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trans-Bis[acetone (2-hydroxybenzoyl)-hydrazonato-κ^2N',O]bis(pyridine-κN)-zinc(II)

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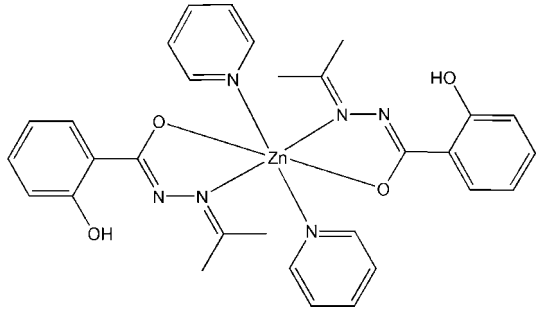
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.033; wR factor = 0.097; data-to-parameter ratio = 17.5.

In the title compound, $[Zn(C_{10}H_{11}N_2O_2)_2(C_5H_5N)_2]$, the Zn^{II} atom lies on an inversion centre, and is coordinated in a distorted octahedral geometry by two carbonyl O atoms and two imino N atoms from two anionic bidentate acetone (2-hydroxybenzoyl)hydrazone ligands and by two N atoms from two pyridine molecules. The hydroxyl group acts as a donor, forming an intramolecular O—H···N hydrogen bond.

Related literature

For general background, see: Bai *et al.* (2006); Gao *et al.* (1998); Grove *et al.* (2004); Liu & Gao (1998); Ma *et al.* (1989). For related structures, see: Chen & Liu (2004); Domiano *et al.* (1975); Hu *et al.* (2006, 2007); Li *et al.* (2006); Liu *et al.* (1999); Samanta *et al.* (2007); Wen *et al.* (2000); Wu *et al.* (2006); Xiao *et al.* (2000).



Experimental

Crystal data

$[Zn(C_{10}H_{11}N_2O_2)_2(C_5H_5N)_2]$
M_r = 605.99
Monoclinic, $P2_1/n$
a = 7.8225 (8) Å
b = 10.0381 (10) Å
c = 18.8201 (18) Å
β = 96.21 (4)°
V = 1469.1 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.88 mm^{-1}
T = 293 (2) K
0.35 × 0.26 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: none
13028 measured reflections
3282 independent reflections
2334 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.097
S = 0.98
3282 reflections
188 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O2	2.0319 (14)	Zn1—N3	2.3013 (18)
Zn1—N2	2.1912 (16)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.99	1.61	2.535 (2)	154

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2173).

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supplementary materials

Acta Cryst. (2009). E**65**, m219-m220 [**doi:10.1107/S1600536809001949**]

trans-Bis[acetone (2-hydroxybenzoyl)hydrazonato-κ^2N',O]bis(pyridine-κN)zinc(II)

M.-X. Yang, S. Lin, L.-J. Chen and X.-H. Chen

Comment

Hydrazones have been attracting much attention by chemists in recent years because of their biological activities, chemical and industrial versatility, and strong tendency to chelate transition metals (Bai *et al.*, 2006; Grove *et al.*, 2004), lanthanide metals (Ma *et al.*, 1989) and main group metals (Gao *et al.*, 1998; Liu & Gao, 1998). In particular, salicyloylhydrazone can be very flexible and finely tuned at the molecular level to take versatile bonding modes. It can act as a bi-, tri-, tetra- and even pentadentate ligand. A number of zinc(II) complexes with salicyloylhydrazone ligands have been studied (Hu *et al.*, 2006; Hu *et al.*, 2007; Li *et al.*, 2006; Samanta *et al.*, 2007; Wu *et al.*, 2006). As an extension of the work on the structural characterization of salicyloylhydrazone complexes, the preparation and crystal structure of the title zinc(II) complex are reported here.

The molecular structure of the title compound is shown in Fig. 1. The Zn^{II} atom lies on an inversion centre and has an axially elongated octahedral coordination geometry. The two carbonyl O atoms and the two imino N atoms make up the equatorial plane and the two N atoms of two pyridine molecules occupy the axial positions at longer distances (Table 1). Double-bond character is present in C7—N1 and C8—N2, as judged from their bond lengths [1.322 (2) and 1.286 (2) Å] (Domiano *et al.*, 1975; Liu *et al.*, 1999; Xiao *et al.*, 2000). The C7—O2 bond length of 1.273 (2) Å approaches the value of 1.263 Å expected for an enolic form of the hydrazone ligand (Chen & Liu, 2004; Wen *et al.*, 2000). The data suggest enolization and deprotonation of the hydrazone groups, which is different from the analogous Zn^{II} complex with the same ligand (Li *et al.*, 2006). There exists an intramolecular O—H···N hydrogen bond (Table 2).

Experimental

All reagents were commercially available and of analytical grade. To a solution of $Zn(CH_3COO)_2.2H_2O$ (0.110 g, 0.5 mmol) in pyridine (5 ml) was slowly added a suspension of acetone-N-salicyloylhydrazone (0.192 g, 1.0 mmol) in DMF(5 ml). The resulting red solution was stirred for 20 min and then filtered. After standing for 5 d, yellow crystals were separated from the filtrate.

Refinement

H atoms bonded to C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic) and 0.96 (CH_3) Å and with $U_{iso}(H) = xU_{eq}(C)$, where x=1.2 for aromatic and 1.5 for methyl H atoms. H atom of the hydroxyl group was located in difference Fourier map and refined isotropically with its coordinates fixed.

Figures

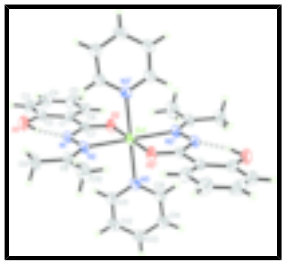


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines. [Symmetry code: (i) 1 - *x*, -*y*, -*z*.]

trans-Bis[acetone (2-hydroxybenzoyl)hydrazonato-κ^2*N*',*O*]bis(pyridine- κ*N*)zinc(II)

Crystal data

$[Zn(C_{10}H_{11}N_2O_2)_2(C_5H_5N)_2]$	F_{000} = 632
M_r = 605.99	D_x = 1.370 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3282 reflections
a = 7.8225 (8) Å	θ = 2.3–27.5º
b = 10.0381 (10) Å	μ = 0.88 mm^{-1}
c = 18.8201 (18) Å	T = 293 (2) K
β = 96.21 (4)º	Block, yellow
V = 1469.1 (3) Å^3	0.35 × 0.26 × 0.15 mm
Z = 2	

Data collection

Rigaku R-AXIS RAPID diffractometer	2334 reflections with $I > 2\sigma(I)$
Radiation source: 18 kW rotation anode	R_{int} = 0.034
Monochromator: graphite	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 2.3º
ω scans	h = 0→10
Absorption correction: none	k = 0→13
13028 measured reflections	l = −24→24
3282 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.033	H-atom parameters constrained
$wR(F^2)$ = 0.097	$w = 1/[\sigma^2(F_o^2) + (0.058P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 0.98	$(\Delta/\sigma)_{max} < 0.001$
3282 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
188 parameters	$\Delta\rho_{min} = -0.33$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.5000	0.0000	0.0000	0.04214 (12)
O1	0.4610 (2)	0.49143 (15)	0.11896 (11)	0.0690 (5)
H1	0.5171	0.4215	0.0926	0.113 (11)*
O2	0.35166 (17)	0.09309 (14)	0.06705 (8)	0.0492 (3)
N1	0.5358 (2)	0.27234 (16)	0.06295 (8)	0.0423 (4)
N2	0.6294 (2)	0.19207 (16)	0.02003 (8)	0.0433 (4)
N3	0.6638 (2)	−0.09222 (17)	0.09654 (9)	0.0469 (4)
C1	0.2948 (2)	0.2914 (2)	0.12902 (10)	0.0435 (4)
C2	0.3302 (3)	0.4273 (2)	0.14421 (11)	0.0525 (5)
C3	0.2284 (4)	0.4958 (3)	0.18860 (14)	0.0694 (7)
H3A	0.2484	0.5859	0.1977	0.083*
C4	0.1004 (4)	0.4326 (3)	0.21861 (15)	0.0755 (8)
H4A	0.0372	0.4790	0.2496	0.091*
C5	0.0628 (4)	0.3007 (3)	0.20383 (15)	0.0753 (7)
H5A	−0.0267	0.2587	0.2237	0.090*
C6	0.1600 (3)	0.2321 (2)	0.15905 (12)	0.0567 (5)
H6A	0.1342	0.1433	0.1487	0.068*
C7	0.3987 (2)	0.21174 (19)	0.08292 (10)	0.0397 (4)
C8	0.7671 (3)	0.2453 (2)	0.00115 (12)	0.0511 (5)
C9	0.8255 (3)	0.3833 (2)	0.02229 (16)	0.0741 (7)
H9A	0.7457	0.4226	0.0515	0.111*
H9B	0.8308	0.4364	−0.0198	0.111*
H9C	0.9374	0.3792	0.0487	0.111*
C10	0.8761 (3)	0.1689 (3)	−0.04426 (17)	0.0835 (9)
H10A	0.8262	0.0826	−0.0543	0.125*
H10B	0.9893	0.1587	−0.0195	0.125*
H10C	0.8833	0.2159	−0.0883	0.125*
C11	0.7532 (3)	−0.0149 (2)	0.14528 (13)	0.0584 (6)
H11A	0.7448	0.0771	0.1401	0.070*
C12	0.8567 (3)	−0.0653 (3)	0.20266 (13)	0.0659 (7)
H12A	0.9172	−0.0082	0.2352	0.079*
C13	0.8699 (3)	−0.2014 (3)	0.21143 (13)	0.0647 (6)

H13A	0.9398	−0.2380	0.2496	0.078*
C14	0.7773 (3)	−0.2813 (2)	0.16238 (13)	0.0624 (6)
H14A	0.7824	−0.3735	0.1667	0.075*
C15	0.6764 (3)	−0.2228 (2)	0.10655 (12)	0.0549 (5)
H15A	0.6134	−0.2781	0.0739	0.066*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.04131 (17)	0.03917 (18)	0.04726 (19)	−0.01003 (14)	0.01086 (12)	−0.00788 (15)
O1	0.0754 (11)	0.0435 (8)	0.0881 (12)	−0.0109 (8)	0.0086 (10)	−0.0158 (9)
O2	0.0496 (7)	0.0406 (7)	0.0606 (9)	−0.0129 (6)	0.0201 (6)	−0.0087 (7)
N1	0.0429 (8)	0.0400 (8)	0.0437 (8)	−0.0079 (7)	0.0031 (7)	−0.0041 (7)
N2	0.0410 (8)	0.0441 (9)	0.0447 (9)	−0.0106 (7)	0.0046 (7)	−0.0030 (7)
N3	0.0466 (9)	0.0486 (10)	0.0449 (9)	−0.0068 (8)	0.0024 (7)	−0.0018 (8)
C1	0.0495 (10)	0.0437 (10)	0.0360 (9)	0.0032 (9)	−0.0008 (8)	−0.0007 (8)
C2	0.0589 (12)	0.0486 (12)	0.0476 (12)	0.0048 (11)	−0.0056 (10)	−0.0054 (10)
C3	0.0841 (17)	0.0553 (14)	0.0669 (15)	0.0167 (14)	−0.0013 (13)	−0.0165 (13)
C4	0.0821 (18)	0.0784 (19)	0.0683 (16)	0.0286 (16)	0.0177 (14)	−0.0098 (14)
C5	0.0811 (17)	0.0750 (18)	0.0756 (17)	0.0154 (15)	0.0344 (14)	0.0028 (14)
C6	0.0617 (13)	0.0532 (13)	0.0582 (13)	0.0043 (11)	0.0201 (10)	0.0016 (11)
C7	0.0435 (9)	0.0391 (9)	0.0355 (9)	−0.0050 (8)	−0.0003 (7)	−0.0001 (8)
C8	0.0447 (10)	0.0505 (12)	0.0587 (12)	−0.0168 (9)	0.0076 (9)	0.0020 (10)
C9	0.0645 (14)	0.0572 (15)	0.102 (2)	−0.0289 (12)	0.0137 (14)	0.0001 (14)
C10	0.0660 (15)	0.0813 (19)	0.111 (2)	−0.0259 (14)	0.0433 (15)	−0.0134 (17)
C11	0.0641 (13)	0.0516 (13)	0.0571 (13)	−0.0078 (11)	−0.0041 (11)	−0.0051 (10)
C12	0.0678 (15)	0.0684 (16)	0.0573 (14)	−0.0087 (13)	−0.0130 (12)	−0.0074 (12)
C13	0.0652 (14)	0.0717 (16)	0.0536 (13)	−0.0039 (13)	−0.0107 (11)	0.0098 (12)
C14	0.0699 (15)	0.0526 (13)	0.0626 (14)	−0.0059 (12)	−0.0032 (12)	0.0078 (12)
C15	0.0588 (12)	0.0526 (12)	0.0511 (12)	−0.0104 (11)	−0.0039 (10)	−0.0007 (10)

Geometric parameters (Å, °)

Zn1—O2^{i}	2.0319 (14)	C4—H4A	0.9300
Zn1—O2	2.0319 (14)	C5—C6	1.379 (3)
Zn1—N2	2.1912 (16)	C5—H5A	0.9300
Zn1—N2^{i}	2.1912 (16)	C6—H6A	0.9300
Zn1—N3^{i}	2.3013 (18)	C8—C10	1.485 (3)
Zn1—N3	2.3013 (18)	C8—C9	1.498 (3)
O1—C2	1.338 (3)	C9—H9A	0.9600
O1—H1	0.99	C9—H9B	0.9600
O2—C7	1.273 (2)	C9—H9C	0.9600
N1—C7	1.322 (2)	C10—H10A	0.9600
N1—N2	1.402 (2)	C10—H10B	0.9600
N2—C8	1.286 (2)	C10—H10C	0.9600
N3—C15	1.326 (3)	C11—C12	1.374 (3)
N3—C11	1.339 (3)	C11—H11A	0.9300
C1—C6	1.384 (3)	C12—C13	1.379 (4)

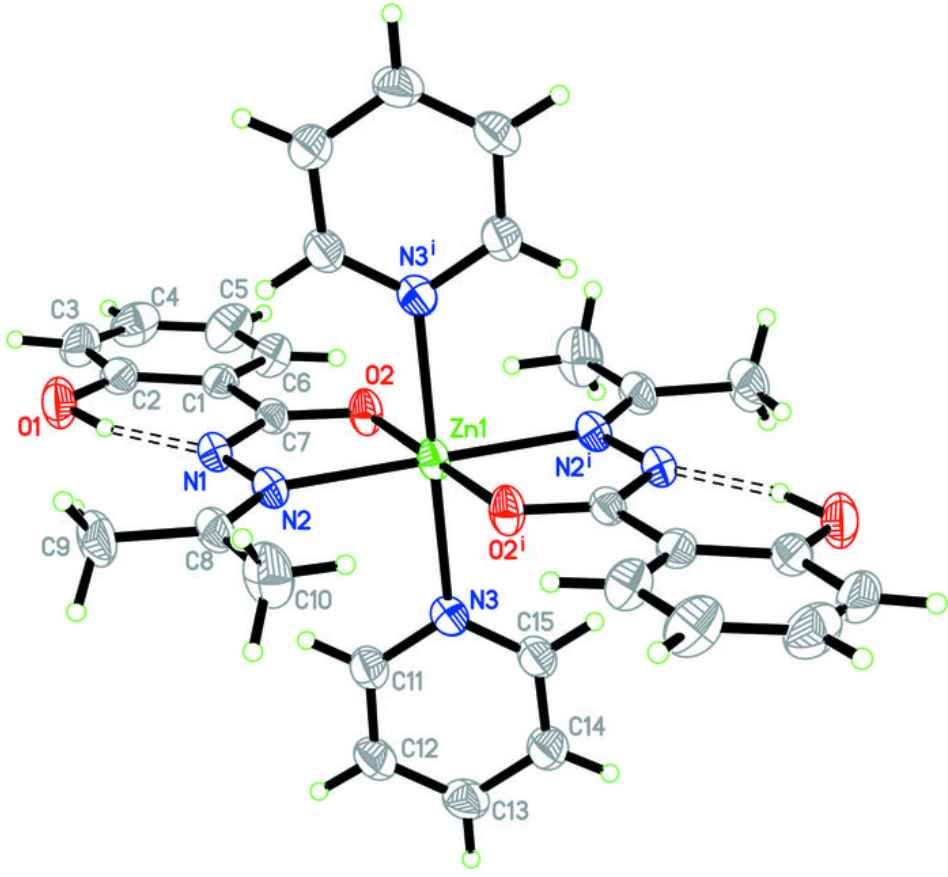
C1—C2	1.415 (3)	C12—H12A	0.9300
C1—C7	1.485 (3)	C13—C14	1.369 (3)
C2—C3	1.396 (3)	C13—H13A	0.9300
C3—C4	1.359 (4)	C14—C15	1.375 (3)
C3—H3A	0.9300	C14—H14A	0.9300
C4—C5	1.378 (4)	C15—H15A	0.9300
$O2^{i}$—Zn1—O2	180.00 (6)	C6—C5—H5A	120.5
$O2^{i}$—Zn1—N2	103.14 (6)	C5—C6—C1	122.0 (2)
O2—Zn1—N2	76.86 (6)	C5—C6—H6A	119.0
$O2^{i}$—Zn1—$N2^{i}$	76.86 (6)	C1—C6—H6A	119.0
O2—Zn1—$N2^{i}$	103.14 (6)	O2—C7—N1	125.93 (18)
N2—Zn1—$N2^{i}$	180.00 (9)	O2—C7—C1	118.57 (17)
$O2^{i}$—Zn1—$N3^{i}$	90.07 (6)	N1—C7—C1	115.49 (17)
O2—Zn1—$N3^{i}$	89.93 (6)	N2—C8—C10	119.64 (19)
N2—Zn1—$N3^{i}$	89.38 (6)	N2—C8—C9	123.4 (2)
$N2^{i}$—Zn1—$N3^{i}$	90.62 (6)	C10—C8—C9	116.92 (19)
$O2^{i}$—Zn1—N3	89.93 (6)	C8—C9—H9A	109.5
O2—Zn1—N3	90.07 (6)	C8—C9—H9B	109.5
N2—Zn1—N3	90.62 (6)	H9A—C9—H9B	109.5
$N2^{i}$—Zn1—N3	89.38 (6)	C8—C9—H9C	109.5
$N3^{i}$—Zn1—N3	180.00 (10)	H9A—C9—H9C	109.5
C2—O1—H1	103.6	H9B—C9—H9C	109.5
C7—O2—Zn1	113.95 (12)	C8—C10—H10A	109.5
C7—N1—N2	112.91 (15)	C8—C10—H10B	109.5
C8—N2—N1	115.16 (17)	H10A—C10—H10B	109.5
C8—N2—Zn1	134.68 (15)	C8—C10—H10C	109.5
N1—N2—Zn1	110.16 (11)	H10A—C10—H10C	109.5
C15—N3—C11	116.73 (19)	H10B—C10—H10C	109.5
C15—N3—Zn1	122.43 (14)	N3—C11—C12	123.0 (2)
C11—N3—Zn1	120.83 (15)	N3—C11—H11A	118.5
C6—C1—C2	118.3 (2)	C12—C11—H11A	118.5
C6—C1—C7	119.76 (18)	C11—C12—C13	119.3 (2)
C2—C1—C7	121.98 (19)	C11—C12—H12A	120.4
O1—C2—C3	118.9 (2)	C13—C12—H12A	120.4
O1—C2—C1	122.2 (2)	C14—C13—C12	118.2 (2)
C3—C2—C1	119.0 (2)	C14—C13—H13A	120.9
C4—C3—C2	120.8 (2)	C12—C13—H13A	120.9
C4—C3—H3A	119.6	C13—C14—C15	118.9 (2)
C2—C3—H3A	119.6	C13—C14—H14A	120.6
C3—C4—C5	121.0 (3)	C15—C14—H14A	120.6
C3—C4—H4A	119.5	N3—C15—C14	123.9 (2)
C5—C4—H4A	119.5	N3—C15—H15A	118.0
C4—C5—C6	118.9 (3)	C14—C15—H15A	118.0
C4—C5—H5A	120.5		

Symmetry codes: (i) −*x*+1, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.99	1.61	2.535 (2)	154

Fig. 1


N3i
C3
C4
C5
C6
O2
O1
C2
C1
C7
Zn1
N2i
N1
N2
O2i
C9
C8
C10
N3
C15
C11
C14
C12
C13