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cis-Diaquabis(*trans*-cinnamato-*O*,*O*′)-zinc(II)

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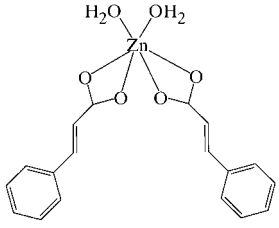
The title complex, $[Zn(C_9H_7O_2)_2(H_2O)_2]$, shows a distorted octahedral coordination and has a crystallographic twofold rotation axis. Intermolecular O—H···O hydrogen bonding forms a two-dimensional network in the *ab* plane.

Comment

Metal–ligand interaction is one of the possible ways of controlling the relative arrangement of the *trans*-cinnamate



(I)

ions in the crystals to yield the desired photodimer (Ito, 1998). The structure of *cis*-diaquabis(*trans*-cinnamato-*O*,*O*′)zinc(II), (I), has been determined and is presented here.

Experimental

Crystals of (I) were grown from an aqueous solution. The crystal specimen was sealed in a capillary to avoid efflorescence.

Crystal data

$[Zn(C_9H_7O_2)_2(H_2O)_2]$
M_r = 395.72
Monoclinic, *C*2
a = 11.728 (4) Å
b = 5.105 (3) Å
c = 14.547 (2) Å
β = 99.83 (2)°
V = 858.2 (5) Å^3
Z = 2
D_x = 1.531 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 25 reflections
θ = 14.5–15.0°
μ = 1.462 mm^{-1}
T = 299 (1) K
Needle, colourless
0.70 × 0.15 × 0.10 mm

Data collection

Rigaku AFC-7*R* diffractometer
θ–2θ scans
Absorption correction: by integration (Coppens *et al.*, 1965)
T_{min} = 0.802, T_{max} = 0.872
1448 measured reflections
1383 independent reflections
1084 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 30°
h = 0 → 17
k = −7 → 0
l = −20 → 20
3 standard reflections
every 150 reflections
intensity decay: none

Refinement

Refinement on F^2
$R(F)$ = 0.034
$wR(F^2)$ = 0.088
S = 1.05
1383 reflections
150 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0404P)^2 + 0.4323P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}
Absolute structure: Flack (1983), no Friedel pairs
Flack parameter = 0.13 (2)

Table 1
Selected geometric parameters (Å, °).

Zn1—O2	2.118 (3)	O2—C5	1.275 (5)
Zn1—O3	2.390 (3)	O3—C5	1.246 (5)
Zn1—O4	1.965 (4)		
O2—Zn1—O2^{i}	94.2 (2)	O3—Zn1—O3^{i}	136.8 (2)
O2—Zn1—O3	57.6 (1)	O3—Zn1—O4	127.0 (1)
O2—Zn1—O3^{i}	92.0 (1)	O3—Zn1—O4^{i}	84.3 (1)
O2—Zn1—O4	99.6 (1)	O4—Zn1—O4^{i}	93.8 (2)
O2—Zn1—O4^{i}	139.9 (1)		

Symmetry code: (i) $1-x, y, 2-z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*A*···O3^{i}	0.75 (5)	1.93 (5)	2.681 (5)	175 (6)
O4—H4*B*···O2^{ii}	0.84 (7)	1.90 (7)	2.713 (4)	163 (6)

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

The C—H distances are in the range 0.86 (5)–0.98 (5) Å. The Flack parameter value of 0.13 (2) suggests the correct polar direction.

Data collection and cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *TEXSAN*.

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