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Crystallographic report

Bis(indole-3-acetato)(1,10-phenanthroline) cadmium(II)

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The structure of Cd(phen)(indole-3-acetato)$_2$ has twofold symmetry and features a six-coordinated distorted octahedral geometry around cadmium(II), defined by an N_2O_4 donor set, with Cd–O distances ranging from 2.214(3) to 2.526(3) Å. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; cadmium; indole-3-acetic acid

COMMENT

Indole-3-acetic acid (IAH), a phytohormone of the auxin series and a substance of essential and multifunctional biological significance, has been established as an essential component of associative plant–microbe interactions[1] and has an influence on the availability of cadmium in soils. Although a few crystallographic studies on metal complexes of indole-3-acetate have been performed, such as on $[Pd(IA)(py)]_2 \cdot 4CHCl_3$[2] and $[Pt(bpm)(\text{L-Ala})](IA) \cdot 7H_2O$,[3] thus far, IA complexes with the toxic heavy-metal cadmium(II) have not yet been characterized by X-ray crystallography. The investigation of the crystal structure of cadmium(II) complexes with IAH and derivatives is of fundamental importance in aiding our understanding of its biological function, such as acting as phytochelatin to decrease the toxicity of cadmium.[4] The structure of Cd(phen)(IA)$_2$ (Fig. 1) has crystallographic twofold symmetry and looks like a butterfly, similar to $Cd(S_2CNEt_2)_2$(2,9-Me$_2$-1,10-phen),[5] by virtue of the presence of chelating IAH ligands, and the cadmium center exists in a distorted octahedral environment defined by an N_2O_4 donor set with Cd–O distances ranging from 2.214(3) to 2.526(3) Å.

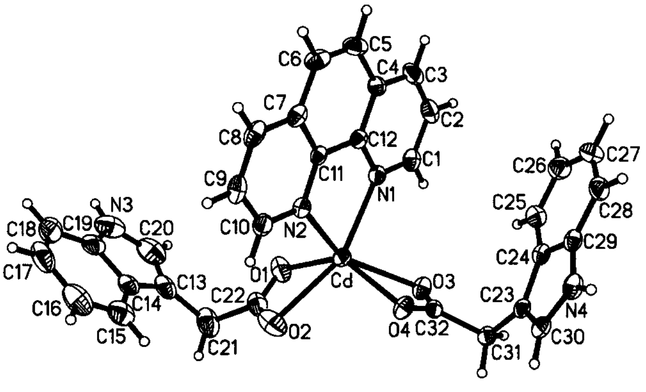

Figure 1. Molecular structure of Cd(phen)(IA)$_2$. Key geometric parameters: Cd — O1 2.234(4), Cd–O2 2.439(4), Cd–O3 2.526(3), Cd–O4 2.214(3), Cd–N1 2.308(4), Cd–N2 2.309(4) Å; O1–Cd–O2 55.81(17), O1–Cd–O3 105.93(13), O1–Cd–4 136.12(15), O1–Cd–N1 113.37(15), O1–Cd–N2 105.23(14), O2–Cd–O3 115.35(15), O2–Cd–O4 94.41(17), O2–Cd–N1 156.68(16), O2–Cd–N2 89.41 (15), O3–Cd–O4 54.58(11), O3–Cd–N1 86.87(13), O3–Cd–N2 147.67(12), O4–Cd–N1 104.90(13), O4–Cd–N2 105.81(12), N1–Cd–N2 73.01(14)°.

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EXPERIMENTAL

To a methanolic solution (5 ml) containing IAH (0.2 mmol), which was adjusted to pH = 7 using 1 mol l^{-1} NaOH, was added an aqueous $Cd(OAc)_2$ (0.2 mmol) solution (10 ml) with stirring at 60 °C. After 3 h, a methanolic solution (10 ml) of 1,10-phenanthroline (0.1 mmol) was added with 6 h stirring. The reaction mixture was filtered and the filtrate was allowed to stand in air; yellow, block crystals were obtained within 3 weeks. Yield 60% (based on IAH). Anal. Found: C, 60.04; H, 3.85; N, 8.69%. Calc. for $C_{32}H_{24}CdN_4O_4$: C, 59.96; H, 3.77; N, 8.74. X-ray diffraction data were collected at 293(2) K on a Siemens SMART CCD area detector diffractometer using graphite-monochromated MoKα radiation on a block $0.20 \times 0.34 \times 0.40$ mm^3. Crystallographic data: $C_{32}H_{24}CdN_4O_4$, $M = 640.95$, monoclinic, space group $P2_1/c$, $a = 12.4378(8)$, $b = 12.3442(8)$, $c = 18.2971(11)$ Å, $\beta = 106.223(1)°$, $V = 2697.4(3)$ Å^3, $Z = 4$, $D_c = 1.578$ Mg m^{-3}, 16 625 reflections collected, 6668 unique and 4752 with $I > 2\sigma(I)$.R (obs. data on F^2) 0.070, wR (all data) 0.132, $\rho_{\max} = 1.03$ e$^-$. Å^{-3}. Programs used: SHELXTL97, ORTEP. CCDC deposition number: CCDC 216 213.

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