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(Acetato-κO)[benzoylacetone (4-methoxybenzoyl)hydrazonato-$\kappa^3 O,O',N$](quinoline-κN)zinc(II)

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Key indicators

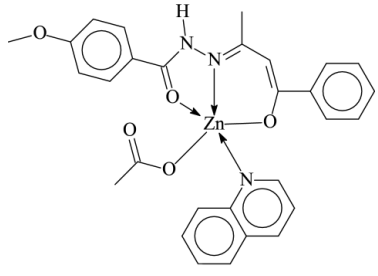
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.120
Data-to-parameter ratio = 17.4

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

In the title complex, $[Zn(C_{18}H_{17}N_2O_3)(C_2H_3O_2)(C_9H_7N)]$, the Zn^{II} atom is coordinated by two O atoms and one N atom from the tridentate hydrazone ligand, the N atom from the quinoline molecule and one O atom from the acetate group, leading to a distorted trigonal bipyramidal environment for the metal atom. The two O atoms of the deprotonated hydrazone ligand occupy the axial sites. A hydrogen-bonded dimer is formed through intermolecular hydrogen bonds across a center of inversion.

Comment

Although a number of metal hydrazonates have been structurally characterized (Chen *et al.*, 1999; Gao *et al.*, 1998), there are few zinc complexes in the list (Müller & Robson, 2000). The ligands themselves are readily synthesized by condensing thiosemicarbazone and its derivatives with, for example, acetylacetone (Toshev *et al.*, 1991) and salicylaldehyde (Gerbeleu *et al.*, 1990; Cui & Hu, 1994; Zelenin *et al.*, 1990). On the other hand, benzoylacetone (4-methoxybenzoyl)-hydrazone is a potentially tridentate chelating agent. This coordination mode is present in the title zinc complex, (I) (Fig. 1).



(I)

The hydrazone ligand is mono-deprotonated; it uses two O atoms and one N atom to bind to the Zn atom. The N atom from the quinoline molecule and one O atom from the acetate anion complete the distorted trigonal bipyramidal ZnN_2O_3 geometry. The equatorial plane is defined by atoms N2, N3 and O4; the axial sites are occupied by the O atoms of the hydrazone entity. The quinoline molecule is nearly perpendicular to the hydrazone entity [dihedral angle = 86.0 (4)°], probably to avoid steric congestion. A hydrogen-bonded dimer [N···O = 2.909 (3) Å, H···O = 2.10 Å, N—H···O = 156.7°] results from the interaction of the hydrazone N atom with the free carbonyl O atom of the actetate group across a center of symmetry (Fig. 2).

Experimental

Benzoylacetone (4-methoxybenzoyl)hydrazone was synthesized by condensing benzoylacetone with an equimolar quantity of 4-methoxybenzoylhydrazine in ethanol. The title compound was prepared by the addition of zinc(II) acetate dihydrate (6.048 mg, 0.04 mmol) and quinoline (1 ml) to a methanol solution of benzoylacetone (4-methoxybenzoyl)hydrazone (6.640 mg, 0.04 mmol). The mixture was refluxed for 30 min, then cooled slowly to room temperature and filtered. Yellow crystals separated from the solution after several days. CHN analysis calculated for $C_{29}H_{27}N_3O_5Zn$: C 61.88, H 4.83, N 14.21%; found: C 61.54, H 4.99, N 14.05%.

Crystal data

$[Zn(C_{18}H_{17}N_2O_3)(C_2H_3O_2)(C_9H_7N)]$	$Z = 2$
$M_r = 562.93$	$D_x = 1.402$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 9.529$ (1) Å	Cell parameters from 6783 reflections
$b = 11.471$ (1) Å	$\theta = 3.0$–$27.3°$
$c = 12.633$ (2) Å	$\mu = 0.97$ mm^{-1}
$\alpha = 94.391$ (9)°	$T = 293$ (2) K
$\beta = 95.409$ (8)°	Prism, yellow
$\gamma = 102.888$ (5)°	0.37 × 0.24 × 0.19 mm
$V = 1333.2$ (3) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	6036 independent reflections
ω scans	4880 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$R_{int} = 0.026$
$T_{min} = 0.717$, $T_{max} = 0.838$	$\theta_{max} = 27.5°$
12738 measured reflections	$h = -11 \rightarrow 12$
	$k = -14 \rightarrow 14$
	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0716P)^2 + 0.2421P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.045$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.120$	$\Delta\rho_{max} = 0.67$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.34$ e Å^{-3}
6036 reflections	
346 parameters	
All H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.058 (2)	O2—C11	1.252 (3)
Zn1—N3	2.176 (2)	C7—C8	1.390 (3)
Zn1—O1	1.987 (2)	N1—N2	1.395 (2)
Zn1—O2	2.174 (2)	N2—C11	1.344 (3)
Zn1—O4	2.027 (2)	O1—C7	1.283 (3)
N1—C9	1.322 (3)	C8—C9	1.419 (3)
N1—Zn1—N3	105.54 (8)	O1—Zn1—O4	97.59 (7)
N1—Zn1—O2	75.77 (7)	O2—Zn1—N3	88.04 (7)
O1—Zn1—N1	90.07 (7)	O4—Zn1—N1	149.27 (8)
O1—Zn1—N3	95.17 (8)	O4—Zn1—N3	103.35 (7)
O1—Zn1—O2	165.82 (7)	O4—Zn1—O2	95.08 (7)

The H atoms were placed in calculated positions, with C—H = 0.93 (aromatic) or 0.96 Å (methyl) and N—H = 0.86 Å (imino group), and with U_{iso}(H) = 1.2U_{eq}(C,N) or 1.5U_{eq}(methyl), in the riding-model approximation.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

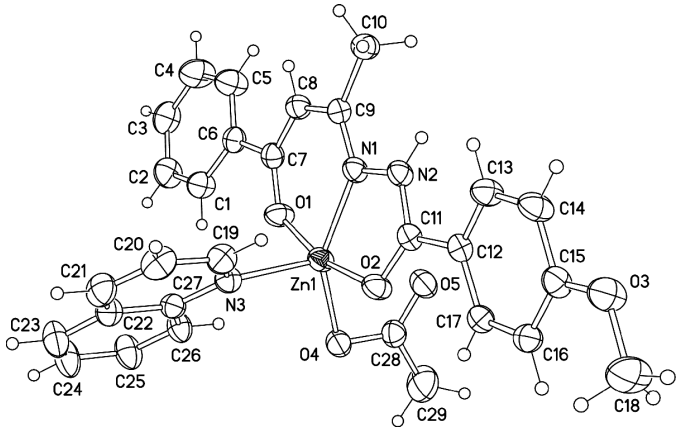


Figure 1
*ORTEP*II plot (Johnson, 1976) of the title complex, with displacement ellipsoids drawn at the 30% probability level.

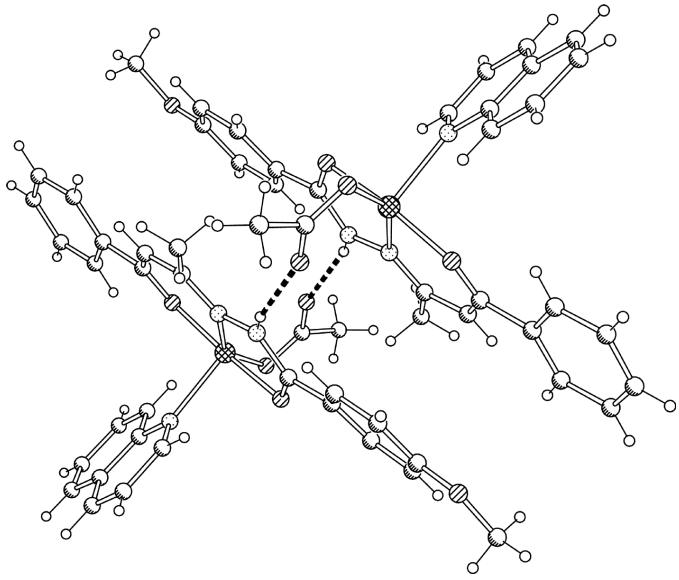


Figure 2
The hydrogen-bonded (dashed lines) dimeric structure of the title complex.

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