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Diaquadiacetylacetonatozinc(II)

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.020
wR factor = 0.056
Data-to-parameter ratio = 18.0

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

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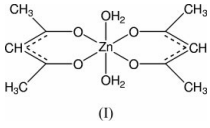
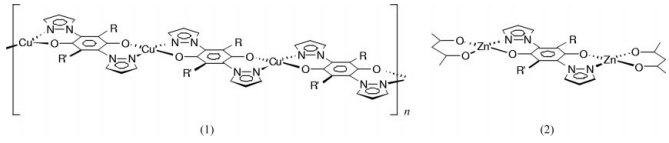
The title compound, $[Zn(C_5H_7O_2)_2(H_2O)_2]$, crystallizes with the Zn atom on a centre of inversion and one acetylacetonato and one water molecule in the asymmetric unit. It is isostructural with the Co, Mg, Ni, Mn and Fe complexes.

Comment

We report here the X-ray crystal structure analysis of diaquadiacetylacetonatozinc(II), (I). We have recently synthesized the purple coordination polymer (1) (see Scheme) from $CuBr_2$ and 2,5-bis(pyrazol-1-yl)-1,4-dihydroxybenzene (Dinnebier *et al.*, 2002) and have now become interested in the physical and chemical properties of the dinuclear transition metal complex (2) (see Scheme). We have therefore prepared (I), the synthesis of which has been achieved according to a literature procedure (Rudolph & Henry, 1967) as indicated in the reaction Scheme.



(I)



(1) (2)

$$ZnSO_4 + 2CH_3COCH_2COCH_3 \xrightarrow{NaOH/H_2O} [Zn(C_5H_7O_2)_2(H_2O)_2]$$

In (I), the Zn atom is located on a centre of inversion and the asymmetric unit contains one acetylacetonate anion and one water molecule. The acetylacetonate is almost planar (r.m.s.d. = 0.043 Å for all seven non-H atoms). The Zn atom is displaced from this plane by 0.466 (1) Å. The bond from Zn to the water molecule is significantly longer than the bonds to the acetylacetonatee O atoms (see Table 1). The crystal packing is stabilized by hydrogen bonds (see Table 2) from the water molecule to the two acetylacetonate O atoms.

The title compound is isostructural with the Co (Bullen, 1959; Laugier & Mathieu, 1975), Mg (Morosin, 1967), Ni (Montgomery & Lingafelter, 1964), Mn (Montgomery & Lingafelter, 1968; Onuma & Shibata, 1970) and Fe (Laugier & Mathieu, 1975; Tsodikov *et al.*, 1995) complexes.

Experimental

The title compound was synthesized by stirring a slurry of $ZnSO_4$, 2,4-pentanedione, NaOH and water at ambient temperature. After 1 h, (I) precipitated quantitatively and was filtered off. After washing, the title compound was recrystallized from ethyl acetate (yield 64%).

Crystal data

$[Zn(C_5H_7O_2)_2(H_2O)_2]$
M_r = 299.61
Monoclinic, $P2_1/c$
a = 10.7987 (9) Å
b = 5.3744 (4) Å
c = 11.1259 (11) Å
β = 105.781 (7)°
V = 621.37 (9) Å^3
Z = 2
D_x = 1.601 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 15112 reflections
θ = 3.7–28.5°
μ = 1.99 mm^{-1}
T = 100 (2) K
Block, colourless
0.34 × 0.25 × 0.23 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 1990; Blessing, 1995)
T_{min} = 0.495, T_{max} = 0.631
10 528 measured reflections
1601 independent reflections
1476 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 28.7°
$h = -14 \rightarrow 13$
$k = -7 \rightarrow 7$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.056
S = 1.06
1601 reflections
89 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0336P)^2 + 0.0697P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

Table 1
Selected geometric parameters (Å).

Zn1—O2	2.0319 (8)	O2—C4	1.2700 (14)
Zn1—O1	2.0491 (8)	C2—C3	1.4122 (15)
Zn1—O3	2.1849 (8)	C3—C4	1.4088 (15)
O1—C2	1.2661 (14)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O1^{i}	0.79 (2)	2.09 (2)	2.8715 (12)	170 (2)
O3—H3B···O2^{ii}	0.78 (2)	2.122 (19)	2.8656 (11)	158.3 (19)

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

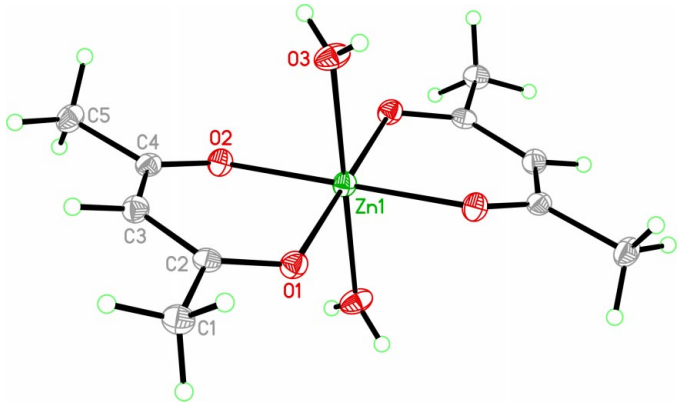


Figure 1
Perspective view of the title compound, with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

H atoms bonded to C atoms were refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C) or 1.5 U_{eq}(C_{methyl})] using a riding model, with C—H = 0.95 Å or methyl C—H = 0.98 Å, respectively. The methyl groups were allowed to rotate but not to tip. The H atoms bonded to O were refined isotropically.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97 (Sheldrick, 1997).

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