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Bis{2-[(2-aminophenyl)iminomethyl]-6-carboxyphenolato-κ^3*O*,*N*,*N*′}zinc(II)

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The title compound, $[Zn(C_{14}H_{17}N_2O_3)_2]$, is a complex of Zn^{II} and the Schiff base 2-[(2-aminophenyl)iminomethyl]-6-carboxyphenol synthesized by the reaction of 3-carboxylsalicylaldehyde and (1*R*,2*R*)-diaminocyclohexane in equimolar ratio. In the crystal structure, the Zn^{II} ion is six-coordinated in an octahedral environment (N_4O_2) formed by two monovalent anions. Each anion acts as a tridentate *NON*-chelator and occupies a coordination plane. The two NON coordination planes formed are nearly perpendicular to each other.

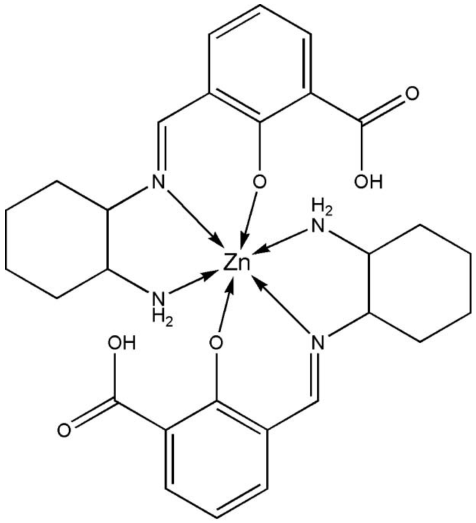
Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.007 Å
R factor = 0.055
wR factor = 0.130
Data-to-parameter ratio = 18.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Complexes of Schiff bases play an important role in modern chemistry, because they show abundant bioactivity (Dios *et al.*, 2002), medicinal activity (Sharma, 2004) and catalytic activity. The Schiff bases of 3-carboxylsalicylaldehyde and diamines (1,2-diaminoethane, 1,2-diaminopropane, 1,3-diaminopropane, *etc.*) have many coordination modes, so they can form many mono- and polynuclear complexes (Tao *et al.*, 2002; Li *et al.*, 2006). Recently, our interest has been focused on asymmetric Schiff bases and their complexes (Zhang *et al.*, 2005; Yu *et al.*, 2006). Here, we report the crystal structure of the title mononuclear zinc(II) complex, (I), in which the ligand is the Schiff base of (1*R*,2*R*)-diaminocyclohexane mono-condensed with one equivalent of 3-carboxylsalicylaldehyde.



(I)

Complex (I) is formed by a Zn^{II} cation and two univalent anions. The Zn^{II} cation is coordinated by four N atoms and two O atoms in an octahedral geometry. Each anionic ligand

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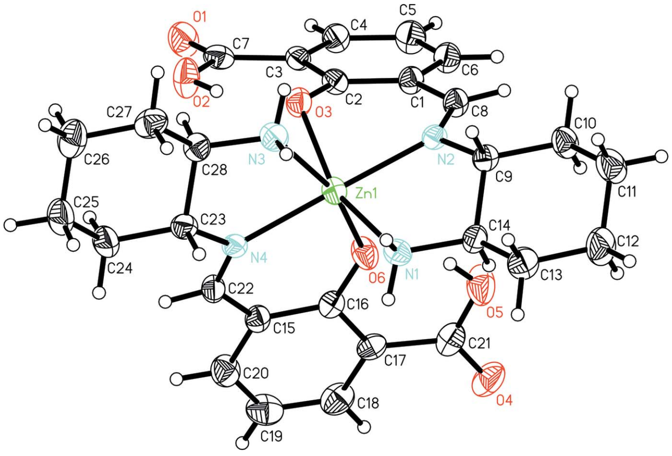

Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

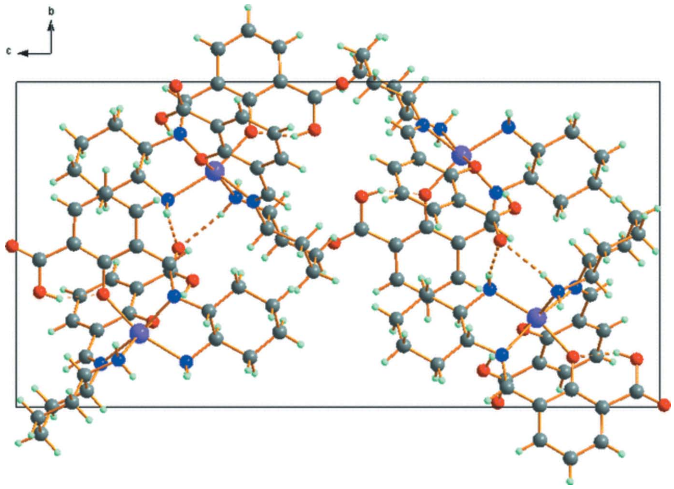

Figure 2
The molecular packing of (I), viewed along the *a* axis. Hydrogen bonds are indicated by dashed lines.

acts as a tridentate chelator *via* two N atoms and one phenolate O atom, and occupies a coordination plane. The two NON coordination planes formed are nearly perpendicular to each other, with a dihedral angle of 88.08 (13)°.

The carboxy group in the ligand does not coordinate to the central atom, but forms an intramolecular hydrogen bond with the phenolate O atom. Intermolecular hydrogen bonds are formed through the H atoms of the amine groups to carboxyl O atoms and link the molecules into chains running parallel to the *b* axis (Table 1, Fig. 2).

Experimental

3-Carboxylsalicylaldehyde (0.332 g, 2.0 mmol) was dissolved in methanol (30 ml). To this solution, an aqueous solution (10 ml) containing NaOH (0.160 g, 4.0 mmol) and cyclohexane-1,2-diammonium (1*R*,2*R*)-tartrate (0.5286 g, 2.0 mmol) was added. The mixed solution was stirred at 333 K for 1 h and then filtered to give a clear yellow solution. To this yellow solution, zinc acetate [$Zn(OOCCH_3)_2\cdot2H_2O$; 0.439 g, 2.0 mmol] dissolved in methanol (30 ml) was added. The system was stirred at 333 K for 2 h, then cooled and filtered. The filtrate was sealed and kept at room temperature. After 30 d, yellow block-shaped crystals of (I), suitable for X-ray diffraction, were obtained.

Crystal data

$[Zn(C_{14}H_{17}N_2O_3)_2]$
$M_r = 587.96$
Orthorhombic, $P2_12_12_1$
$a = 8.858$ (2) Å
$b = 12.610$ (3) Å
$c = 25.008$ (6) Å
$V = 2793.5$ (11) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.93$ mm^{-1}
$T = 273$ (2) K
0.15 × 0.12 × 0.11 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{\min} = 0.873$, $T_{\max} = 0.905$
17440 measured reflections
6561 independent reflections
3447 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.083$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.130$
$S = 0.97$
6561 reflections
354 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 0.52$ e Å^{-3}
$\Delta\rho_{\min} = -0.50$ e Å^{-3}
Absolute structure: Flack (1983), with 3755 Friedel pairs
Flack parameter: 0.018 (17)

Table 1
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O5—H5⋯O6	0.82	1.71	2.473 (4)	153
O2—H2⋯O3	0.82	1.67	2.439 (5)	155
N3—H3*A*⋯O1$^{\rm i}$	0.90	2.37	3.253 (6)	168
N1—H1*A*⋯O1$^{\rm i}$	0.90	2.22	3.114 (5)	170

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

All H atoms were included in calculated positions, with C—H distances ranging from 0.93 to 0.98 Å, N—H distances of 0.90 Å and O—H distances of 0.82 Å. They were refined in the riding-model approximation, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C,N})$ or $1.5U_{\rm eq}({\rm O})$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2005); software used to prepare material for publication: *SHELXTL*.

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References

Bruker (2005). *APEX2*, *SAINT*, *SHELXTL* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dios, A., Mitchell, R. A., Aljabari, B., Lubetsky, J., O'Connor, K., Liao, H., Senter, P. D., Manogue, K. R., Lolis, E., Metz, C., Bucala, R., Callaway, D. J. E. & Al-Abed, Y. (2002). *J. Med. Chem.* **45**, 2410–2416.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Li, F. A., Mei, C. Z. & Tao, R. J. (2006). *J. Henan Univ. (Nat. Sci.)*, **36**, 32–36.
Sharma, V. (2004). *Bioconjugate Chem.* **15**, 1464–1474.

m1564 Yu *et al.* • $[Zn(C_{14}H_{17}N_2O_3)_2]$ *Acta Cryst.* (2007). E**63**, m1563–m1565

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Tao, R. J., Zhang, S. Q., Niu, J. Y., Yu, Z. W. & Zhou, X. Y. (2002). *Chin. J. Inorg. Chem.* **18**, 409–412.

Yu, Z.-W., Hao, Y.-L., Zhang, W. & Cui, Q.-X. (2006). *Acta Cryst.* E**62**, m2786–m2788.

Zhang, W., Hao, Y. L., Yao, L. & Yu, Z. W. (2005). *Chem. Res.* **16**, 49–51.

Acta Cryst. (2007). E**63**, m1563–m1565 Yu *et al.* • [Zn($C_{14}H_{17}N_2O_3$)$_2$] **m1565**