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A new monoclinic polymorph of anhydrous zinc acetate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.035
wR factor = 0.097
Data-to-parameter ratio = 15.3

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

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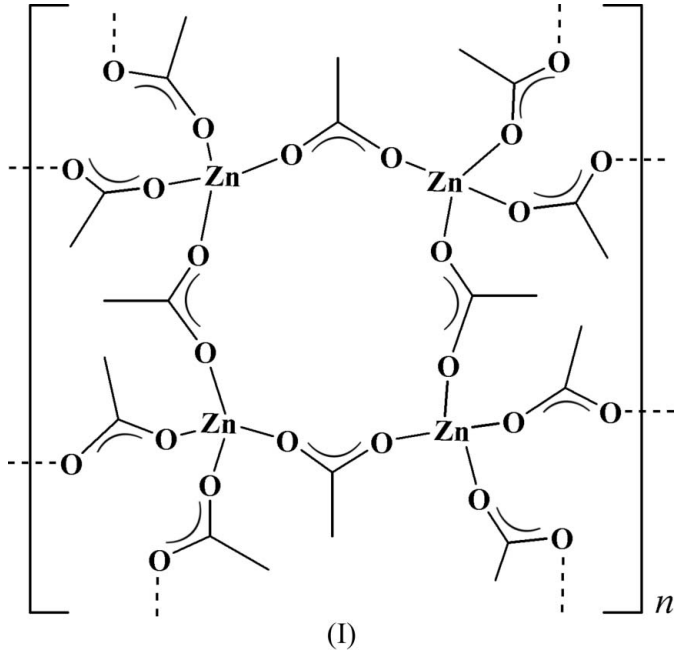
A new monoclinic polymorph of anhydrous zinc acetate, poly[di-μ_2-acetato-zinc(II)], $[Zn(C_2H_3O_2)_2]$, crystallizes in the space group $P2_1/c$. The structure contains two-dimensional sheets identical to those in the known $C2/c$ polymorph, but exhibits a different sheet-stacking sequence.

Comment

The crystal structure of zinc acetate was studied as early as 1926 (Wyart, 1926). In 1979, Valero Capilla & Alcala Aranda (1979) determined the structure of anhydrous zinc acetate and found that the compound crystallizes in the orthorhombic space group *Fdd*2. In that structure, the Zn atoms lie in a distorted tetrahedral environment, and they are linked by acetate bridges into a three-dimensional network. Subsequently, Clegg *et al.* (1986) reported a monoclinic polymorph of anhydrous zinc acetate, which adopts space group $C2/c$. There, the Zn coordination geometry is very similar to that found in the orthorhombic polymorph, but the network in the monoclinic case is two-dimensional. We are interested in zinc complexes due to the biorelevance of this metal ion. During a study in which zinc acetate hydrate was reacted with a phenolate-containing ligand, several crystals of a new monoclinic polymorph of anhydrous zinc acetate, (I), were obtained.



(I)

The title complex, (I) (Fig. 1), crystallizes in space group $P2_1/c$. Each Zn atom is bridged by four acetate groups to

neighbouring Zn atoms, forming two-dimensional sheets parallel to the (100) planes (Fig. 2) that are closely comparable with those in the *C*2/*c* polymorph (Clegg *et al.*, 1986). Within these sheets, the distances between neighbouring Zn atoms, approximately along [001] and exactly along [010], are 4.6411 (9) and 4.7967 (10) Å, respectively. The distinction between the two monoclinic polymorphs lies in the stacking sequence of the two-dimensional sheets: in (I), every second sheet is related by translation along *a*, while in the *C*2/*c* polymorph, it is every fourth sheet.

Experimental

Equimolar quantities of zinc acetate dihydrate (0.22 g, 0.1 mmol) and dimethyl-2,5-dihydroxyterephthalate (0.22 g, 0.1 mmol) were separately dissolved in 2 ml and 5 ml methanol, respectively. The solutions were mixed and stirred magnetically for 30 min. Single crystals of (I) were obtained after slow evaporation of the solvent at room temperature for 1 week.

Crystal data

$[Zn(C_2H_3O_2)_2]$
M_r = 183.46
Monoclinic, $P2_1/c$
a = 15.096 (3) Å
b = 4.7967 (10) Å
c = 9.2361 (18) Å
β = 98.10 (3)°
V = 662.1 (2) Å^3
Z = 4
D_x = 1.840 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.65 mm^{-1}
T = 293 (2) K
Prism, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.417, T_{max} = 0.476
5931 measured reflections
1285 independent reflections
1146 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.097
S = 1.06
1285 reflections
84 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0601P)^2 + 0.4165P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.88 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

H atoms were positioned geometrically and allowed to ride during refinement with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C), while the methyl groups were allowed to rotate about their local threefold axes.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; 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: *WinGX* (Farrugia, 1999).

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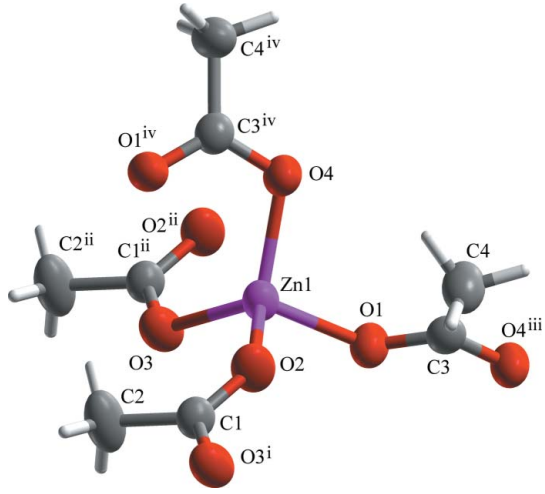

Figure 1
The coordination environment of Zn in (I), showing displacement ellipsoids at the 50% probability level. [Symmetry codes: (i) $x, -1+y, z$; (ii) $x, 1+y, z$; (iii) $x, \frac{1}{2}-y, -\frac{1}{2}+z$; (iv) $x, \frac{1}{2}-y, \frac{1}{2}+z$.]

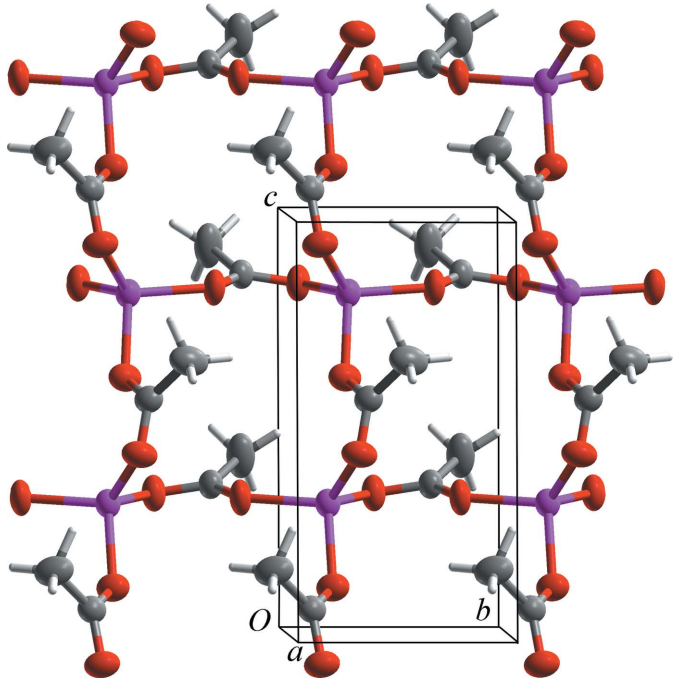

Figure 2
A view of (I), approximately along the *a* axis, showing a single two-dimensional layer.

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