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Aqua(2,2′-diamino-4,4′-bi-1,3-thiazole-κ^2N,N')(malonato-κ^2O,O')zinc(II) monohydrate

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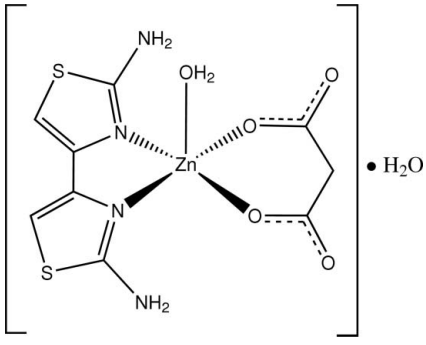
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; R factor = 0.038; wR factor = 0.086; data-to-parameter ratio = 12.5.

In the asymmetric unit of the crystal structure of the title compound, $[Zn(C_3H_2O_4)(C_6H_6N_4S_2)(H_2O)]\cdot H_2O$, there are two independent Zn^{II} complex molecules. Each Zn^{II} ion assumes a distorted square-pyramidal coordination geometry formed by a diaminobithiazole (DABT) ligand, a malonate dianion and a water molecule. Within the chelating DABT ligand, the two thiazole rings are twisted with respect to each other, with dihedral angles of 3.23 (19) and 2.54 (18)°. O—H···O and N—H···O hydrogen bonding occurs in the crystal structure.

Related literature

For general background, see: Sun *et al.* (1997); Liu & Xu (2004); Luo *et al.* (2004). For related structures, see: Wu *et al.* (2003).



Experimental

Crystal data

$[Zn(C_3H_2O_4)(C_6H_6N_4S_2)(H_2O)]\cdot H_2O$
M_r = 401.72
Triclinic, $P\overline{1}$
a = 8.4695 (11) Å
b = 12.5509 (15) Å
c = 14.8615 (19) Å
α = 68.895 (1)°
β = 88.074 (2)°
γ = 78.337 (2)°
V = 1442.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.03 mm^{-1}
T = 295 (2) K
0.25 × 0.22 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.628, T_{max} = 0.735
7536 measured reflections
4992 independent reflections
3768 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.086
S = 1.08
4992 reflections
398 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O1	2.023 (2)	Zn2—O2	2.016 (3)
Zn1—O11	2.013 (2)	Zn2—O21	2.026 (3)
Zn1—O13	2.016 (2)	Zn2—O23	2.023 (2)
Zn1—N11	2.098 (3)	Zn2—N21	2.076 (3)
Zn1—N13	2.077 (3)	Zn2—N23	2.097 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O24^{i}	0.84	1.86	2.694 (4)	173
O1—H1B···O1W	0.83	1.80	2.619 (4)	168
O2—H2A···O2W	0.80	1.88	2.673 (4)	168
O2—H2B···O22^{i}	0.86	1.83	2.687 (4)	175
O1W—H1WA···O12^{ii}	0.85	2.06	2.855 (4)	154
O1W—H1WB···O12^{iii}	0.84	1.93	2.774 (4)	174
O2W—H2WA···O14^{iii}	0.82	2.07	2.839 (4)	156
O2W—H2WB···O1	0.82	2.15	2.957 (4)	173
N12—H12A···O22^{iv}	0.87	2.06	2.910 (4)	168
N14—H14B···O24^{v}	0.88	2.05	2.905 (4)	163
N22—H22B···O14^{vi}	0.86	2.02	2.854 (4)	164
N24—H24B···O12^{ii}	0.87	2.06	2.880 (4)	156

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2284).

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supplementary materials

Acta Cryst. (2007). E**63**, m2054-m2055 [**doi:10.1107/S1600536807031741**]

Aqua(2,2'-diamino-4,4'-bi-1,3-thiazole-κ^2N,N')(malonato-κ^2O,O')zinc(II) monohydrate

B.-X. Liu, G.-H. Chen, Y.-P. Yu and Y.-Y. Lin

Comment

Transition metal complexes of 2,2'-diamino-4,4'-bi-1,3-thiazole (DABT) have shown potential application in the field of soft magnetic material (Sun *et al.*, 1997). As part of serial structural investigation of metal complexes with DABT (Liu & Xu, 2004; Luo *et al.*, 2004), the title Zn^{II} complex was recently prepared and its X-ray structure is presented here.

Asymmetric unit of the crystal of the title compound contains two independent Zn^{II} complexes (Fig. 1). Each Zn^{II} ion has a distorted square pyramid coordination geometry (Table 1) formed by one of DABT ligand, one of malonate dianion and one water molecules. The O atom of coordinated water lies on the apical position of square pyramid. The The Zn1 and Zn2 atoms are out of the base plane of pyramidal by 0.437 (2) Å and 0.413 (2) Å, respectively.

Within the complex, each DABT moiety is approximately coplanar with a dihedral angles of 3.23 (19)° for Zn1 complex and 2.54 (18)° for Zn1 and Zn2 complex respectively. The average distances of 1.334 (4) Å of *C*—*N*(amino) within Zn1 complex and 1.329 (4) Å of *C*—*N*(amino) within Zn2 complex imply the existence of electron delocalization between thiazole rings and amino groups. This feature of electron delocalization of DABT agrees with reported Cu^{II} complex of DABT (Wu *et al.*, 2003).

The malonate dianion chelates to the Zn^{II} atom with a nearly planar configuration with the maximum atomic deviation of 0.025 (2) Å (C17) to the mean plane defined by O11 O13 C17 C18 C19 and 0.071 (3) Å (C29) to the mean plane defined by O21 O23 C27 C28 C29. The extensive hydrogen bonding between lattice water and complex molecules helps to stabilize the crystal structure (Fig. 1. and Table 2).

Experimental

An ethanol solution (20 ml) containing DABT (0.20 g, 1 mmol) and $ZnCl_2$ (0.14 g, 1 mmol) was mixed with an aqueous solution (10 ml) of malonic acid (0.21 g, 2 mmol) and NaOH (0.16 g, 4 mmol). The mixture was refluxed for 6 h. After cooling to room temperature the solution was filtered. Single crystals of the title compound were obtained from the filtrate after 2 d.

Refinement

H atoms on carbon atoms were placed in calculated positions, with C—H distances = 0.93 Å (aromatic) or C—H = 0.97 (methylene), and were included in the final cycles of refinement in riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms on amino groups and coordinated water molecules were located in a difference Fourier map and included in the structure factor calculations with fixed positional and isotropic displacement parameters $U_{iso}(H) = 0.05$ Å^2. H atoms of lattice water were located in a difference Fourier map and included in the final cycles of refinement in riding mode with $U_{iso}(H) = 1.5U_{eq}(O)$.

Figures

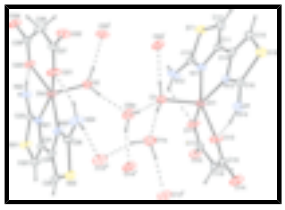


Fig. 1. The molecular structure of (I) with 25% probability displacement ellipsoids (arbitrary spheres for H atoms), dashed lines showing the hydrogen bonding [symmetry code: (i) $1-x$, $1-y$, $-z$; (ii) $2-x$, $-y$, $1-z$; (iii) $-1+x$, y, z].

Aqua(2,2'-diamino-4,4'-bi-1,3-thiazole-κ^2N,N')(malonato-κ^2O,O')zinc(II) monohydrate

Crystal data

$[Zn(C_3H_2O_4)(C_6H_6N_4S_2)(H_2O)]\cdot H_2O$	$Z = 4$
$M_r = 401.72$	$F_{000} = 816$
Triclinic, $P\overline{1}$	$D_x = 1.850$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.4695$ (11) Å	Cell parameters from 4880 reflections
$b = 12.5509$ (15) Å	$\theta = 2.4$–25.0°
$c = 14.8615$ (19) Å	$\mu = 2.03$ mm^{-1}
$\alpha = 68.895$ (1)°	$T = 295$ (2) K
$\beta = 88.074$ (2)°	Prism, yellow
$\gamma = 78.337$ (2)°	0.25 × 0.22 × 0.15 mm
$V = 1442.1$ (3) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	4992 independent reflections
Radiation source: fine-focus sealed tube	3768 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.024$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 25.0^\circ$
$T = 295$(2) K	$\theta_{min} = 2.4^\circ$
ω scans	$h = -4\rightarrow10$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -13\rightarrow14$
$T_{min} = 0.628$, $T_{max} = 0.735$	$l = -17\rightarrow17$
7536 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.038$	H-atom parameters constrained
$wR(F^2) = 0.086$	$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
4992 reflections	$\Delta\rho_{max} = 0.41$ e Å^{-3}
398 parameters	$\Delta\rho_{min} = -0.40$ 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.88504 (5)	0.31911 (3)	0.43082 (3)	0.02935 (14)
Zn2	0.56845 (6)	0.21371 (3)	0.00971 (3)	0.03282 (14)
O1	0.7108 (3)	0.3062 (2)	0.34771 (16)	0.0329 (6)
H1A	0.6546	0.3730	0.3207	0.050*
H1B	0.6473	0.2649	0.3787	0.050*
O2	0.7538 (3)	0.2748 (2)	0.04109 (18)	0.0449 (7)
H2A	0.7802	0.2460	0.0973	0.050*
H2B	0.7539	0.3481	0.0215	0.050*
O11	1.0722 (3)	0.2090 (2)	0.40389 (18)	0.0435 (7)
O12	1.2746 (3)	0.0620 (2)	0.42855 (19)	0.0468 (8)
O13	0.8758 (3)	0.1976 (2)	0.56278 (18)	0.0444 (7)
O14	0.9634 (4)	0.0497 (2)	0.69622 (18)	0.0543 (8)
O21	0.3790 (4)	0.3220 (2)	0.03881 (18)	0.0488 (8)
O22	0.2502 (4)	0.4952 (2)	0.03062 (18)	0.0487 (8)
O23	0.5257 (3)	0.3127 (2)	−0.13198 (17)	0.0375 (7)
O24	0.4464 (3)	0.4715 (2)	−0.25955 (17)	0.0427 (7)
O1W	0.5480 (3)	0.1515 (2)	0.4527 (2)	0.0537 (8)
H1WA	0.4756	0.1321	0.4266	0.080*
H1WB	0.6035	0.0889	0.4913	0.080*
O2W	0.8814 (4)	0.1887 (2)	0.22125 (19)	0.0658 (10)
H2WA	0.8984	0.1175	0.2440	0.099*
H2WB	0.8361	0.2155	0.2600	0.099*
N11	0.9577 (4)	0.4616 (2)	0.3251 (2)	0.0305 (7)
N12	1.0922 (4)	0.3928 (3)	0.2089 (2)	0.0526 (10)
H12A	1.1403	0.4132	0.1546	0.050*
H12B	1.0719	0.3237	0.2330	0.050*

N13	0.7881 (3)	0.4519 (2)	0.4811 (2)	0.0269 (7)
N14	0.6448 (4)	0.3689 (3)	0.6174 (2)	0.0370 (8)
H14A	0.6717	0.3002	0.6188	0.050*
H14B	0.5762	0.3871	0.6580	0.050*
N21	0.6930 (3)	0.0708 (2)	−0.02042 (19)	0.0270 (7)
N22	0.7906 (4)	0.1492 (3)	−0.1752 (2)	0.0374 (8)
H22A	0.7284	0.2120	−0.1813	0.050*
H22B	0.8373	0.1333	−0.2221	0.050*
N23	0.5398 (4)	0.0760 (2)	0.1367 (2)	0.0332 (8)
N24	0.3770 (4)	0.1607 (3)	0.2345 (2)	0.0560 (11)
H24A	0.3584	0.2254	0.1907	0.050*
H24B	0.3253	0.1501	0.2879	0.050*
S11	1.08320 (13)	0.61328 (9)	0.19332 (7)	0.0411 (3)
S12	0.65560 (13)	0.59502 (8)	0.56222 (7)	0.0373 (3)
S21	0.87839 (14)	−0.08109 (9)	−0.07459 (8)	0.0464 (3)
S22	0.48746 (14)	−0.07143 (9)	0.30120 (7)	0.0417 (3)
C11	0.9206 (4)	0.5639 (3)	0.3433 (3)	0.0291 (9)
C12	0.9765 (5)	0.6532 (3)	0.2810 (3)	0.0383 (10)
H12	0.9602	0.7271	0.2844	0.046*
C13	1.0418 (5)	0.4746 (3)	0.2469 (3)	0.0336 (9)
C14	0.8246 (4)	0.5596 (3)	0.4274 (3)	0.0285 (8)
C15	0.7636 (5)	0.6456 (3)	0.4602 (3)	0.0354 (9)
H15	0.7777	0.7221	0.4318	0.043*
C16	0.6984 (4)	0.4580 (3)	0.5546 (2)	0.0276 (8)
C17	1.1553 (4)	0.1141 (3)	0.4571 (2)	0.0276 (8)
C18	1.1183 (4)	0.0575 (3)	0.5623 (2)	0.0307 (9)
H18A	1.1101	−0.0217	0.5714	0.037*
H18B	1.2133	0.0514	0.5999	0.037*
C19	0.9751 (5)	0.1053 (3)	0.6098 (3)	0.0309 (9)
C21	0.7058 (4)	−0.0363 (3)	0.0549 (3)	0.0297 (9)
C22	0.7968 (5)	−0.1257 (3)	0.0372 (3)	0.0448 (11)
H22	0.8140	−0.2027	0.0799	0.054*
C23	0.7787 (4)	0.0603 (3)	−0.0939 (3)	0.0282 (8)
C24	0.6192 (4)	−0.0337 (3)	0.1401 (3)	0.0291 (9)
C25	0.6045 (5)	−0.1218 (3)	0.2222 (3)	0.0388 (10)
H25	0.6514	−0.1997	0.2347	0.047*
C26	0.4637 (5)	0.0694 (3)	0.2172 (3)	0.0332 (9)
C27	0.3292 (5)	0.4292 (3)	−0.0072 (3)	0.0339 (9)
C28	0.3635 (5)	0.4842 (3)	−0.1126 (3)	0.0464 (12)
H28A	0.2600	0.5246	−0.1460	0.056*
H28B	0.4233	0.5439	−0.1168	0.056*
C29	0.4506 (4)	0.4174 (3)	−0.1717 (2)	0.0277 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0343 (3)	0.0237 (2)	0.0243 (2)	−0.0011 (2)	0.00842 (19)	−0.00496 (19)
Zn2	0.0455 (3)	0.0231 (2)	0.0225 (2)	0.0025 (2)	0.0076 (2)	−0.00518 (19)

O1	0.0318 (15)	0.0292 (14)	0.0308 (14)	−0.0005 (12)	0.0044 (12)	−0.0062 (12)
O2	0.070 (2)	0.0277 (15)	0.0331 (16)	−0.0085 (14)	−0.0064 (14)	−0.0061 (12)
O11	0.0491 (18)	0.0325 (15)	0.0308 (15)	0.0100 (14)	0.0134 (13)	−0.0007 (12)
O12	0.0482 (18)	0.0398 (16)	0.0350 (16)	0.0096 (14)	0.0164 (14)	−0.0041 (13)
O13	0.0508 (18)	0.0331 (15)	0.0300 (15)	0.0095 (14)	0.0192 (13)	0.0001 (12)
O14	0.069 (2)	0.0470 (17)	0.0237 (15)	0.0155 (16)	0.0163 (14)	−0.0006 (13)
O21	0.070 (2)	0.0270 (15)	0.0307 (15)	0.0098 (14)	0.0227 (14)	0.0000 (12)
O22	0.078 (2)	0.0261 (14)	0.0360 (16)	−0.0020 (15)	0.0293 (15)	−0.0110 (13)
O23	0.0520 (18)	0.0281 (14)	0.0237 (14)	0.0078 (13)	0.0059 (12)	−0.0080 (12)
O24	0.0509 (18)	0.0408 (16)	0.0191 (14)	0.0118 (14)	0.0089 (13)	−0.0023 (12)
O1W	0.0516 (19)	0.0375 (16)	0.056 (2)	−0.0105 (15)	−0.0030 (16)	0.0026 (14)
O2W	0.098 (3)	0.0513 (19)	0.0321 (17)	0.0173 (18)	0.0027 (17)	−0.0139 (15)
N11	0.0317 (18)	0.0269 (17)	0.0268 (17)	−0.0026 (14)	0.0137 (14)	−0.0056 (14)
N12	0.076 (3)	0.0297 (19)	0.050 (2)	−0.0131 (19)	0.039 (2)	−0.0127 (17)
N13	0.0268 (17)	0.0264 (16)	0.0251 (16)	−0.0019 (14)	0.0049 (14)	−0.0086 (13)
N14	0.043 (2)	0.0363 (19)	0.0308 (18)	−0.0071 (16)	0.0177 (16)	−0.0125 (15)
N21	0.0307 (18)	0.0220 (16)	0.0226 (16)	0.0000 (14)	0.0065 (14)	−0.0049 (13)
N22	0.046 (2)	0.0349 (18)	0.0275 (18)	−0.0055 (16)	0.0147 (16)	−0.0097 (15)
N23	0.042 (2)	0.0300 (17)	0.0212 (16)	−0.0002 (15)	0.0091 (15)	−0.0061 (14)
N24	0.080 (3)	0.044 (2)	0.0281 (19)	0.009 (2)	0.0252 (19)	−0.0081 (16)
S11	0.0486 (7)	0.0357 (6)	0.0340 (6)	−0.0127 (5)	0.0187 (5)	−0.0058 (5)
S12	0.0432 (6)	0.0350 (6)	0.0352 (6)	−0.0034 (5)	0.0111 (5)	−0.0178 (5)
S21	0.0559 (7)	0.0343 (6)	0.0405 (6)	0.0091 (5)	0.0123 (5)	−0.0141 (5)
S22	0.0538 (7)	0.0376 (6)	0.0256 (5)	−0.0099 (5)	0.0104 (5)	−0.0020 (4)
C11	0.025 (2)	0.029 (2)	0.029 (2)	−0.0022 (17)	0.0013 (17)	−0.0071 (17)
C12	0.044 (3)	0.034 (2)	0.037 (2)	−0.011 (2)	0.010 (2)	−0.0127 (19)
C13	0.034 (2)	0.027 (2)	0.029 (2)	−0.0031 (18)	0.0053 (18)	0.0002 (17)
C14	0.026 (2)	0.029 (2)	0.027 (2)	−0.0060 (17)	0.0013 (17)	−0.0073 (17)
C15	0.043 (2)	0.031 (2)	0.032 (2)	−0.0102 (19)	0.0073 (19)	−0.0104 (18)
C16	0.024 (2)	0.031 (2)	0.024 (2)	−0.0004 (17)	0.0037 (16)	−0.0093 (17)
C17	0.031 (2)	0.027 (2)	0.027 (2)	−0.0074 (18)	0.0052 (17)	−0.0114 (17)
C18	0.032 (2)	0.030 (2)	0.025 (2)	−0.0012 (17)	0.0060 (17)	−0.0066 (17)
C19	0.038 (2)	0.025 (2)	0.025 (2)	−0.0013 (18)	0.0074 (18)	−0.0071 (17)
C21	0.034 (2)	0.025 (2)	0.029 (2)	−0.0055 (17)	0.0037 (17)	−0.0089 (17)
C22	0.058 (3)	0.028 (2)	0.036 (2)	0.004 (2)	0.009 (2)	−0.0044 (19)
C23	0.028 (2)	0.028 (2)	0.028 (2)	−0.0013 (17)	0.0041 (17)	−0.0119 (17)
C24	0.031 (2)	0.0252 (19)	0.027 (2)	−0.0037 (17)	0.0017 (17)	−0.0065 (17)
C25	0.049 (3)	0.026 (2)	0.031 (2)	−0.0023 (19)	0.0037 (19)	−0.0007 (17)
C26	0.039 (2)	0.033 (2)	0.0206 (19)	−0.0034 (18)	0.0033 (17)	−0.0029 (17)
C27	0.039 (2)	0.027 (2)	0.031 (2)	−0.0031 (18)	0.0064 (18)	−0.0067 (18)
C28	0.065 (3)	0.038 (2)	0.023 (2)	0.009 (2)	0.010 (2)	−0.0076 (18)
C29	0.030 (2)	0.025 (2)	0.023 (2)	−0.0004 (17)	0.0032 (17)	−0.0066 (16)

Geometric parameters (Å, °)

Zn1—O1	2.023 (2)	N21—C23	1.323 (4)
Zn1—O11	2.013 (2)	N21—C21	1.392 (4)
Zn1—O13	2.016 (2)	N22—C23	1.334 (4)
Zn1—N11	2.098 (3)	N22—H22A	0.8308

Zn1—N13	2.077 (3)	N22—H22B	0.8556
Zn2—O2	2.016 (3)	N23—C26	1.324 (4)
Zn2—O21	2.026 (3)	N23—C24	1.388 (4)
Zn2—O23	2.023 (2)	N24—C26	1.333 (4)
Zn2—N21	2.076 (3)	N24—H24A	0.8259
Zn2—N23	2.097 (3)	N24—H24B	0.8748
O1—H1A	0.8365	S11—C12	1.725 (4)
O1—H1B	0.8334	S11—C13	1.737 (4)
O2—H2A	0.8010	S12—C15	1.728 (4)
O2—H2B	0.8594	S12—C16	1.729 (4)
O11—C17	1.248 (4)	S21—C22	1.721 (4)
O12—C17	1.238 (4)	S21—C23	1.729 (3)
O13—C19	1.265 (4)	S22—C25	1.722 (4)
O14—C19	1.232 (4)	S22—C26	1.735 (4)
O21—C27	1.258 (4)	C11—C12	1.332 (5)
O22—C27	1.239 (4)	C11—C14	1.459 (5)
O23—C29	1.268 (4)	C12—H12	0.9300
O24—C29	1.234 (4)	C14—C15	1.343 (5)
O1W—H1WA	0.8536	C15—H15	0.9300
O1W—H1WB	0.8432	C17—C18	1.517 (5)
O2W—H2WA	0.8169	C18—C19	1.511 (5)
O2W—H2WB	0.8148	C18—H18A	0.9700
N11—C13	1.319 (4)	C18—H18B	0.9700
N11—C11	1.379 (4)	C21—C22	1.331 (5)
N12—C13	1.334 (4)	C21—C24	1.449 (5)
N12—H12A	0.8687	C22—H22	0.9300
N12—H12B	0.8623	C24—C25	1.342 (5)
N13—C16	1.326 (4)	C25—H25	0.9300
N13—C14	1.391 (4)	C27—C28	1.513 (5)
N14—C16	1.324 (4)	C28—C29	1.501 (5)
N14—H14A	0.8392	C28—H28A	0.9700
N14—H14B	0.8809	C28—H28B	0.9700
O11—Zn1—O13	88.83 (10)	C12—C11—N11	115.4 (3)
O11—Zn1—O1	99.45 (11)	C12—C11—C14	129.0 (3)
O13—Zn1—O1	106.13 (11)	N11—C11—C14	115.6 (3)
O11—Zn1—N13	152.32 (12)	C11—C12—S11	111.0 (3)
O13—Zn1—N13	91.05 (11)	C11—C12—H12	124.5
O1—Zn1—N13	107.14 (10)	S11—C12—H12	124.5
O11—Zn1—N11	90.47 (11)	N11—C13—N12	125.7 (3)
O13—Zn1—N11	157.42 (12)	N11—C13—S11	113.5 (3)
O1—Zn1—N11	96.25 (11)	N12—C13—S11	120.8 (3)
N13—Zn1—N11	79.29 (11)	C15—C14—N13	114.7 (3)
O2—Zn2—O23	100.60 (11)	C15—C14—C11	129.3 (3)
O2—Zn2—O21	100.53 (11)	N13—C14—C11	116.0 (3)
O23—Zn2—O21	88.22 (10)	C14—C15—S12	111.0 (3)
O2—Zn2—N21	100.54 (11)	C14—C15—H15	124.5
O23—Zn2—N21	92.46 (10)	S12—C15—H15	124.5
O21—Zn2—N21	158.42 (12)	N14—C16—N13	124.3 (3)
O2—Zn2—N23	104.88 (11)	N14—C16—S12	121.9 (3)

O23—Zn2—N23	154.14 (11)	N13—C16—S12	113.8 (3)
O21—Zn2—N23	91.35 (11)	O12—C17—O11	122.5 (3)
N21—Zn2—N23	78.76 (11)	O12—C17—C18	115.9 (3)
Zn1—O1—H1A	107.9	O11—C17—C18	121.6 (3)
Zn1—O1—H1B	114.0	C19—C18—C17	123.9 (3)
H1A—O1—H1B	105.9	C19—C18—H18A	106.4
Zn2—O2—H2A	111.8	C17—C18—H18A	106.4
Zn2—O2—H2B	122.1	C19—C18—H18B	106.4
H2A—O2—H2B	108.8	C17—C18—H18B	106.4
C17—O11—Zn1	131.8 (2)	H18A—C18—H18B	106.4
C19—O13—Zn1	131.3 (2)	O14—C19—O13	123.0 (3)
C27—O21—Zn2	127.8 (3)	O14—C19—C18	115.9 (3)
C29—O23—Zn2	129.8 (2)	O13—C19—C18	121.1 (3)
H1WA—O1W—H1WB	106.5	C22—C21—N21	114.5 (3)
H2WA—O2W—H2WB	110.0	C22—C21—C24	130.0 (3)
C13—N11—C11	111.2 (3)	N21—C21—C24	115.5 (3)
C13—N11—Zn1	134.3 (2)	C21—C22—S21	111.5 (3)
C11—N11—Zn1	114.4 (2)	C21—C22—H22	124.2
C13—N12—H12A	117.3	S21—C22—H22	124.2
C13—N12—H12B	123.1	N21—C23—N22	124.2 (3)
H12A—N12—H12B	119.3	N21—C23—S21	113.5 (3)
C16—N13—C14	111.1 (3)	N22—C23—S21	122.3 (3)
C16—N13—Zn1	134.4 (2)	C25—C24—N23	115.0 (3)
C14—N13—Zn1	114.5 (2)	C25—C24—C21	129.5 (3)
C16—N14—H14A	123.7	N23—C24—C21	115.5 (3)
C16—N14—H14B	114.8	C24—C25—S22	111.0 (3)
H14A—N14—H14B	121.5	C24—C25—H25	124.5
C23—N21—C21	111.3 (3)	S22—C25—H25	124.5
C23—N21—Zn2	133.1 (2)	N23—C26—N24	124.5 (3)
C21—N21—Zn2	115.2 (2)	N23—C26—S22	113.6 (3)
C23—N22—H22A	115.3	N24—C26—S22	121.9 (3)
C23—N22—H22B	117.7	O22—C27—O21	122.4 (3)
H22A—N22—H22B	124.2	O22—C27—C28	116.4 (3)
C26—N23—C24	111.0 (3)	O21—C27—C28	121.1 (3)
C26—N23—Zn2	134.2 (2)	C29—C28—C27	124.1 (3)
C24—N23—Zn2	114.8 (2)	C29—C28—H28A	106.3
C26—N24—H24A	119.6	C27—C28—H28A	106.3
C26—N24—H24B	120.1	C29—C28—H28B	106.3
H24A—N24—H24B	119.4	C27—C28—H28B	106.3
C12—S11—C13	88.98 (19)	H28A—C28—H28B	106.4
C15—S12—C16	89.39 (17)	O24—C29—O23	123.1 (3)
C22—S21—C23	89.26 (18)	O24—C29—C28	115.8 (3)
C25—S22—C26	89.37 (18)	O23—C29—C28	121.0 (3)

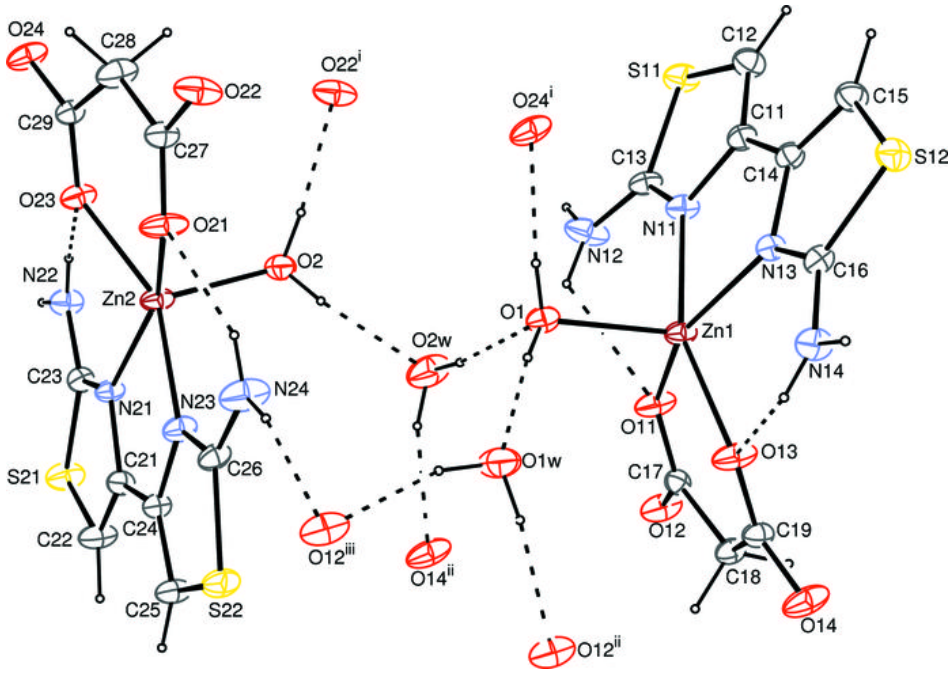
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···O24^{i}	0.84	1.86	2.694 (4)	173
O1—H1B···O1W	0.83	1.80	2.619 (4)	168

O2—H2A···O2W	0.80	1.88	2.673 (4)	168
O2—H2B···O22^{i}	0.86	1.83	2.687 (4)	175
O1W—H1WA···O12^{ii}	0.85	2.06	2.855 (4)	154
O1W—H1WB···O12^{iii}	0.84	1.93	2.774 (4)	174
O2W—H2WA···O14^{iii}	0.82	2.07	2.839 (4)	156
O2W—H2WB···O1	0.82	2.15	2.957 (4)	173
N12—H12A···O22^{iv}	0.87	2.06	2.910 (4)	168
N14—H14B···O24^{v}	0.88	2.05	2.905 (4)	163
N22—H22B···O14^{vi}	0.86	2.02	2.854 (4)	164
N24—H24B···O12^{ii}	0.87	2.06	2.880 (4)	156

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) *x*−1, *y*, *z*; (iii) −*x*+2, −*y*, −*z*+1; (iv) *x*+1, *y*, *z*; (v) *x*, *y*, *z*+1; (vi) *x*, *y*, *z*−1.

Fig. 1


O24
C28
O22
C29
C27
O23
O21
N22
Zn2
O2
C23
N21
N23
N24
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C26
C22
C24
C25
S22
O22i
O12iii
O14ii
O2w
O1w
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O1
C12
S11
C11
C15
C13
C14
S12
N12
N11
N13
C16
Zn1
N14
O11
O13
C17
O12
C19
C18
O14