5 2.328(4), Cd–N1 2.339(4), Cd–N6A 2.349(5), Cd–N10 2.370(4), Cd–N9 2.372(4) Å; N1–Cd–N5 151.96(14), N1–Cd–N9 73.53(13), N1–Cd–N10 90.61(14), N5–Cd–N9 88.68(13), N5–Cd–N10, 74.25(14), N9–Cd–N10 108.17(15), N2A–Cd–N5 101.10(13), N2A–Cd–N6A 80.43(15)°. Symmetry operation A: $\frac{1}{2} - x$, $\frac{3}{2} - y$, $-z$; B: $-x$, $1 - y$, $-z$.

EXPERIMENTAL

Hydrothermal treatment of $Cd(ClO_4)_2{\cdot}6H_2O$ (2.0 mmol), 2-aminobenzonitrile (2.0 mmol), NaN_3 (3.0 mmol), and water (3.0 ml) over 1 day at 105 °C yielded colourless needles. The yield was about 75%, based on 2-aminobenzonitrile. Intensity data were collected at 293(2) K on a Bruker AXS SMART CCD for a colourless block $0.10 \times 0.15 \times 0.23$ mm^3. $C_{14}H_{12}CdN_{10}$, $M = 432.74$, monoclinic, $C2/c$, $a = 10.6586(19)$, $b = 11.1828(18)$, $c = 25.769(4)$ Å, $\beta = 94.624(3)°$, $V = 3061.5(9)$Å^3, $Z = 8$, 2996 unique data ($\theta_{max} = 26.1°$), $R = 0.042$ (2143 [$I \geq 2\sigma(I)$] reflections), $wR = 0.092$ (all data). Programs used: SAINT, SADABS, SHELX-97, ORTEP. CCDC deposition number: 235635.

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