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Key indicators

Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$
 R factor = 0.058
 wR factor = 0.131
Data-to-parameter ratio = 17.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Bis(μ -5-chloro-2-hydroxyacetophenone 4-nitro-
benzoylhydrazonato)bis[dipyridinecadmium(II)]

The title dinuclear complex, $[\text{Cd}_2(\text{C}_{15}\text{H}_{10}\text{ClN}_3\text{O}_4)_2(\text{C}_5\text{H}_5\text{N})_4]$, lies on a centre of inversion. The deprotonated Schiff base spans the meridional sites of the octahedron surrounding the Cd atom through its O, N and O atoms; the hydroxy O atom of the symmetry-related anion forms a square plane with these atoms, and the other two sites of the octahedron are occupied by the N atoms of the pyridine ligands.

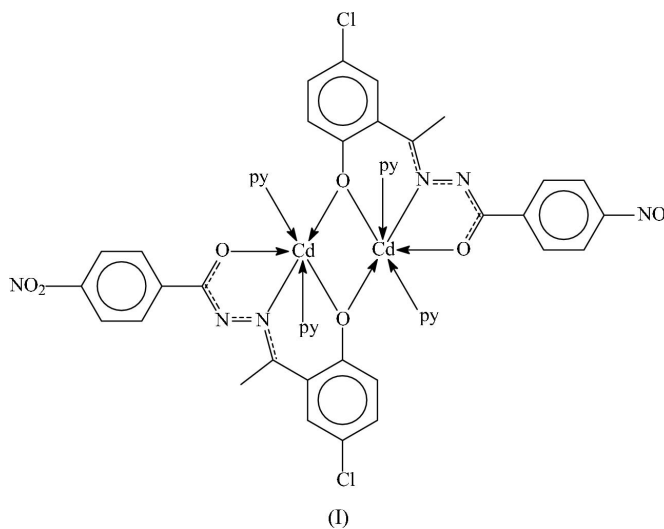
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Comment

The Schiff bases that are synthesized by condensing salicylaldehyde and related compounds with aroylhydrazides typically chelate through their O, N, O' -atoms in their metal complexes (Cambridge Structural Database, Version 5.26; Allen, 2002). The crystallographically verified examples have one Schiff base binding to a metal atom; it is probably too sterically crowded for two of the ligands to chelate simultaneously, and the complexes have other ligands or counter-ions in their coordination sphere. The salicylaldehyde benzoylhydrazone Schiff base in its monodeprotonated form has been reported to chelate to a Cu atom; the positive charge is balanced by a coordinated perchlorate ion. However, the hydroxy O-atom site additionally functions as a bridging site to furnish a dinuclear compound (Ainscough *et al.*, 1998). Such dimeric hydrazonates are not commonly encountered; the title cadmium derivative, (I), represents the second example of a dinuclear compound in which the hydroxy site of the ligand serves to link the monomeric complexes into a dinuclear species.



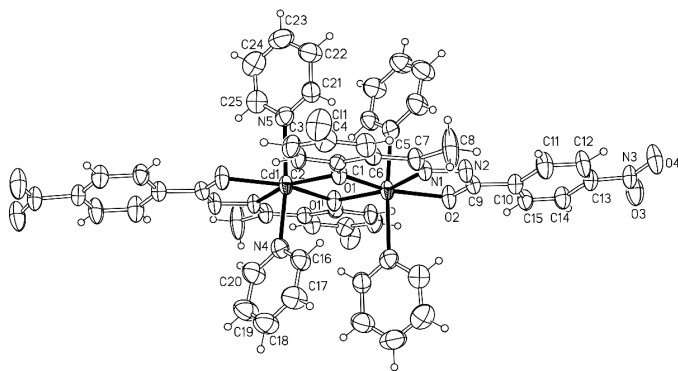


Figure 1
ORTEP plot (Johnson, 1976) of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii. Unlabelled atoms are related to labelled atoms by $(1-x, 1-y, 1-z)$.

meridional sites of the octahedron surrounding the Cd atom in the centrosymmetric dinuclear compound; these three atoms and the hydroxy O atom of the symmetry-related Schiff base constitute a square plane, above and below which are the N atoms of the pyridine molecules (Fig. 1).

Experimental

The Schiff base was synthesized by the condensation of 4-nitrobenzoylhydrazine with 5-chloro-2-hydroxyacetophenone. Cadmium chloride hydrate (0.07 g, 0.32 mmol) dissolved in ethanol (30 ml) was added to the ligand (0.22 g, 0.64 mmol) dissolved in ethanol (30 ml) and the mixture was refluxed for 3 h. The orange precipitate was recrystallized from pyridine. Crystallization took several weeks to complete.

Crystal data

$[\text{Cd}_2(\text{C}_{15}\text{H}_{10}\text{ClN}_3\text{O}_4)_2(\text{C}_5\text{H}_5\text{N})_4]$	$D_x = 1.579 \text{ Mg m}^{-3}$
$M_r = 1204.62$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 4294 reflections
$a = 19.115(2) \text{ \AA}$	$\theta = 1.9\text{--}27.5^\circ$
$b = 12.012(1) \text{ \AA}$	$\mu = 1.01 \text{ mm}^{-1}$
$c = 22.071(2) \text{ \AA}$	$T = 298(2) \text{ K}$
$\beta = 90.024(1)^\circ$	Plate, orange
$V = 5067.8(8) \text{ \AA}^3$	$0.29 \times 0.26 \times 0.07 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART APEX area-detector diffractometer	5692 independent reflections
φ and ω scans	4632 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$R_{\text{int}} = 0.034$
$T_{\text{min}} = 0.759, T_{\text{max}} = 0.933$	$\theta_{\text{max}} = 27.5^\circ$
14 778 measured reflections	$h = -24 \rightarrow 24$
	$k = -15 \rightarrow 14$
	$l = -14 \rightarrow 28$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.058$
 $wR(F^2) = 0.131$
 $S = 1.15$
 5692 reflections
 326 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 1.6639P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 1.09 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.92 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters ($\text{\AA}, ^\circ$).

Cd1—O1	2.273 (3)	Cd1—N1 ⁱ	2.321 (3)
Cd1—O1 ⁱ	2.232 (3)	Cd1—N4	2.415 (4)
Cd1—O2 ⁱ	2.227 (3)	Cd1—N5	2.382 (4)
O1—Cd1—O1 ⁱ	78.4 (1)	O1—Cd1—N5	85.7 (1)
O1—Cd1—O2 ⁱ	129.9 (1)	O2 ⁱ —Cd1—N1 ⁱ	72.7 (1)
O1—Cd1—N1 ⁱ	157.3 (1)	O2 ⁱ —Cd1—N4	86.0 (1)
O1—Cd1—N4	86.1 (1)	O2 ⁱ —Cd1—N5	84.0 (1)
O1 ⁱ —Cd1—N5	100.9 (1)	N1 ⁱ —Cd1—N4	95.1 (1)
O1 ⁱ —Cd1—O2 ⁱ	151.71 (1)	N1 ⁱ —Cd1—N5	100.1 (1)
O1 ⁱ —Cd1—N1 ⁱ	78.9 (1)	N4—Cd1—N5	158.5 (1)
O1 ⁱ —Cd1—N4	97.0 (1)		

Symmetry code: (i) $1-x, 1-y, 1-z$.

The aromatic H atoms were placed in calculated positions ($C-H = 0.93 \text{ \AA}$) and were included in the refinement in the riding-model approximation, with $U_{\text{iso}}(\text{H})$ values set at 1.2 times $U_{\text{eq}}(\text{C})$. The methyl group was rotated to fit the electron density; $C-H = 0.96 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$. The final difference Fourier map had a large peak at about 1 \AA from Cd1.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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