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# Diaquabis(2,4-dibromo-6-formylphenolato-$\kappa^2N,N'$)zinc(II)

**Xian-Ming Chen,[a] Shu-Hua Zhang,[b]* Li-Xia Jin,[b] Zheng Liu[b] and Yang Yan[a]**

[a]Yulin Teachers' College, Yulin, Guangxi 537000, People's Republic of China, and [b]Key Laboratory of Non-Ferrous Metal Materials and Processing Technology, Department of Materials and Chemical Engineering, Guilin University of Technology, Ministry of Education, Guilin 541004, People's Republic of China
Correspondence e-mail: zsh720108@21cn.com

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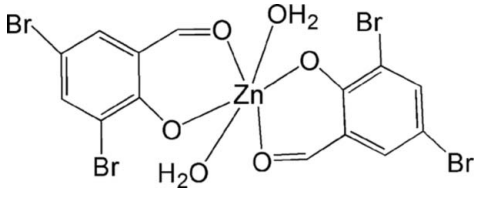
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.009 Å; $R$ factor = 0.041; $wR$ factor = 0.127; data-to-parameter ratio = 18.5.

In the title compound, $[Zn(C_7H_3Br_2O_2)_2(H_2O)_2]$, the $Zn^{II}$ atom is six-coordinated in a slightly distorted octahedral coordination geometry by four O atoms of two 3,5-dibromo-2-hydroxybenzaldehyde ligands and by two water molecules. The Zn—O bond lengths lie in the range 2.040 (4)–2.121 (4) Å, and the angles subtended at the $Zn^{II}$ atom range from 84.10 (18) to 96.64 (17)°. The molecules are linked into a chain along the $a$ axis by O—H···O and O—H···Br hydrogen bonds.

## Related literature

A similar cobalt(II) complex also forms a distorted octahedral geometry (Xiao *et al.*, 2002). For related literature, see: Cohen *et al.* (1964); Desiraju (1989); Schmidt (1964); Zordan *et al.* (2005).




## Experimental

*Crystal data*

$[Zn(C_7H_3Br_2O_2)_2(H_2O)_2]$
$M_r$ = 659.23
Monoclinic, $P2_1/c$
$a$ = 7.6486 (15) Å
$b$ = 28.095 (6) Å
$c$ = 8.6716 (17) Å
$\beta$ = 101.25 (3)°
$V$ = 1827.6 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 10.12 mm$^{-1}$
$T$ = 293 (2) K
0.40 × 0.16 × 0.14 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.107, $T_{max}$ = 0.332
(expected range = 0.078–0.243)
12164 measured reflections
4189 independent reflections
2577 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.066

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.127
$S$ = 1.03
4189 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.76 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.77 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H1$WB$···O4$^{i}$ | 0.85 | 2.01 | 2.751 (6) | 144 |
| O1$W$—H1$WA$···O2$^{i}$ | 0.85 | 2.31 | 3.065 (6) | 148 |
| O2$W$—H2$WA$···O2$^{ii}$ | 0.85 | 2.24 | 2.773 (6) | 121 |
| O2$W$—H2$WB$···O4$^{ii}$ | 0.85 | 2.17 | 2.932 (6) | 149 |
| O1$W$—H1$WA$···Br2$^{i}$ | 0.85 | 2.89 | 3.596 (5) | 141 |
| O2$W$—H2$WA$···Br2$^{ii}$ | 0.85 | 2.81 | 3.637 (5) | 166 |
| O2$W$—H2$WB$···Br4$^{ii}$ | 0.85 | 2.84 | 3.509 (5) | 137 |

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); 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: CI2359).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m1321 [ **doi:10.1107/S1600536807018259** ]

# Diaquabis(2,4-dibromo-6-formylphenolato-$\kappa^2N,N'$)zinc(II)

**X.-M. Chen, S.-H. Zhang, L.-X. Jin, Z. Liu and Y. Yan**

## Comment

Interest in packing arrangements of halogenated compounds goes back many years to what Schmidt (1964) called the "chloro effect",

wherein the presence of chloro substituents on aromatic compounds frequently results in stacking arrangements with a short (*ca* 4 Å) crystallographic axis (Cohen *et al.*, 1964; Zordan *et al.*, 2005; Desiraju, 1989). We report here the crystal structure of the title mononuclear zinc(II) complex, $Zn(L)_2(H_2O)_2$ (I), where LH is 3,5-dibromo-2-hydroxy-benzaldehyde, a dibrominated ligand with two Br atoms accessible at the periphery of each ligand.

The asymmetric unit of (I) contains one unique $Zn^{II}$ centre, two independent $L^-$ ligands and two coordinated water molecules (Fig. 1). The $Zn^{II}$ atom is coordinated by four O atoms from two $L^-$ ligands and two O atoms from two water molecules, forming slightly distorted octahedral geometry (Table 1). The $L^-$ ligand is present in the chelating bidentate mode.

The molecules are linked into a chain along the *a* axis by O—H···O and O—H···Br hydrogen bonds (Table 2).

## Experimental

A solution of taurine (2 mmol, 0.253 g) and caustic potash (2 mmol, 0.112 g) in distilled water (10 ml) was slowly added to a solution of 3,5-dibromo- 2-hydroxy-benzaldehyde (2 mmol, 0.560 g) in ethanol (10 ml). The mixture was stirred for 30 min at room temperature, then the solution was slowly added to a solution of zinc nitrate (1 mmol, 0.297 g) in distilled water (10 ml). The mixture was stirred and refluxed for 4 h at room temperature. Colourless needle-shaped single-crystal of (I) were obtained by slow evaporation at room temperature (yield 68%, based on zinc).

## Refinement

H atoms of the water molecule were located in a difference Fourier map. The O—H distances were normalized to 0.85 Å and the H atoms were allowed to ride during subsequent refinement, with $U_{iso}(H) = 1.5\ U_{eq}(O)$.

All other H atoms were positioned geometrically and were treated as riding atoms, with C–H = 0.93 Å and $U_{iso}(H) = 1.2\ U_{eq}(C)$.

## Figures

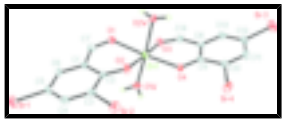

Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids. For clarity, all but water H atoms have been omitted.

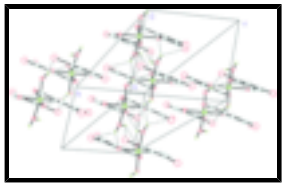

Fig. 2. The crystal packing of (I). Dashed lines indicate hydrogen bonds. C-bound H atoms have been omitted for clarity.

**Diaquabis(2,4-dibromo-6-formylphenolato-κ$^2$*N*,*N*')zinc(II)**

*Crystal data*

| | |
|---|---|
| $[Zn(C_7H_3Br_2O_2)_2(H_2O)_2]$ | $F_{000}$ = 1248 |
| $M_r$ = 659.23 | $D_x$ = 2.396 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 5376 reflections |
| $a$ = 7.6486 (15) Å | θ = 1–27.5º |
| $b$ = 28.095 (6) Å | μ = 10.12 mm$^{-1}$ |
| $c$ = 8.6716 (17) Å | $T$ = 293 (2) K |
| β = 101.25 (3)º | Needle, colourless |
| $V$ = 1827.6 (6) Å$^3$ | 0.40 × 0.16 × 0.14 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 4189 independent reflections |
| Radiation source: fine-focus sealed tube | 2577 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.066 |
| $T$ = 293(2) K | $\theta_{max}$ = 27.6º |
| φ and ω scans | $\theta_{min}$ = 1.5º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −9→9 |
| $T_{min}$ = 0.107, $T_{max}$ = 0.332 | $k$ = −36→33 |
| 12164 measured reflections | $l$ = −10→11 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.041 | H-atom parameters constrained |
| $wR(F^2)$ = 0.127 | $w = 1/[\sigma^2(F_o^2) + (0.0561P)^2]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.03 | $(\Delta/\sigma)_{max}$ = 0.001 |
| 4189 reflections | $\Delta\rho_{max}$ = 0.76 e Å$^{-3}$ |
| 226 parameters | $\Delta\rho_{min}$ = −0.77 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.55634 (12) | 0.25086 (3) | 0.72223 (10) | 0.0510 (2) |
| Br2 | 0.38278 (11) | 0.43461 (3) | 0.91144 (8) | 0.0425 (2) |
| Br3 | −0.07491 (13) | 0.72472 (3) | 0.08867 (13) | 0.0708 (3) |
| Br4 | 0.23829 (11) | 0.63158 (3) | 0.65207 (8) | 0.0425 (2) |
| C1 | 0.3092 (8) | 0.3676 (2) | 0.4757 (7) | 0.0254 (14) |
| C2 | 0.3114 (8) | 0.4041 (2) | 0.5911 (7) | 0.0223 (13) |
| C3 | 0.3828 (8) | 0.3896 (2) | 0.7481 (7) | 0.0279 (15) |
| C4 | 0.4534 (9) | 0.3450 (2) | 0.7876 (8) | 0.0338 (16) |
| H4 | 0.5017 | 0.3377 | 0.8918 | 0.041* |
| C5 | 0.4518 (10) | 0.3107 (2) | 0.6699 (9) | 0.0357 (17) |
| C6 | 0.3789 (9) | 0.3217 (2) | 0.5193 (8) | 0.0327 (16) |
| H6 | 0.3744 | 0.2985 | 0.4421 | 0.039* |
| C7 | 0.2336 (9) | 0.3744 (3) | 0.3118 (8) | 0.0352 (17) |
| H7 | 0.2289 | 0.3474 | 0.2489 | 0.042* |
| C8 | 0.1252 (9) | 0.5882 (2) | 0.1838 (8) | 0.0304 (15) |
| C9 | 0.1785 (8) | 0.5864 (2) | 0.3508 (7) | 0.0247 (14) |
| C10 | 0.1614 (9) | 0.6300 (2) | 0.4297 (8) | 0.0300 (15) |
| C11 | 0.0909 (9) | 0.6704 (3) | 0.3535 (9) | 0.0399 (18) |
| H11 | 0.0802 | 0.6979 | 0.4103 | 0.048* |
| C12 | 0.0361 (10) | 0.6701 (3) | 0.1931 (9) | 0.0393 (18) |
| C13 | 0.0548 (9) | 0.6299 (3) | 0.1089 (8) | 0.0385 (18) |
| H13 | 0.0199 | 0.6303 | 0.0000 | 0.046* |
| C14 | 0.1414 (9) | 0.5481 (3) | 0.0829 (8) | 0.0318 (16) |
| H14 | 0.1159 | 0.5544 | −0.0244 | 0.038* |
| O1 | 0.1748 (6) | 0.41087 (16) | 0.2442 (5) | 0.0305 (10) |
| O2 | 0.2526 (6) | 0.44684 (15) | 0.5594 (5) | 0.0303 (10) |
| O3 | 0.1838 (6) | 0.50740 (17) | 0.1193 (5) | 0.0325 (11) |
| O4 | 0.2395 (6) | 0.54800 (15) | 0.4281 (5) | 0.0291 (10) |
| O1W | 0.4842 (6) | 0.47247 (17) | 0.3266 (5) | 0.0328 (11) |
| H1WB | 0.5531 | 0.4541 | 0.3888 | 0.049* |
| H1WA | 0.5434 | 0.4977 | 0.3190 | 0.049* |

| | | | | |
|---|---|---|---|---|
| O2W | −0.0665 (6) | 0.48299 (16) | 0.3156 (5) | 0.0291 (10) |
| H2WA | −0.1464 | 0.5033 | 0.2793 | 0.044* |
| H2WB | −0.1136 | 0.4639 | 0.3719 | 0.044* |
| Zn1 | 0.21512 (10) | 0.47942 (3) | 0.34528 (8) | 0.02439 (19) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0589 (5) | 0.0313 (4) | 0.0632 (5) | 0.0112 (4) | 0.0130 (4) | 0.0182 (4) |
| Br2 | 0.0587 (5) | 0.0441 (5) | 0.0252 (4) | −0.0025 (4) | 0.0089 (3) | −0.0051 (3) |
| Br3 | 0.0697 (7) | 0.0406 (5) | 0.0988 (8) | 0.0178 (5) | 0.0080 (6) | 0.0331 (5) |
| Br4 | 0.0599 (5) | 0.0325 (4) | 0.0371 (4) | −0.0081 (4) | 0.0142 (4) | −0.0102 (3) |
| C1 | 0.025 (3) | 0.024 (3) | 0.029 (3) | 0.002 (3) | 0.009 (3) | −0.002 (3) |
| C2 | 0.023 (3) | 0.018 (3) | 0.029 (3) | −0.002 (2) | 0.012 (3) | −0.001 (3) |
| C3 | 0.025 (4) | 0.032 (4) | 0.027 (3) | −0.003 (3) | 0.006 (3) | 0.002 (3) |
| C4 | 0.035 (4) | 0.037 (4) | 0.028 (4) | −0.002 (3) | 0.004 (3) | 0.008 (3) |
| C5 | 0.041 (4) | 0.021 (4) | 0.045 (4) | 0.005 (3) | 0.008 (3) | 0.012 (3) |
| C6 | 0.040 (4) | 0.021 (4) | 0.037 (4) | 0.004 (3) | 0.008 (3) | 0.001 (3) |
| C7 | 0.042 (4) | 0.029 (4) | 0.033 (4) | 0.003 (3) | 0.005 (3) | −0.010 (3) |
| C8 | 0.029 (4) | 0.028 (4) | 0.031 (4) | −0.005 (3) | −0.002 (3) | 0.003 (3) |
| C9 | 0.019 (3) | 0.023 (3) | 0.032 (4) | −0.002 (3) | 0.003 (3) | 0.004 (3) |
| C10 | 0.029 (4) | 0.028 (4) | 0.035 (4) | −0.001 (3) | 0.011 (3) | −0.002 (3) |
| C11 | 0.035 (4) | 0.029 (4) | 0.058 (5) | 0.000 (3) | 0.016 (4) | 0.000 (4) |
| C12 | 0.037 (4) | 0.027 (4) | 0.057 (5) | 0.007 (3) | 0.014 (4) | 0.016 (4) |
| C13 | 0.033 (4) | 0.041 (5) | 0.036 (4) | −0.003 (3) | −0.006 (3) | 0.014 (3) |
| C14 | 0.034 (4) | 0.038 (4) | 0.020 (3) | 0.000 (3) | −0.002 (3) | 0.001 (3) |
| O1 | 0.033 (3) | 0.029 (3) | 0.025 (2) | 0.001 (2) | −0.004 (2) | −0.002 (2) |
| O2 | 0.044 (3) | 0.023 (2) | 0.024 (2) | 0.005 (2) | 0.007 (2) | −0.0003 (18) |
| O3 | 0.038 (3) | 0.035 (3) | 0.023 (2) | 0.003 (2) | 0.005 (2) | −0.001 (2) |
| O4 | 0.033 (3) | 0.022 (2) | 0.029 (2) | 0.0020 (19) | −0.003 (2) | 0.0015 (19) |
| O1W | 0.025 (2) | 0.036 (3) | 0.035 (3) | 0.000 (2) | 0.000 (2) | −0.001 (2) |
| O2W | 0.023 (2) | 0.032 (3) | 0.032 (2) | 0.000 (2) | 0.0040 (19) | 0.000 (2) |
| Zn1 | 0.0266 (4) | 0.0229 (4) | 0.0223 (4) | 0.0022 (3) | 0.0015 (3) | −0.0017 (3) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Br1—C5 | 1.880 (6) | C9—O4 | 1.308 (7) |
| Br2—C3 | 1.899 (6) | C9—C10 | 1.420 (9) |
| Br3—C12 | 1.896 (7) | C10—C11 | 1.370 (10) |
| Br4—C10 | 1.904 (7) | C11—C12 | 1.372 (10) |
| C1—C6 | 1.418 (9) | C11—H11 | 0.93 |
| C1—C2 | 1.431 (8) | C12—C13 | 1.369 (11) |
| C1—C7 | 1.439 (9) | C13—H13 | 0.93 |
| C2—O2 | 1.292 (7) | C14—O3 | 1.214 (8) |
| C2—C3 | 1.424 (8) | C14—H14 | 0.93 |
| C3—C4 | 1.383 (9) | O1—Zn1 | 2.114 (4) |
| C4—C5 | 1.401 (10) | O2—Zn1 | 2.040 (4) |
| C4—H4 | 0.93 | O3—Zn1 | 2.081 (4) |
| C5—C6 | 1.353 (9) | O4—Zn1 | 2.052 (4) |

| | | | |
|---|---|---|---|
| C6—H6 | 0.93 | O1W—Zn1 | 2.105 (4) |
| C7—O1 | 1.223 (8) | O1W—H1WB | 0.85 |
| C7—H7 | 0.93 | O1W—H1WA | 0.85 |
| C8—C13 | 1.394 (9) | O2W—Zn1 | 2.121 (4) |
| C8—C9 | 1.426 (9) | O2W—H2WA | 0.85 |
| C8—C14 | 1.447 (9) | O2W—H2WB | 0.85 |
| C6—C1—C2 | 120.9 (6) | C13—C12—Br3 | 119.8 (6) |
| C6—C1—C7 | 116.2 (6) | C11—C12—Br3 | 120.0 (6) |
| C2—C1—C7 | 122.9 (6) | C12—C13—C8 | 121.0 (7) |
| O2—C2—C3 | 121.4 (5) | C12—C13—H13 | 119.5 |
| O2—C2—C1 | 124.2 (6) | C8—C13—H13 | 119.5 |
| C3—C2—C1 | 114.4 (6) | O3—C14—C8 | 128.8 (6) |
| C4—C3—C2 | 123.7 (6) | O3—C14—H14 | 115.6 |
| C4—C3—Br2 | 118.4 (5) | C8—C14—H14 | 115.6 |
| C2—C3—Br2 | 117.9 (5) | C7—O1—Zn1 | 123.7 (4) |
| C3—C4—C5 | 119.7 (6) | C2—O2—Zn1 | 126.3 (4) |
| C3—C4—H4 | 120.2 | C14—O3—Zn1 | 125.2 (4) |
| C5—C4—H4 | 120.2 | C9—O4—Zn1 | 126.6 (4) |
| C6—C5—C4 | 119.4 (6) | Zn1—O1W—H1WB | 120.1 |
| C6—C5—Br1 | 120.9 (5) | Zn1—O1W—H1WA | 118.3 |
| C4—C5—Br1 | 119.7 (5) | H1WB—O1W—H1WA | 106.3 |
| C5—C6—C1 | 121.9 (6) | Zn1—O2W—H2WA | 135.8 |
| C5—C6—H6 | 119.1 | Zn1—O2W—H2WB | 115.8 |
| C1—C6—H6 | 119.1 | H2WA—O2W—H2WB | 106.3 |
| O1—C7—C1 | 128.6 (6) | O2—Zn1—O4 | 96.64 (17) |
| O1—C7—H7 | 115.7 | O2—Zn1—O3 | 175.22 (18) |
| C1—C7—H7 | 115.7 | O4—Zn1—O3 | 87.75 (18) |
| C13—C8—C9 | 120.8 (6) | O2—Zn1—O1W | 93.58 (19) |
| C13—C8—C14 | 116.3 (6) | O4—Zn1—O1W | 95.20 (18) |
| C9—C8—C14 | 123.0 (6) | O3—Zn1—O1W | 84.10 (18) |
| O4—C9—C10 | 121.4 (6) | O2—Zn1—O1 | 87.25 (17) |
| O4—C9—C8 | 123.6 (6) | O4—Zn1—O1 | 175.34 (17) |
| C10—C9—C8 | 115.0 (6) | O3—Zn1—O1 | 88.45 (18) |
| C11—C10—C9 | 123.1 (6) | O1W—Zn1—O1 | 87.10 (17) |
| C11—C10—Br4 | 118.9 (5) | O2—Zn1—O2W | 95.20 (18) |
| C9—C10—Br4 | 118.0 (5) | O4—Zn1—O2W | 91.08 (17) |
| C10—C11—C12 | 119.9 (7) | O3—Zn1—O2W | 86.59 (18) |
| C10—C11—H11 | 120.0 | O1W—Zn1—O2W | 168.55 (17) |
| C12—C11—H11 | 120.0 | O1—Zn1—O2W | 85.99 (17) |
| C13—C12—C11 | 120.1 (7) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1W—H1WB···O4$^{i}$ | 0.85 | 2.01 | 2.751 (6) | 144 |
| O1W—H1WA···O2$^{i}$ | 0.85 | 2.31 | 3.065 (6) | 148 |
| O2W—H2WA···O2$^{ii}$ | 0.85 | 2.24 | 2.773 (6) | 121 |
| O2W—H2WB···O4$^{ii}$ | 0.85 | 2.17 | 2.932 (6) | 149 |

| | | | | |
|---|---|---|---|---|
| O1W—H1WA···Br2$^{i}$ | 0.85 | 2.89 | 3.596 (5) | 141 |
| O2W—H2WA···Br2$^{ii}$ | 0.85 | 2.81 | 3.637 (5) | 166 |
| O2W—H2WB···Br4$^{ii}$ | 0.85 | 2.84 | 3.509 (5) | 137 |

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

**Fig. 1**

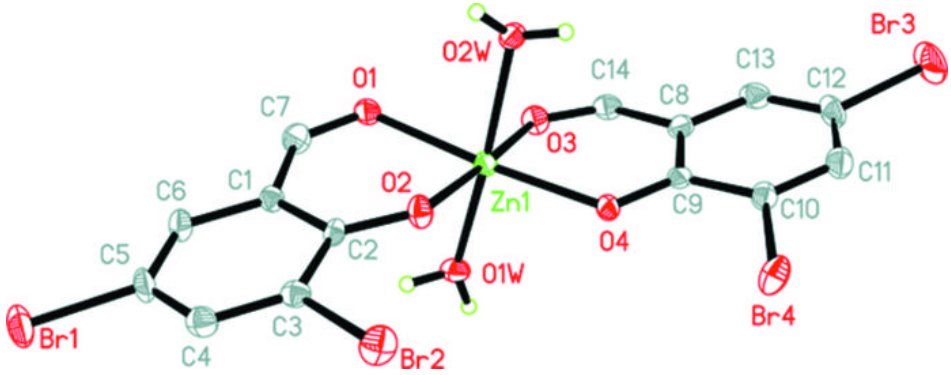
O2W
Br3
C14
C13
C12
O1
C8
C7
O3
C11
C6
C1
O2
Zn1
C9
C10
C5
C2
O4
O1W
Br4
Br1
C3
C4
Br2

**Fig. 2**