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Crystallographic report

Bis[tris(2-pyridyl)amine]cadmium(II)-di-μ-chloro-dichloro-cadmium(II), $[(C_5H_4N)_3N]_2CdCl_2CdCl_2$

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In the dinuclear molecule of $[(C_5H_4N)_3N]_2CdCl_2CdCl_2$, one cadmium is octahedrally coordinated by a Cl_2N_4 donor set and the other cadmium is tetrahedrally coordinated by four chlorine atoms. The dinuclear units are connected by $\pi-\pi$ interactions to give a two-dimensional network. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; cadmium complex; $\pi-\pi$ interactions; two-dimensional network

COMMENT

The structure of the title compound was determined in connection with the study of dimensional cadmium(II) complexes as potential optical materials.[1] In the dinuclear structure of $[(C_5H_4N)_3N]_2CdCl_2CdCl_2$ (**1**), the coordination geometries about Cd(1) and Cd(2) are pseudo-octahedral and pseudotetrahedral, respectively. It is worth noting that intramolecular face-to-face $\pi-\pi$ interactions[2] occur between the tris(2-pyridyl)amine (TPA) ligands coordinated to the same cadmium(II) atom. Furthermore, the binuclear moieties are connected into a two-dimensional network by intermolecular $\pi-\pi$ interactions (Fig. 1). The plane–plane angles and the centroid–centroid distances between the interacting pyridyl rings lie in the ranges of 0–6.9° and 3.33–3.71 Å, respectively.

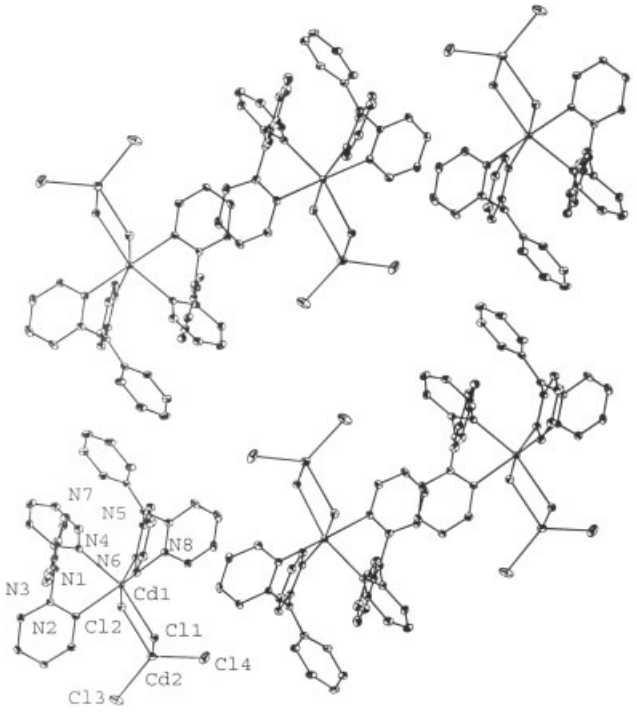

Figure 1. Two-dimensional network structure of **1**.

EXPERIMENTAL

1 was synthesized by the reaction of equimolar amounts of $CdCl_2$ and TPA in methanol. The concentrated solution was left undisturbed for slow evaporation of the solvent to give colorless crystals. Anal. Found C, 45.69; H, 2.98; N, 14.22. Calc. for $C_{30}H_{24}Cd_2Cl_4N_8$: C, 45.48; H, 3.05; N, 14.14%.

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Intensity data were collected at 291 K on a Rigaku RAXIS–IV diffractometer for a colorless crystal $0.20 \times 0.20 \times 0.30$ mm^3. $C_{30}H_{24}Cd_2Cl_4N_8$, $M = 863.17$, monoclinic, $P2_1/n$, $a = 10.993(2)$, $b = 25.688(5)$, $c = 11.787(2)$ Å, $\beta = 99.78(3)°$, $V = 3280.2(11)$ Å^3, $Z = 4$, 5215 unique data (θ_{max}27.5°), 4528 data with $I \geq 2\sigma(I)$, $R_{obs} = 0.046$,

$wR = 0.127$ (all data), $\rho_{max} = 0.79\ e^{-}\ Å^{-3}$. Programs used: *SHELXS-97*, *SHELXL-97*. CCDC deposition number: 193 090.

REFERENCES

1. Ayyappan P, Evans OR, Cui Y, Wheeler KA, Lin WB. *Inorg. Chem.* 2002; **41**: 4978.
2. Guo D, Pang KL, Duan CY, He C, Meng QJ. *Inorg. Chem.* 2002; **41**: 5978.