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## Structure Reports

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## Key indicators

Single-crystal X-ray study
$T=173 \mathrm{~K}$
Mean $\sigma(\mathrm{C}-\mathrm{C})=0.005 \AA$
$R$ factor $=0.043$
$w R$ factor $=0.100$
Data-to-parameter ratio $=13.8$

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

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## trans-Bis[acetone (2-oxidobenzoyl)hydrazonato$\left.\kappa^{2} N, O\right]$ diaquazinc(II)

In the title compound, $\left[\mathrm{Zn}\left(\mathrm{C}_{10} \mathrm{H}_{11} \mathrm{~N}_{2} \mathrm{O}_{2}\right)_{2}\left(\mathrm{H}_{2} \mathrm{O}\right)_{2}\right]$, the $\mathrm{Zn}^{\text {II }}$ atom lies on an inversion centre, and is coordinated in a distorted octahedral geometry by two carbonyl O atoms and two imine N atoms from two anionic bidentate acetone (2oxidobenzoyl)hydrazone ligands and two aqua ligands. The complexes are linked together via $\mathrm{O}-\mathrm{H} \cdots \mathrm{O}$ hydrogen bonds, leading to a two-dimensional network.

## Comment

Recently, there has been considerable interest in the chemistry of metal complexes with Schiff base ligands containing N and O atoms as donors (Ali \& Livingstone, 1974; Li et al., 2004; Rodriguez-Arguelles et al., 2004). Here, we report the crystal structure of the title compound, (I).


In compound (I), $\mathrm{Zn}^{\mathrm{II}}$ atom lies on an inversion centre and exhibits a distorted octahedral coordination geometry, with carbonyl atom O 2 and imine atom N 2 of the anionic acetoneN -salicyloylhydrazone ligands in the equatorial plane, and water molecules (O3) in the axial positions (Fig. 1). The phenol group of the ligand is deprotonated, in contrast with the $\mathrm{Cu}^{\text {II }}$ complex with an analogous ligand (Kraudelt et al., 1996). The C $7-\mathrm{O} 2$ and $\mathrm{C} 8-\mathrm{N} 2$ bond distances (Table 1) are mostly consistent with double-bond character. In contrast, the $\mathrm{C} 1-\mathrm{O} 1$ and $\mathrm{C} 7-\mathrm{N} 1$ bond lengths are within the range for normal single bonds (Hu et al., 2006).
There is an intramolecular $\mathrm{N} 1-\mathrm{H} 1 A \cdots \mathrm{O} 1$ hydrogen bond (Table 2). The complexes are linked via $\mathrm{O}-\mathrm{H} \cdots \mathrm{O}$ hydrogen bonds, forming a two-dimensional network (Fig. 2).

## Experimental

All reagents were commercially available and of analytical grade. To a solution of $\mathrm{Zn}\left(\mathrm{CH}_{3} \mathrm{COO}\right)_{2} \cdot 2 \mathrm{H}_{2} \mathrm{O}(0.110 \mathrm{~g}, 0.5 \mathrm{mmol})$ in methanol ( 5 ml ) was slowly added a suspension of acetone-N-salicyloylhydrazone ( $0.192 \mathrm{~g}, 1.0 \mathrm{mmol}$ ) in methanol $(10 \mathrm{ml})$. The suspension dissolved partially, and after stirring for 24 h , the reaction mixture

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Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the $50 \%$ probability level. Atoms $\mathrm{N} 2 A, \mathrm{O} 2 A$ and $\mathrm{O} W A$ and unlabelled atoms are related to atoms $\mathrm{N} 2, \mathrm{O} 2$ and $\mathrm{O} W$ and other labelled atoms by the symmetry operation $(2-x,-y$, $1-z$ ).
was filtered. Crystals of (I) suitable for X-ray diffraction analysis were obtained from the filtrate by slow evaporation at room temperature. Elemental analysis, calculated for $\mathrm{C}_{20} \mathrm{H}_{26} \mathrm{~N}_{4} \mathrm{O}_{6} \mathrm{Zn}$ : C49.65, H 5.42, N $11.58 \%$; found: C 49.44, H 5.33, N $11.45 \%$.

## Crystal data

| $\left[\mathrm{Zn}\left(\mathrm{C}_{10} \mathrm{H}_{11} \mathrm{~N}_{2} \mathrm{O}_{2}\right)_{2}\left(\mathrm{H}_{2} \mathrm{O}\right)_{2}\right]$ | $Z=4$ |
| :--- | :--- |
| $M_{r}=483.82$ | $D_{x}=1.412 \mathrm{Mg} \mathrm{m}^{-3}$ |
| Monoclinic, $C 2 / c$ | Mo $K \alpha$ radiation |
| $a=12.246(3) \AA$ | $\mu=1.12 \mathrm{~mm}^{-1}$ |
| $b=8.6666(18) \AA$ | $T=173(2) \mathrm{K}$ |
| $c=21.714(4) \AA$ | Irregular fragment, colourless |
| $\beta=98.955(4)^{\circ}$ | $0.20 \times 0.16 \times 0.12 \mathrm{~mm}$ |
| $V=2276.3(8) \AA^{3}$ |  |

## Data collection

Bruker SMART APEX CCD areadetector diffractometer

## $\omega$ scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2001)
$T_{\text {min }}=0.807, T_{\text {max }}=0.877$

## Refinement

| Refinement on $F^{2}$ | H-atom parameters constrained |
| :--- | :--- |
| $R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.043$ | $w=1 /\left[\sigma^{2}\left(F_{\mathrm{o}}{ }^{2}\right)+(0.048 P)^{2}\right]$ |
| $w R\left(F^{2}\right)=0.100$ | where $P=\left(F_{\mathrm{o}}{ }^{2}+2 F_{\mathrm{c}}{ }^{2}\right) / 3$ |
| $S=1.00$ | $(\Delta / \sigma)_{\max }<0.001$ |
| 1990 reflections | $\Delta \rho_{\max }=0.46 \mathrm{e}^{-3}$ |
| 144 parameters | $\Delta \rho_{\min }=-0.25 \mathrm{e}^{-3}$ |

Table 1
Selected geometric parameters $\left(\AA,{ }^{\circ}\right)$.

| $\mathrm{Zn} 1-\mathrm{O} 2$ | $2.062(2)$ | $\mathrm{C} 7-\mathrm{O} 2$ | $1.243(4)$ |
| :--- | :--- | :--- | :--- |
| $\mathrm{Zn} 1-\mathrm{O} W$ | $2.074(2)$ | $\mathrm{C} 7-\mathrm{N} 1$ | $1.341(4)$ |
| $\mathrm{Zn} 1-\mathrm{N} 2$ | $2.204(3)$ | $\mathrm{C} 8-\mathrm{N} 2$ | $1.278(4)$ |
| $\mathrm{C} 1-\mathrm{O} 1$ | $1.318(4)$ | $\mathrm{N} 1-\mathrm{N} 2$ | $1.384(3)$ |
|  |  |  |  |
| $\mathrm{O} 2-\mathrm{Zn} 1-\mathrm{OW}$ | $90.23(11)$ | $\mathrm{O} W-\mathrm{Zn} 1-\mathrm{N} 2$ | $87.17(9)$ |
| $\mathrm{O} 2-\mathrm{Zn} 1-\mathrm{N} 2$ | $77.14(9)$ |  |  |



The crystal structure of $\stackrel{\text { (I) }}{(\mathrm{I}) \text {. Dashed lines indicate hydrogen bonds. H }}$ atoms not participating in the hydrogen bonding have been omitted for clarity.

Table 2
Hydrogen-bond geometry ( $\AA{ }^{\circ},{ }^{\circ}$ ).

| $D-\mathrm{H} \cdots A$ | $D-\mathrm{H}$ | $\mathrm{H} \cdots A$ | $D \cdots A$ | $D-\mathrm{H} \cdots A$ |
| :--- | :--- | :--- | :--- | :--- |
| $\mathrm{~N} 1-\mathrm{H} 1 A \cdots \mathrm{O} 1$ | 0.88 | 1.82 | $2.545(3)$ | 138 |
| $\mathrm{O}^{\mathrm{i}}-\mathrm{H} W A \cdots 1^{\mathrm{i}}$ | 0.85 | 2.13 | $2.659(3)$ | 120 |
| $\mathrm{O}^{\mathrm{H}}-\mathrm{H} W B \cdots \mathrm{O}^{\mathrm{ii}}$ | 0.85 | 1.94 | $2.699(3)$ | 148 |

Symmetry codes: (i) $-x+2,-y+1,-z+1$; (ii) $x+\frac{1}{2}, y-\frac{1}{2}, z$.
H atoms were positioned geometrically and refined using a riding model, with $\mathrm{C}-\mathrm{H}=0.95-0.98 \AA, \mathrm{~N}-\mathrm{H}=0.88 \AA$ and $\mathrm{O}-\mathrm{H}=0.85 \AA$, and with $U_{\text {iso }}(\mathrm{H})=1.2 U_{\text {eq }}(\mathrm{C}, \mathrm{N})$, or $1.5 U_{\text {eq }}(\mathrm{C}, \mathrm{O})$ for methyl groups and water molecules.

Data collection: SMART (Bruker, 2001); cell refinement: SAINTPlus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXL97; software used to prepare material for publication: SHELXL97.

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