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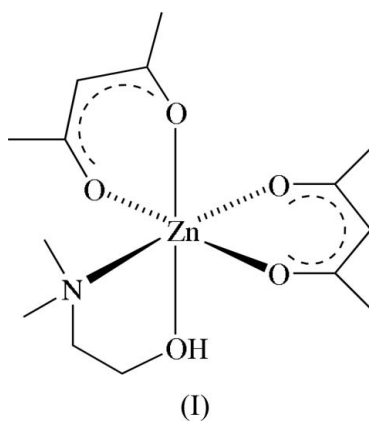
Key indicators

Single-crystal X-ray study
 $T = 110$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.047
 wR factor = 0.131
Data-to-parameter ratio = 20.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Bis(acetylacetonato- $\kappa^2\text{O},\text{O}'$)(N,N -dimethylaminoethanol- $\kappa^2\text{N},\text{O}$)zinc(II)

The title crystalline complex, $[\text{Zn}(\text{C}_5\text{H}_7\text{O}_2)_2(\text{C}_4\text{H}_{11}\text{NO})]$, was prepared as a result of our efforts to synthesize ZnO precursors for chemical vapor deposition. Two acetylacetonate and one N,N -dimethylaminoethanol ligands are coordinated to the Zn^{II} atom in a slightly distorted octahedral environment.

Comment

The solid state structures of octahedral complexes of the type $M(\text{acac})_2(\text{dmaeH})$ (acac is acetylacetonate and dmaeH is N,N -dimethylaminoethanol) have recently been reported for the Ni^{II} (Williams *et al.*, 2001) and Co^{II} derivatives (Tanase *et al.*, 2004). Such complexes are potential precursors for chemical vapor deposition to form ceramic oxides, for example, ZnO, which is used in diverse applications including gas sensors (Roy & Basu, 2002), solar cells (Keis *et al.*, 2002) and transparent conducting oxide electrodes (Jayaraj *et al.*, 2002). The melting point of the title compound, (I), $\text{Zn}(\text{acac})_2(\text{dmaeH})$ (393–398 K), is lower than that of the parent reagent $\text{Zn}(\text{acac})_2 \cdot \text{H}_2\text{O}$ (409–411 K), making (I) a promising candidate as a precursor for thin films of ZnO by aerosol-assisted chemical vapor deposition, which will be studied in detail later.



Compound (I) is isostructural with its Ni and Co analogs, $\text{Ni}(\text{acac})_2(\text{dmaeH})$ and $\text{Co}(\text{acac})_2(\text{dmaeH})$. The geometric environment around the central metal atom is a distorted octahedron with O–Zn–O ‘bite’ angles close to 90° [$89.48(6)^\circ$ and $87.75(6)^\circ$; Table 1] for the acac groups. In contrast, the dmaeH ligand, which forms a five-membered chelate ring, has a smaller O–Zn–N bite angle [$77.51(6)^\circ$]. The Zn–O bond lengths for the acac ligands range from 2.0429 (15) to 2.0739 (15) Å (Table 1). These are slightly longer than the corresponding distances (2.01–2.05 Å) found

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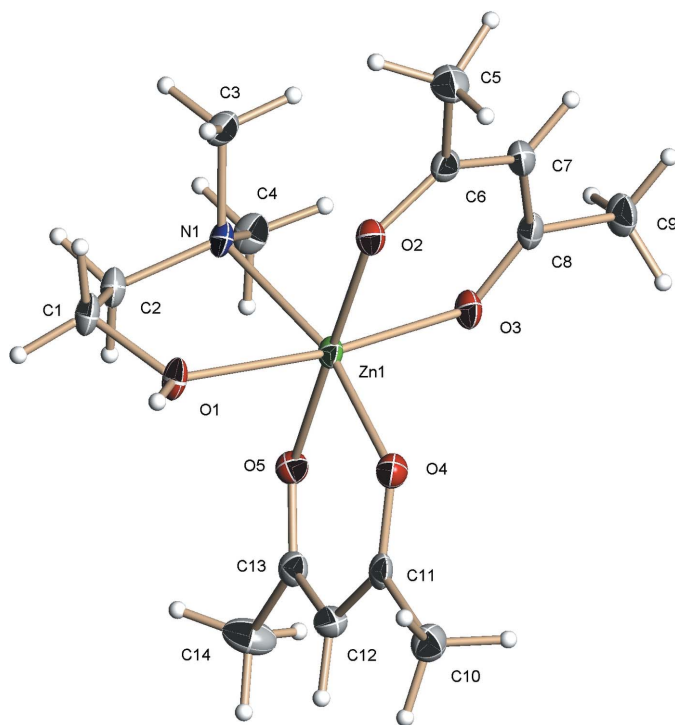


Figure 1
The atom-numbering scheme in the title complex. Displacement ellipsoids are drawn at the 50% probability level.

for $\text{Zn}(\text{acac})_2 \cdot \text{H}_2\text{O}$ (Montgomery & Lingafelter, 1963) and $\text{Zn}(\text{acac})_2 \cdot 2\text{H}_2\text{O}$ (Harbach *et al.*, 2003). The Zn–N bond length observed here is 2.2195 (17) Å, while those for the octahedral complex $[\text{pyda-H}][\text{Zn}(\text{pydc})(\text{pydc-H})] \cdot 3\text{H}_2\text{O}$ (pyda is 2,6-pyridinediamine and pydc-H2 is pyridinedicarboxylic acid; Ranjbar *et al.*, 2002) are 2.015 and 2.032 Å. Pairs of symmetry-related molecules in the unit cell are bridged by two O1–H1···O2 hydrogen bonds between the hydroxy group and one of the acac O atoms (Fig. 2 and Table 2).

Experimental

N,N-Dimethylaminoethanol (0.1 ml, 1.0 mmol) was added to a stirred solution of $\text{Zn}(\text{acac})_2 \cdot \text{H}_2\text{O}$ (0.281 g, 1.0 mmol) in tetrahydrofuran (THF, 20 ml). Three hours of continuous stirring at 323 K, followed by removal of all volatiles in vacuum, gave a dry powder of (I). Pink block-like crystals suitable for single-crystal X-ray analysis were harvested from a concentrated solution in THF at room temperature after two weeks.

Crystal data

$[\text{Zn}(\text{C}_5\text{H}_7\text{O}_2)_2(\text{C}_4\text{H}_{11}\text{NO})]$	$Z = 2$
$M_r = 352.72$	$D_x = 1.385 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.6131$ (7) Å	Cell parameters from 7241 reflections
$b = 10.3234$ (10) Å	$\theta = 2.3\text{--}30.5^\circ$
$c = 11.7736$ (11) Å	$\mu = 1.47 \text{ mm}^{-1}$
$\alpha = 105.837$ (2)°	$T = 110$ (2) K
$\beta = 103.790$ (2)°	Block, pink
$\gamma = 97.422$ (2)°	$0.45 \times 0.4 \times 0.35 \text{ mm}$
$V = 845.65$ (14) Å ³	

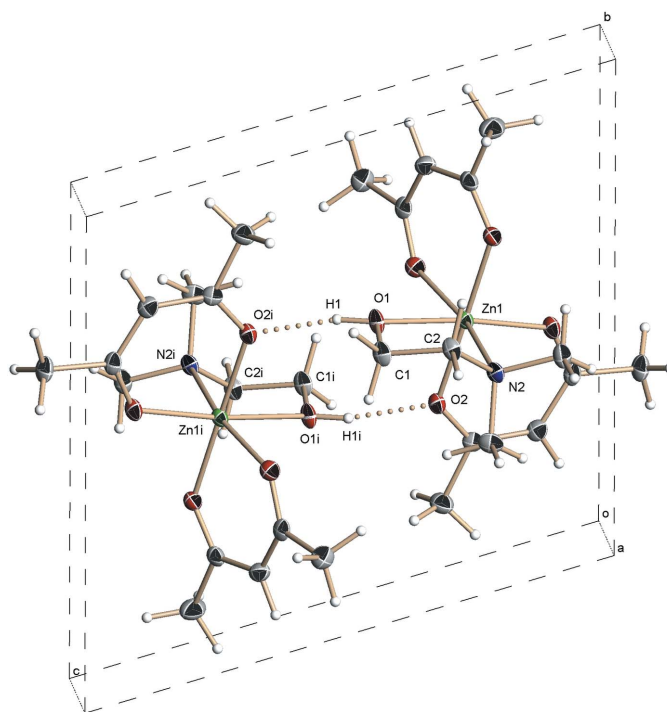


Figure 2
The packing of (I). Hydrogen bonds are shown as dotted lines.

Data collection

Bruker SMART APEX CCD diffractometer	4166 independent reflections
ω scans	3852 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS in SAINTE-Plus; Bruker, 2003)	$R_{\text{int}} = 0.040$
$T_{\text{min}} = 0.394$, $T_{\text{max}} = 0.60$	$\theta_{\text{max}} = 28.3^\circ$
8704 measured reflections	$h = -10 \rightarrow 10$
	$k = -13 \rightarrow 13$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.047$	$w = 1/[\sigma^2(F_o^2) + (0.0976P)^2]$
$wR(F^2) = 0.131$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{\text{max}} < 0.001$
4166 reflections	$\Delta\rho_{\text{max}} = 1.94 \text{ e } \text{Å}^{-3}$
200 parameters	$\Delta\rho_{\text{min}} = -1.22 \text{ e } \text{Å}^{-3}$

Table 1
Selected geometric parameters (Å, °).

Zn1–N1	2.2195 (17)	Zn1–O3	2.0429 (15)
Zn1–O1	2.1901 (15)	Zn1–O4	2.0502 (14)
Zn1–O2	2.0739 (15)	Zn1–O5	2.0450 (15)
O3–Zn1–O5	92.41 (6)	O4–Zn1–O1	87.00 (6)
O3–Zn1–O4	99.64 (6)	O2–Zn1–O1	89.92 (6)
O5–Zn1–O4	89.48 (6)	O3–Zn1–N1	95.95 (6)
O3–Zn1–O2	87.75 (6)	O5–Zn1–N1	88.13 (6)
O5–Zn1–O2	179.08 (5)	O4–Zn1–N1	164.32 (7)
O4–Zn1–O2	89.60 (6)	O2–Zn1–N1	92.75 (6)
O3–Zn1–O1	172.95 (5)	O1–Zn1–N1	77.51 (6)
O5–Zn1–O1	90.03 (6)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1-H1\cdots O2^i$	0.85 (2)	1.87 (2)	2.685 (2)	161 (3)

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

The hydroxy H atom was located in a difference Fourier map and was refined isotropically. The O—H bond distance was restrained to be 0.90 (2) Å. All other H atoms were placed in calculated positions (C—H = 0.98 and 0.99 Å) and were refined with $U_{\text{iso}}(\text{H})$ values of 1.5 (methyl) or 1.2 times (methylene) U_{eq} of the adjacent C atom. Methyl H atoms were allowed to rotate to best fit the experimental electron density. The s.u. values of the cell parameters are taken from the software, recognizing that the values are unreasonably small (Herbstein, 2000). The highest peak and deepest hole are located 0.86 and 0.88 Å, respectively, from atom Zn1.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINTE-Plus* (Bruker, 2003); data reduction: *SAINTE-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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