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Key indicators

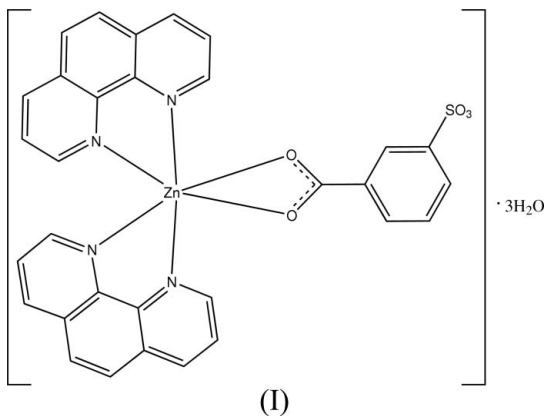
Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.011$ Å
H-atom completeness 89%
 R factor = 0.073
 wR factor = 0.198
Data-to-parameter ratio = 12.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Bis(1,10-phenanthroline)(3-sulfonato-
benzoato)zinc(II) trihydrate

In the title complex, $[\text{Zn}(\text{C}_7\text{H}_4\text{O}_5\text{S})(\text{C}_{12}\text{H}_8\text{N}_2)_2] \cdot 3\text{H}_2\text{O}$, the two crystallographically distinct Zn atoms are both coordinated by four N atoms from two 1,10-phenanthroline ligands and two O atoms from the carboxylate group in a distorted octahedral geometry. The 3-sulfonatobenzoate ligand only chelates to the Zn atom using its carboxylate group. Several $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds stabilize the crystal packing.

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Comment

2-Sulfonatobenzoate or 4-sulfonatobenzoate metal complexes have shown interesting structural assemblies (Fan, Xiao, Zhang & Zhu, 2004; Fan, Xiao, Zhang, Cai & Zhu, 2004; Li & Yang, 2004; Zhang & Zhu, 2005; Zhang *et al.*, 2005). However, 3-sulfobenzoate–metal complexes are rare (Cai & Zhu, 2005).



In the title complex, (I), there are two crystallographically independent Zn atoms in the asymmetric unit, and both are coordinated by four N atoms from two 1,10-phenanthroline residues and two O atoms from the carboxylate group of the 3-sulfobenzoate ligand in a distorted octahedral geometry (Fig. 1 and Table 1). The 3-sulfobenzoate ligand chelates the metal atom using its carboxylate group, while hydrogen bonds are formed between the sulfonate O atoms and water molecules. There are several $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds stabilizing the crystal packing.

Experimental

A mixture of $\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ (0.103 g, 0.47 mmol), sodium hydrogen 3-sulfonatobenzoate (0.130 g, 0.58 mmol) and 1,10-phenanthroline monohydrate (0.107 g, 0.54 mmol) in water (30 ml) was heated at about 363 K for 5 min. The clear solution that was obtained was allowed to evaporate at room temperature. After four days, colorless block-shaped crystals of (I) were obtained.

Crystal data

[Zn(C₇H₄O₅S)(C₁₂H₈N₂)₂] \cdot 3H₂O
M_r = 679.99
 Triclinic, *P* $\bar{1}$
a = 13.9620 (18) Å
b = 15.403 (2) Å
c = 16.157 (2) Å
 α = 73.823 (2)°
 β = 72.460 (2)°
 γ = 68.580 (2)°
V = 3028.3 (7) Å³

Z = 4
D_x = 1.491 Mg m⁻³
 Mo *K* α radiation
 Cell parameters from 2112 reflections
 θ = 2.5–18.3°
 μ = 0.94 mm⁻¹
T = 295 (2) K
 Block, colorless
 0.14 \times 0.10 \times 0.08 mm

Data collection

Bruker APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
T_{min} = 0.880, *T_{max}* = 0.929
 21863 measured reflections

10538 independent reflections
 6339 reflections with *I* > 2 σ (*I*)
R_{int} = 0.061
 θ_{\max} = 25.0°
h = -16 \rightarrow 16
k = -18 \rightarrow 18
l = -19 \rightarrow 18

Refinement

Refinement on *F*²
R [*F*² > 2 σ (*F*²)] = 0.073
wR (*F*²) = 0.198
S = 1.02
 10538 reflections
 829 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2 + 4.6392P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.70 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.36 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Zn1–O1	2.100 (4)	Zn2–O6	2.461 (5)
Zn1–O2	2.265 (4)	Zn2–O7	2.016 (5)
Zn1–N2	2.117 (5)	Zn2–N5	2.138 (5)
Zn1–N1	2.133 (5)	Zn2–N6	2.111 (5)
Zn1–N3	2.142 (5)	Zn2–N7	2.094 (5)
Zn1–N4	2.114 (5)	Zn2–N8	2.158 (5)
O1–Zn1–N4	95.05 (18)	O7–Zn2–N7	147.3 (2)
O1–Zn1–N2	154.48 (19)	O7–Zn2–N6	100.34 (19)
N4–Zn1–N2	109.3 (2)	N7–Zn2–N6	111.2 (2)
O1–Zn1–N1	91.35 (19)	O7–Zn2–N5	97.5 (2)
N4–Zn1–N1	96.66 (19)	N7–Zn2–N5	96.8 (2)
N2–Zn1–N1	78.7 (2)	N6–Zn2–N5	78.93 (19)
O1–Zn1–N3	97.84 (18)	O7–Zn2–N8	90.9 (2)
N4–Zn1–N3	78.55 (19)	N7–Zn2–N8	78.3 (2)
N2–Zn1–N3	94.46 (19)	N6–Zn2–N8	94.90 (18)
N1–Zn1–N3	169.9 (2)	N5–Zn2–N8	170.3 (2)
O1–Zn1–O2	59.85 (16)	O7–Zn2–O6	57.32 (18)
N4–Zn1–O2	151.00 (18)	N7–Zn2–O6	94.1 (2)
N2–Zn1–O2	98.02 (19)	N6–Zn2–O6	152.57 (18)
N1–Zn1–O2	98.12 (18)	N5–Zn2–O6	87.96 (18)
N3–Zn1–O2	90.06 (17)	N8–Zn2–O6	100.68 (18)

The aromatic H atoms were placed in calculated positions, with C–H = 0.93 Å, and refined as riding, with *U*_{iso}(H) = 1.2*U*_{eq}(C). The O-bound H atoms were located in difference Fourier maps and were refined with a distance restraint of O–H = 0.85 (1) Å, with *U*_{iso}(H) =

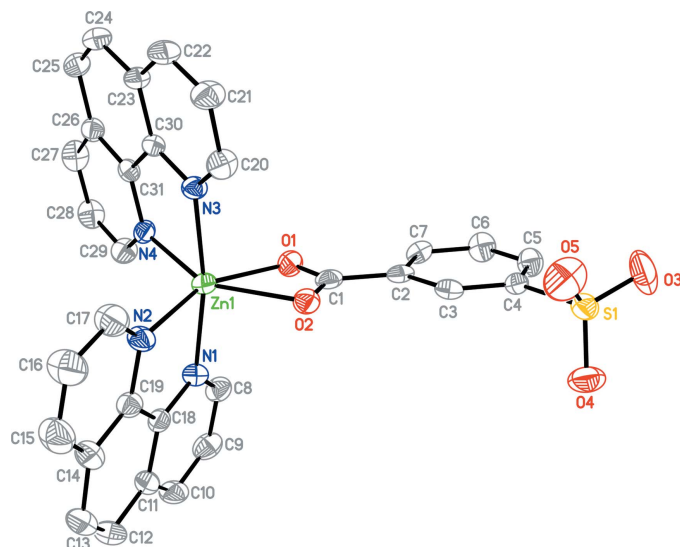


Figure 1

The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. Only one of the two molecules in the asymmetric unit is shown. H atoms and water molecules have been omitted for clarity.

0.08 Å². H atoms on atoms O4W, O5W and O6W could not be located.

Data collection: *SMART* (Bruker, 2002); cell refinement: *S SAINT* (Bruker, 2002); data reduction: *S SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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