

Bis(5-chlorosalicylato- κ O)bis(1,10-phenanthroline- κ^2 N,N')cadmium(II)

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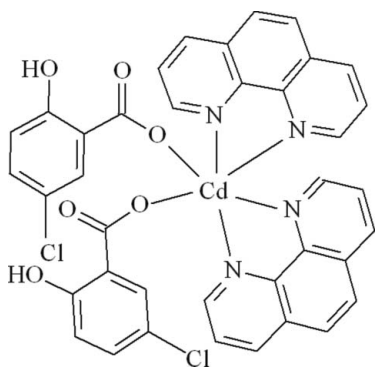
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.045; wR factor = 0.087; data-to-parameter ratio = 16.7.

In the title complex, $[\text{Cd}(\text{C}_7\text{H}_4\text{ClO}_3)_2(\text{C}_{12}\text{H}_8\text{N}_2)_2]$, the Cd atom is coordinated by two 5-chlorosalicylate ligands and two 1,10-phenanthroline ligands, displaying a distorted octahedral coordination geometry. The crystal structure is stabilized by O—H...O and C—H...O hydrogen bonds and π – π interactions between the 1,10-phenanthroline ligands and 5-chlorosalicylate ligands, with a centroid–centroid distance between neighbouring aromatic rings of 3.730 (1) Å.

Related literature

For related literature, see: Lemoine *et al.* (2004); Melnik *et al.* (2001); Wen, Liu & Ribas (2007); Wen & Ying (2007); Wen, Ta *et al.* (2007); Yin *et al.* (2004); Zhu *et al.* (2003).



Experimental

Crystal data

 $[\text{Cd}(\text{C}_7\text{H}_4\text{ClO}_3)_2(\text{C}_{12}\text{H}_8\text{N}_2)_2]$
 $M_r = 815.91$ Orthorhombic, $P2_12_1$ $a = 10.812$ (3) Å $b = 16.495$ (4) Å $c = 18.862$ (5) Å $V = 3363.9$ (14) Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 0.86$ mm⁻¹ $T = 293$ (2) K

0.25 × 0.23 × 0.22 mm

Data collection

Rigaku R-Axis RAPID IP

diffractometer

Absorption correction: none

32955 measured reflections

7696 independent reflections

5812 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.086$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.045$ $wR(F^2) = 0.086$ $S = 1.01$

7696 reflections

461 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.64$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.55$ e Å⁻³

Absolute structure: Flack (1983),

with 3402 Friedel pairs

Flack parameter: 0.00 (19)

Table 1

Selected geometric parameters (Å, °).

Cd1—O4	2.261 (3)	Cd1—N2	2.400 (4)
Cd1—O1	2.336 (4)	Cd1—N1	2.422 (3)
Cd1—N4	2.400 (3)	Cd1—N3	2.423 (3)
O4—Cd1—O1	82.14 (12)	N4—Cd1—N1	141.39 (12)
O4—Cd1—N4	125.46 (12)	N2—Cd1—N1	69.12 (12)
O1—Cd1—N4	83.28 (13)	O4—Cd1—N3	164.68 (11)
O4—Cd1—N2	86.00 (13)	O1—Cd1—N3	97.76 (14)
O1—Cd1—N2	156.59 (12)	N4—Cd1—N3	69.51 (11)
N4—Cd1—N2	87.33 (12)	N2—Cd1—N3	98.95 (13)
O4—Cd1—N1	84.29 (12)	N1—Cd1—N3	83.98 (12)
O1—Cd1—N1	129.12 (13)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3...O2	0.82	1.76	2.504 (6)	149
O6—H6...O5	0.82	1.83	2.553 (6)	147
C15—H15A...O2	0.93	2.45	3.181 (6)	136
C36—H36A...O5	0.93	2.34	3.134 (6)	143
C24—H24A...O3 ⁱ	0.93	2.42	3.185 (6)	140

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2261).

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