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Key indicators

Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.026
 wR factor = 0.067
Data-to-parameter ratio = 12.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Tetraaquabis[5-(4-pyridyl)-1,3,4-oxadiazole-2-thiolato- κN^4]zinc(II) dihydrateIn the structure of the title compound, $[\text{Zn}(\text{C}_7\text{H}_4\text{N}_3\text{OS})_2(\text{H}_2\text{O})_4]\cdot 2\text{H}_2\text{O}$, the Zn^{II} atom, located on an inversion centre, is coordinated by the pyridyl groups of two oxadiazole ligands and four water molecules. The packing is dominated by a three-dimensional system of hydrogen bonds.Received 17 October 2005
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Comment

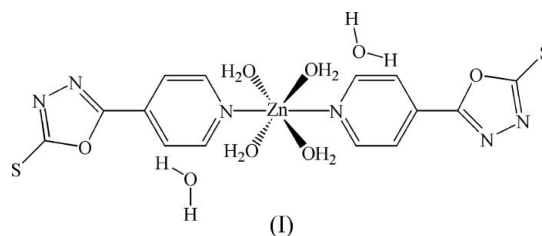
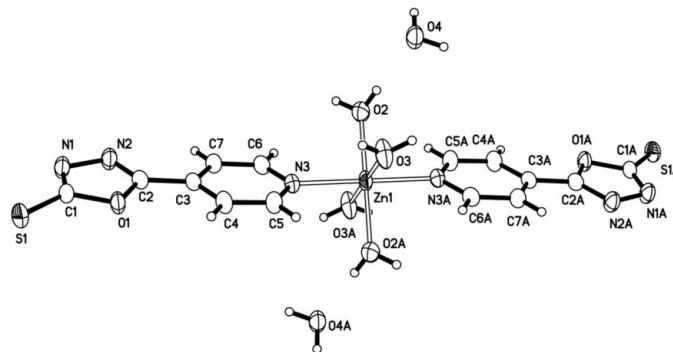
1,3,4-Oxadiazole ring-containing organic spacers are widely used to construct luminescent materials by incorporating them into all-organic or inorganic–organic composite species (Lee *et al.*, 2001; Wang *et al.*, 2001). This paper deals with the preparation and crystal structure of the title coordination compound, (I), which falls into this category (Fig. 1)The Zn^{II} atom of (I), located on an inversion centre, exhibits a distorted octahedral coordination (Table 1). It is coordinated by two pyridyl N atoms from the 5-(4-pyridinyl)-1,3,4-oxadiazole-2-thiolate ligands and four O atoms from water molecules. Two additional water molecules are not directly coordinated to the Zn^{II} atom, but do contribute to the extensive three-dimensional hydrogen-bonded network, which involves all possible donor atoms (Table 2 and Fig. 2).

Figure 1

The structure of (I), drawn with 50% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii. [Symmetry code: (A) $-x + 1, -y + 2, -z + 1$.]

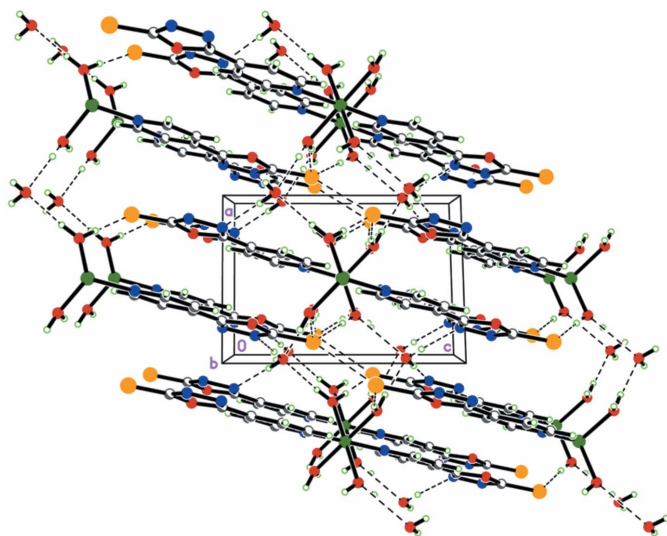


Figure 2
A packing diagram for (I), with hydrogen bonds shown as dashed lines.

Experimental

To a solution (20 ml) of $\text{Zn}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (0.063 g, 0.17 mmol) in water, NaOH (0.0068 g, 0.17 mol) and 5-(4-pyridyl)-1,3,4-oxadiazole-2(3*H*)-thione (0.030 g, 0.17 mol) were added and the solution stirred for a few minutes. The solution was then left for about 2 d at room temperature and yellow crystals of (I) were obtained.

Crystal data

$[\text{Zn}(\text{C}_7\text{H}_4\text{N}_3\text{OS})_2(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$	$Z = 1$
$M_r = 529.85$	$D_x = 1.682 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.028$ (4) Å	Cell parameters from 2297 reflections
$b = 7.981$ (5) Å	$\theta = 2.7\text{--}27.8^\circ$
$c = 9.690$ (6) Å	$\mu = 1.43 \text{ mm}^{-1}$
$\alpha = 90.414$ (8)°	$T = 298$ (2) K
$\beta = 90.672$ (7)°	Block, yellow
$\gamma = 105.677$ (7)°	$0.45 \times 0.20 \times 0.18 \text{ mm}$
$V = 523.2$ (5) Å ³	

Data collection

Bruker SMART CCD area-detector diffractometer	1823 independent reflections
φ and ω scans	1764 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.014$
$T_{\text{min}} = 0.566$, $T_{\text{max}} = 0.783$	$\theta_{\text{max}} = 25.0^\circ$
2684 measured reflections	$h = -8 \rightarrow 8$
	$k = -4 \rightarrow 9$
	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 0.1713P]$
$R[F^2 > 2\sigma(F^2)] = 0.026$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.067$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.20 \text{ e \AA}^{-3}$
1823 reflections	$\Delta\rho_{\text{min}} = -0.31 \text{ e \AA}^{-3}$
142 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—N3	2.1179 (18)	Zn1—O3	2.1515 (18)
Zn1—O2	2.1181 (16)		
N3—Zn1—N3 ⁱ	180	N3 ⁱ —Zn1—O3	91.66 (7)
N3—Zn1—O2 ⁱ	87.25 (7)	O2—Zn1—O3	89.61 (8)
N3—Zn1—O2	92.75 (7)	O2—Zn1—O3 ⁱ	90.39 (8)
O2 ⁱ —Zn1—O2	180	O3—Zn1—O3 ⁱ	180
N3—Zn1—O3	88.34 (7)		

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

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

$D\text{—}H \cdots A$	$D\text{—}H$	$H \cdots A$	$D \cdots A$	$D\text{—}H \cdots A$
$\text{O3—H1O3} \cdots \text{S1}^{\text{ii}}$	0.84	2.42	3.246 (2)	167
$\text{O2—H2O2} \cdots \text{S1}^{\text{iii}}$	0.84	2.42	3.247 (2)	167
$\text{O2—H1O2} \cdots \text{O4}^{\text{iv}}$	0.86	1.94	2.793 (2)	171
$\text{O4—H2O4} \cdots \text{N1}^{\text{v}}$	0.85	1.92	2.778 (3)	179
$\text{O4—H1O4} \cdots \text{N2}^{\text{vi}}$	0.86	2.06	2.915 (2)	177
$\text{O3—H2O3} \cdots \text{O4}$	0.86	1.96	2.773 (2)	158

Symmetry codes: (ii) $-x + 1, -y, -z + 2$; (iii) $x, y, z - 1$; (iv) $x - 1, y, z$; (v) $x + 1, y + 1, z - 1$; (vi) $-x + 1, -y, -z + 1$.

H atoms bonded to C atoms were included in calculated positions. Other H atoms were located in a difference map. All H atoms were refined using a riding model, with $\text{C—H} = 0.93 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$, and $\text{O—H} = 0.71\text{--}0.99 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$.

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

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References

- Bruker (1997). SMART (Version 5.6) and SAINT (Version 5.06a). Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2001). SHELXTL (Version 6.12). Bruker AXS Inc., Madison, Wisconsin, USA.
- Lee, D. W., Kwon, K.-Y., Jin, J.-I., Park, Y., Kim, Y.-R. & Hwang, I.-W. (2001). *Chem. Mater.* **13**, 565–574.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
- Wang, J., Wang, R., Yang, J., Zheng, Z., Carducci, M. D., Cayou, T., Peyghambarian, N. & Jabbour, G. E. (2001). *J. Am. Chem. Soc.* **123**, 6179–6180.