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Bis(3-bromo-1-oxidoanthraquinone-κ^2O^1,O^9)-bis(pyridine-κN)zinc(II)

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Key indicators

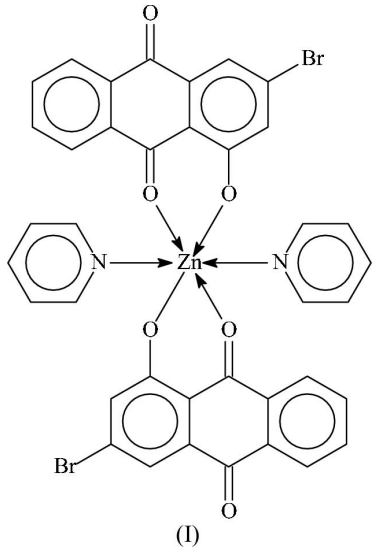
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.006 Å
R factor = 0.044
wR factor = 0.131
Data-to-parameter ratio = 15.3

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

The Zn atom in the title compound, $[Zn(C_{14}H_6BrO_3)_2(C_5H_5N)_2]$, lies on a centre of inversion. It is chelated by the bromo-substituted hydroxyanthroquinone molecule and is coordinated by the pyridine molecules in an all-*trans* octahedral geometry.

Comment

The deprotonated 2-hydroxyanthraquinone anion is a potentially *O*,*O*′-chelating anion, but only a few metal complexes have been crystallographically authenticated (Cambridge Structural Database, Version 5.26; Allen, 2002). 3-Bromo-2-hydroxyanthraquinone is a biologically active compound that can be synthesized through an unusual halogen rearrangement in the Friedel–Crafts acylation of a halophenol (Saha *et al.*, 2005). The deprotonated anion chelates to zinc in the title compound, which crystallizes from pyridine as a bis-pyridine adduct, (I) (Fig. 1). The Zn atom lies on a special position of $\overline{1}$ site symmetry; the chelating O atoms form a square, and the N atoms of the heterocycle occupy the other two octahedral sites around it. The Zn1—O1 bond is marginally shorter than the Zn1—O2 bond; other bond dimensions are unexceptional.



(I)

Experimental

3-Bromo-2-hydroxyanthraquinone (0.50 g, 1.65 mmol; Saha *et al.*, 2005) and zinc acetate dihydrate (0.18 g, 0.82 mmol) were heated in ethanol for several hours. The red solid that was isolated upon removal of the solvent was recrystallized from pyridine to furnish red prism-shaped crystals.

Crystal data

$[Zn(C_{14}H_6BrO_3)_2(C_5H_5N)_2]$	$Z = 1$
$M_r = 827.77$	$D_x = 1.740$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 8.0912$ (6) Å	Cell parameters from 2899 reflections
$b = 9.6445$ (7) Å	$\theta = 2.0$–$27.1°$
$c = 11.3013$ (8) Å	$\mu = 3.36$ mm^{-1}
$\alpha = 105.477$ (1)°	$T = 295$ (2) K
$\beta = 106.119$ (1)°	Prism, red
$\gamma = 99.227$ (1)°	0.48 × 0.28 × 0.11 mm
$V = 789.9$ (1) Å^3	

Data collection

Bruker SMART area-detector diffractometer	3409 independent reflections
φ and ω scans	2670 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	$R_{int} = 0.019$
$T_{min} = 0.404$, $T_{max} = 0.695$	$\theta_{max} = 27.1°$
6723 measured reflections	$h = -9 \rightarrow 10$
	$k = -12 \rightarrow 12$
	$l = -13 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0725P)^2 + 0.6848P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.044$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.131$	$\Delta\rho_{max} = 0.82$ e Å^{-3}
$S = 1.02$	$\Delta\rho_{min} = -0.70$ e Å^{-3}
3409 reflections	
223 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.017 (2)	Zn1—N1	2.219 (3)
Zn1—O2	2.107 (2)		
O1—Zn1—O1^{i}	180	O2—Zn1—O2^{i}	180
O1—Zn1—O2	84.8 (1)	O2—Zn1—N1	91.6 (1)
O1—Zn1—O2^{i}	95.2 (1)	O2—Zn1—N1^{i}	88.4 (1)
O1—Zn1—N1	91.1 (1)	N1—Zn1—N1^{i}	180
O1—Zn1—N1^{i}	88.9 (1)		

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

The H atoms were positioned geometrically (C—H = 0.93 Å) and were included in the refinement in the riding-model approximation, with U_{iso}(H) values set at $1.2U_{eq}$ of the parent atoms.

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: *SHELXL97*.

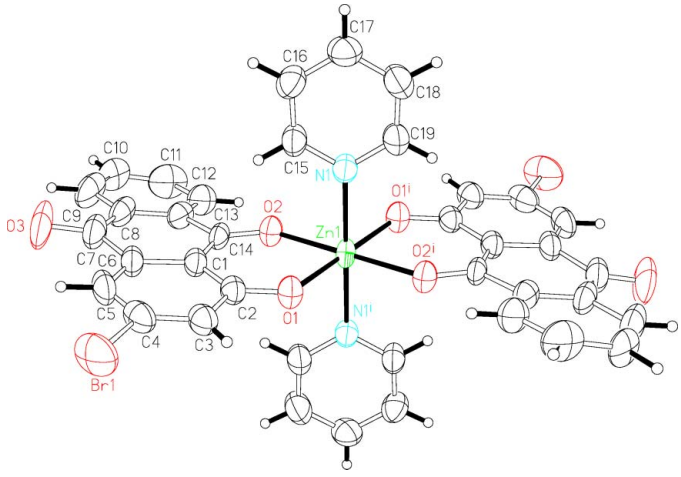


Figure 1
ORTEPII plot (Johnson, 1976) of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii. The Zn atom lies at the centre of inversion ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$). [Symmetry code: (i) $1-x, 1-y, 1-z$.]

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