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Bis(2-chlorobenzoato-*κO*)bis(phenazone-*κO*)-zinc(II) 0.612-hydrate

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Key indicators

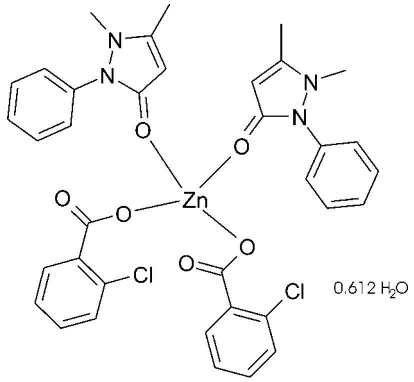
Single-crystal X-ray study
T = 294 K
Mean *σ*(C–C) = 0.008 Å
Disorder in solvent or counterion
R factor = 0.064
wR factor = 0.138
Data-to-parameter ratio = 16.1

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

The title compound, $[Zn(C_7H_4ClO_2)_2(C_{11}H_{12}N_2O)_2]\cdot 0.612H_2O$, is a mononuclear zinc(II) compound. The Zn atom lies on a crystallographic twofold rotation axis. It is coordinated in a distorted tetrahedral arrangement by two O atoms of two phenazone molecules and one carboxylate O atom from each of two 2-chlorobenzoate anions. Intramolecular O—H···O hydrogen bonds may be effective in the stabilization of the structure.

Comment

Zinc is a relatively abundant element in biological organisms and plays an essential role in a large number of enzymatic reactions (Liljas *et al.*, 1972). Zinc(II) benzoate and its halogeno derivatives with organic molecular ligands are interesting because of their potential biological activities. One way to understand metal–drug interactions is to study structures of metal complexes containing the drug as a ligand (*e.g.* papaverine) (Zeleňák *et al.*, 2004). Phenazone has widely been used as analgesic either alone or with other drugs (Verley *et al.*, 2000). In the present paper, we report the crystal structure of the title compound, (I), which has been determined in an attempt to understand the structural behaviour of oxygen-containing ligands when coordinating to zinc carboxylates.



(I)

Compound (I) is a mononuclear zinc(II) compound (Fig. 1). The Zn atom lies on a crystallographic twofold rotation axis. It is coordinated in a distorted tetrahedral arrangement by two O atoms of two phenazone molecules and one carboxylate O atom from each of two 2-chlorobenzoate anions (Table 1). This structure is similar to the structures of other zinc(II) complexes with phenazone as a terminal ligand: $[ZnCl_2(C_{11}H_{12}N_2O)_2]$ (Cingi *et al.*, 1972), $[ZnBr_2(C_{11}H_{12}N_2O)_2]$ (Zeleňák *et al.*, 1999) and $[Zn(NO_3)_2(C_{11}H_{12}N_2O)_2]$ (Brassy *et al.*, 1974).

Intramolecular O—H⋯O hydrogen bonds (Table 2) may be effective in the stabilization of the structure.

Experimental

For the preparation of the title compound, zinc carbonate (0.418 g, 3.33 mmol) and 2-chlorobenzoic acid (1.044 g, 3.33 mmol) were dissolved in ethanol (20 ml) and stirred at room temperature for about 1 h. An aqueous solution of phenazone (1.255 g, 3.33 mmol) was added, and the mixture was again stirred for about 3 h. The final reaction solution was left to stand at ambient temperature. Colourless crystals were collected by filtration, washed with a small amount of cold ethanol and water, and then dried at ambient temperature.

Crystal data

$[Zn(C_7H_4ClO_2)_2(C_{11}H_{12}N_2O)_2]\cdot 0.612H_2O$
$M_r = 763.97$
Monoclinic, $C2/c$
$a = 27.986$ (3) Å
$b = 9.6403$ (12) Å
$c = 14.513$ (4) Å
$\beta = 111.746$ (11)°
$V = 3636.8$ (12) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.87$ mm^{-1}
$T = 294$ (2) K
0.80 × 0.50 × 0.50 mm

Data collection

Siemens P4 diffractometer
Absorption correction: ψ scan (*XEMP*; Siemens, 1990)
$T_{\min} = 0.554$, $T_{\max} = 0.646$
4553 measured reflections
3853 independent reflections
1981 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.067$
3 standard reflections every 97 reflections intensity decay: 8.1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.138$
$S = 1.01$
3853 reflections
240 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max} = 0.44$ e Å^{-3}
$\Delta\rho_{\min} = -0.44$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.956 (3)	Zn1—O3	1.979 (3)
O1—Zn1—O1$^{\rm i}$	125.65 (19)	O1—Zn1—O3$^{\rm i}$	107.71 (12)
O1—Zn1—O3	108.19 (12)	O3—Zn1—O3$^{\rm i}$	95.11 (17)

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

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1W—H1W⋯O2	0.82 (1)	2.36 (1)	2.824 (1)	117 (1)
O1W—H2W⋯O1$^{\rm i}$	0.82 (1)	2.56 (2)	2.970 (1)	113 (2)

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

H atoms of the water molecule were located in a difference synthesis and were refined with distance restraints of 0.82 (2) Å and with $U_{\rm iso}({\rm H}) = 0.107$ Å^2. The remaining H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methyl H atoms, and constrained to ride on their parent atoms, with $U_{\rm iso}({\rm H}) = xU_{\rm eq}({\rm C})$, where $x = 1.2$ for aromatic and $x = 1.5$ for methyl H atoms.

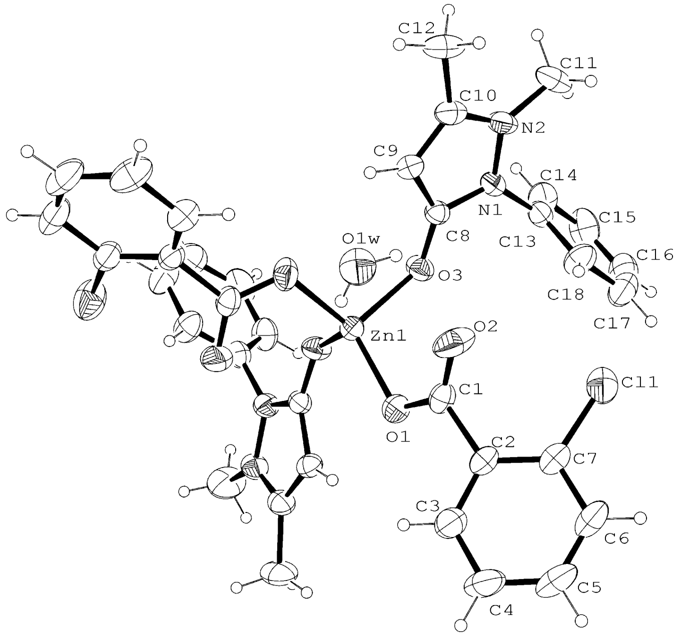


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are related to labelled atoms by $(-x, y, \frac{1}{2} - z)$.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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