Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

catena-Poly[[bis(imidazole-κN)zinc(**II**)]-μ-(2*R*,3*R*)-tartrato-$\kappa^4 O,O':O'',O'''$]

Sy Adama,[a] Gaye Mohamed,[a]* Sall Abdou Salam,[a] Barry Aliou Hamady[b] and Driss Ahmed[c]

[a]Département de Chimie, Faculté des Sciences et Techniques, Université Cheikh Anta Diop, Dakar, Senegal, [b]Département de Chimie, Faculté des Sciences, Université de Nouakchott, Nouakchott, Mauritania, and [c]Campus Universitaire, Département de Chimie, Faculté des Sciences, Université de Tunis, 1060 Tunis, Tunisia

Correspondence e-mail: mlgayeastou@yahoo.fr

Received 30 December 2006
Accepted 16 January 2007

Key indicators

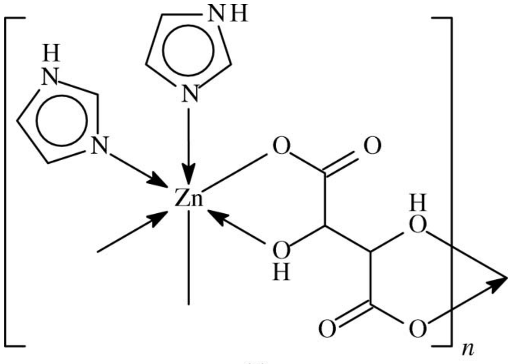
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.027
wR factor = 0.076
Data-to-parameter ratio = 16.2

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

The Zn atom in the title complex, $[Zn(C_4H_4O_6)(C_3H_4N_2)_2]_n$, is in an octahedral environment comprising two N atoms fom the imidazole ligands and four O atoms from the tartrate ligands. The imino groups participate in intramolecular N—H···O hydrogen bonds, as do the O atoms.

Comment

The carboxylate group is well known for its ability to bridge two metal centers and numerous multinuclear carboxylate-bridged systems are known in the literature (Colacio *et al.*, 2000; Dey *et al.*, 2003; Choi *et al.*, 2004; Scherb *et al.*, 2002; Zhang *et al.*, 2003; Li *et al.*, 2004). The structure of a zinc(II) complex, (I), derived from (+)-(2*R*,3*R*)-tartaric acid is described here.



(I)

The coordination environment is made up of the imino N atoms of two neutral monodentate imidazole ligands, two negatively charged O atoms of the tartrate and two hydroxy O atoms of the tartrate (Fig. 1). The tartrate dianion links adjacent Zn atoms into a polymer. The two hydroxy O atoms occupy *cis* positions, in contrast to $[Zn(C_3H_4N_2)(L)]$, where H_2L is methyl-2-lactic acid (Carballo *et al.*, 2004). The two imidazole molecules are also *cis* to each other. The Zn—N distances are simlar to distances found in $[Zn(quin\text{-}2\text{-}c)_2(1\text{-}Meim)_2]$ (quin-2-c is quinoline-2-carboxylate and 1-Meim is 1-methylimidazole; Zevaco *et al.*, 1998) and compares well with typical values found in octahedral complexes (Janiak, 2000). The Zn—O(hydroxy) and Zn—O(carboxylate) distances are typical of Zn—O bonds.

Intermolecular hydrogen-bond contacts involve the NH groups and the coordinated O atoms (Table 2), as well as the hydroxy group and non-coordinated O atoms of the carboxylate groups. The hydrogen bonds connect the chains into a three-dimensional network.

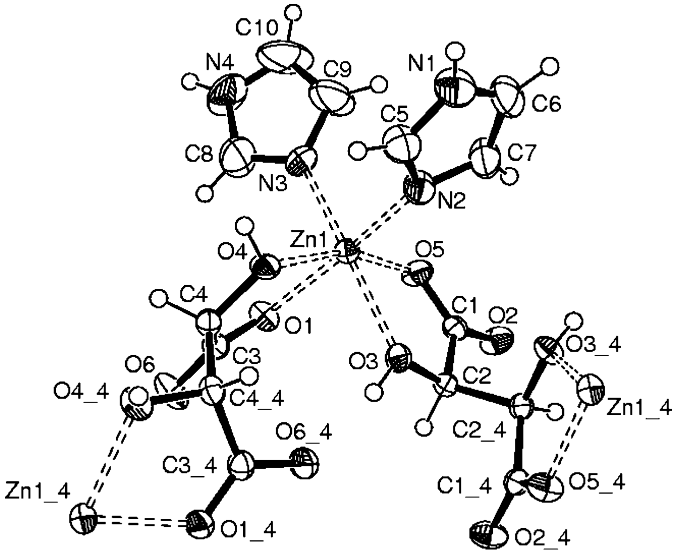


Figure 1
A view of the asymmetric unit of the title compound, with displacement ellipsoids are drawn at the 50% probability level. H atom are shown as small spheres of arbitrary radii.

Experimental

Zinc(II) chloride tetrahydrate (0.44 g, 2 mmol) was dissolved in a mixture of water and ethanol (10 ml, 1:1). This solution was added to a solution of imidazole (0.272 g, 4 mmol) in the same volume of the mixed solvent. A solution of (+)-(2*R*,3*R*)-tartaric acid (0.300 g, 2 mmol) and KOH (0.224 g, 4 mmol) in a mixture of water and ethanol (10 ml, 1:1) was added. The colorless crystals that formed from the filtered solution were collected in 80% yield. Elemental analysis calculated for $C_{10}H_{12}N_4O_6Zn$: C 34.35, H 3.46, N 116.03%; found: C 34.33, H 3.45, N 116.01%.

Crystal data

$[Zn(C_4H_4O_6)(C_3H_4N_2)_2]$
$M_r = 349.61$
Orthorhombic, $C222_1$
$a = 8.949$ (9) Å
$b = 14.175$ (5) Å
$c = 22.128$ (5) Å
$V = 2807$ (3) Å^3

$Z = 8$
$D_x = 1.655$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.78$ mm^{-1}
$T = 293$ (2) K
Prism, colorless
0.6 × 0.4 × 0.3 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.425$, $T_{\max} = 0.580$
3374 measured reflections

3070 independent reflections
2935 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.035$
$\theta_{\max} = 27.0°$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.076$
$S = 1.13$
3070 reflections
190 parameters
H-atom parameters not refined

$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2 + 2.8362P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.022$
$\Delta\rho_{\max} = 0.35$ e Å^{-3}
$\Delta\rho_{\min} = -0.38$ e Å^{-3}
Absolute structure: Flack (1983), no Friedel pairs
Flack parameter: −0.001 (13)

Table 1
Selected geometric parameters (Å, °).

Zn1—N2	2.057 (3)	Zn1—O1	2.104 (2)
Zn1—O5	2.081 (2)	Zn1—O3	2.215 (2)
Zn1—N3	2.093 (3)	Zn1—O4	2.221 (2)
N2—Zn1—O5	97.02 (11)	N3—Zn1—O3	168.64 (10)
N2—Zn1—N3	93.14 (12)	O1—Zn1—O3	84.31 (8)
O5—Zn1—N3	95.33 (10)	N2—Zn1—O4	93.24 (11)
N2—Zn1—O1	167.75 (10)	O5—Zn1—O4	161.54 (8)
O5—Zn1—O1	94.43 (10)	N3—Zn1—O4	99.40 (10)
N3—Zn1—O1	90.12 (10)	O1—Zn1—O4	74.57 (9)
N2—Zn1—O3	94.37 (10)	O3—Zn1—O4	88.68 (8)
O5—Zn1—O3	75.30 (8)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1$^{\rm i}$	0.86	1.90	2.746 (4)	169
N4—H2···O5$^{\rm ii}$	0.86	2.02	2.846 (5)	162
O3—H11···O6$^{\rm iii}$	0.82	1.81	2.617 (4)	168
O4—H12···O2$^{\rm iv}$	0.82	1.85	2.649 (4)	165

Symmetry codes: (i) $x + \frac{1}{2}, y + \frac{1}{2}, z$; (ii) $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (iii) $-x, y, -z + \frac{3}{2}$; (iv) $x - \frac{1}{2}, y + \frac{1}{2}, z$.

All H atoms were treated as riding on their parent atoms [N—H = 0.86, C—H = 0.93–0.98 and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C,N})$]. The H atoms of the hydroxy groups were located in Fourier difference maps and refined using AFIX instructions. The absolute configuration is that of the starting tartaric acid.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors thank the Agence Universitaire de la Francophonie for financial support (AUF-PSCI No. 6301PS48).

References

Carballo, R., Castiñeiras, A., Covelo, B., García-Martínez, E., Niclós, E. J. & Vázquez-López, E. M. (2004). *Polyhedron*, **23**, 1505–1518.
Choi, K.-Y., Jeon, Y.-M., Ryu, H., Oh, J.-J., Lim, H.-H. & Kim, M.-W. (2004). *Polyhedron*, **23**, 903–911.
Colacio, E., Ghazi, M., Kivekäs, R. & Moreno, J. M. (2000). *Inorg. Chem.* **39**, 2882–2890.
Dey, S. K., Bag, B. K., Malik, M. A., El Fallah, M. S., Ribas, J. & Mitra, S. (2003). *Inorg. Chem.* **42**, 4029–4035.
Enraf–Nonius (1994). *CAD-4 EXPRESS*. Enraf–Nonius, Delft, The Netherlands.
Fair, C. K. (1990). *MolEN*. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Janiak, C. (2000). *J. Chem. Soc. Dalton Trans.* pp. 3885–3896.
Li, D.-X., Xu, D.-J. & Xu, Y.-Z. (2004). *Acta Cryst.* E**60**, m1982–m1984.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Scherb, S., Näther, C. & Bensch, W. (2002). *Acta Cryst.* C**58**, m135–m136.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zevaco, T. A., Görls, H. & Dinjus, E. (1998). *Inorg. Chim. Acta*, **269**, 283–286.
Zhang, X.-F., Huang, D.-G., Feng, C., Chen, C.-N., Liu, Q.-T. & Sun, L.-C. (2003). *Acta Cryst.* C**59**, m402–m404.

Acta Cryst. (2007). E**63**, m574–m575 Adama *et al.* • $[Zn(C_4H_4O_6)(C_3H_4N_2)_2]$ **m575**