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Crystallographic report

Bis(acetato-*O*,*O*′){4-[*N*,*N*-bis(2-cyanoethyl)amino]pyridine}bis(methanol)cadmium(II), [Cd($C_{11}H_{12}N_4$)(CH_3CO_2)$_2$(CH_3OH)$_2$]

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The cadmium atom is coordinated in distorted pentagonal bipyramidal geometry by the pyridine-nitrogen atom of the 4-[*N*,*N*-bis(2-cyanoethyl)amino]pyridine ligand, two oxygen atoms of two methanol molecules and four oxygen atoms of two acetate groups. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; cadmium(II); 4-[*N*,*N*-bis(2-cyanoethyl)amino]pyridine

COMMENT

The 4-[*N*,*N*-bis(2-cyanoethyl)amino]pyridine ligand is a good hydrogen-bond acceptor and, as such, it has been used to construct distinct packing arrangements by forming different hydrogen-bonding patterns.[1–3] The cadmium atom in the title compound, Fig. 1, is seven-coordinated, existing in a distorted pentagonal bipyramidal defined by a pyridine-nitrogen atom, two oxygen atoms of two methanol molecules and four oxygen atoms of two bidentate acetate groups.

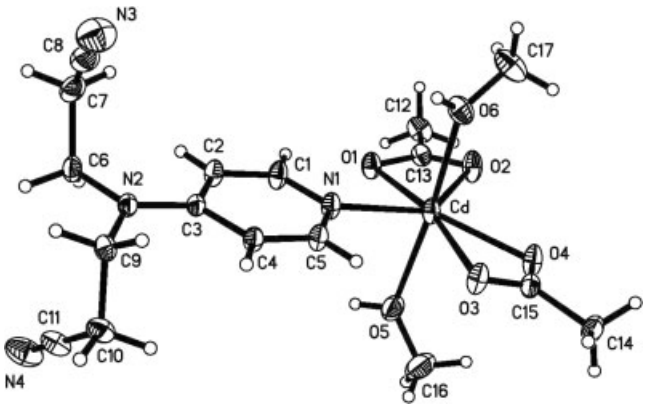

Figure 1. Molecular structure of the Cd(CH_3CO_2)$_2$($C_{11}H_{12}N_4$)($CH3OH$)$_2$. Selected geometric parameters: Cd–O1 2.474(3), Cd–O2 2.337(3), Cd1–O3 2.601(3), Cd–O4 2.281(3), Cd–O5 2.338(3), Cd–O6 2.342(3), Cd–N1 2.293(3) Å; O1–Cd–O3 168.03(8), O1–Cd–N1 85.47(9), O2–Cd–O4 86.30(10), O3–Cd–N1 84.72(9), O5–Cd–O6 171.89(10)°.

EXPERIMENTAL

A mixture of 4-[*N*,*N*-bis(2-cyanoethyl)amino]pyridinium hydrochloride (236.5 mg, 1 mmol) and $Cd(OAc)_2{\cdot}2H_2O$ (266 mg, 1 mmol) was dissolved in the methanol (30 ml). The reaction mixture was refluxed for 3 h and then filtered to yield a white product. Yield: 370 mg (74.8%). Anal. Found: C, 41.10; H, 5.29; N, 11.34. Calc.: C, 41.26; H, 5.30; N, 11.32%. The resultant colorless filtrate was left to stand at room temperature, from which well-defined block-shaped colorless single-crystals were obtained within 1 week. Intensity data for Cd(CH_3CO_2)$_2$($C_{11}H_{12}N_4$)(CH_3OH)$_2$ were collected at 293 K on a Bruker Smart Apex CCD diffractometer for a colorless crystal with dimensions of 0.20 × 0.20 × 0.30 mm^3. $C_{17}H_{26}CdN_4O_6$, $M = 494.82$, space group triclinic, $P\bar{1}$, $a = 9.451(1)$, $b = 10.559(1)$, $c = 12.159(1)$ Å, $\alpha = 76.38(1)$, $\beta = 78.81(1)$, $\gamma = 68.92(1)°$, $V = 1092.3(2)$ Å^3, $Z = 2$, 3791 unique data (θ_{max} 25.0°), 3445 data with $I \geq 2\sigma(I)$. $R = 0.034$ (obs. data), $wR = 0.081$ (all data). Programs used: SMART, SAINT, and SHELXTL. CCDC deposition number: 221585.

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