Bis(3-bromo-1-oxidoanthraquinone-κ²O¹, O⁹)-bis(pyridine-κN)copper(II) dihydrate

The Cu atom in the title compound, \([\text{Cu(C}_14\text{H}_6\text{BrO}_3\text{)}_2(\text{C}_5\text{H}_5\text{N})_2]2\text{H}_2\text{O}\), lies on a center of inversion; it is chelated by the bromo-substituted hydroxyanthraquinone molecule and is coordinated by the pyridine molecules in an all-trans octahedral geometry.

Comment

Our previous study has documented the structure of the zinc derivative of a bromo-substituted 1-hydroxyanthraquinone anion (Ali et al., 2005). This zinc complex crystallizes from pyridine as a bis-pyridine adduct in an all-trans octahedral environment. The corresponding title copper complex, (I), adopts the identical geometry, but the compound crystallizes as a dihydrate (Fig. 1). The Cu atom lies on a special position of \(\bar{1}\) site symmetry; the chelating O atoms form a square, and the N atoms of the heterocycle occupy the other two octahedral sites. Hydrogen bonds (Table 2) link the molecule to the uncoordinated water molecule to give rise to a linear chain.

Experimental

3-Bromo-1-hydroxyanthraquinone (0.50 g, 1.65 mmol) and copper acetate monohydrate (0.16 g, 0.82 mmol) were heated in ethanol for several hours. The solid that was isolated upon removal of the solvent was recrystallized from pyridine to furnish brown prisms.
Data collection

Bruker SMART area-detector
diffractometer
φ and ω scans
Absorption correction: multi-scan
(SADABS; Bruker, 1999)
T_{min} = 0.347, T_{max} = 0.568
6931 measured reflections
3565 independent reflections
2240 reflections with I > 2σ(I)
R_{int} = 0.029
θ_{max} = 27.2
hk0 = 11 12 13
l = −12 13

Refinement

Refinement on F^{2}
R[F^{2} > 2\sigma(F^{2})] = 0.048
wR(F^{2}) = 0.144
S = 1.01
3565 reflections
238 parameters
H atoms treated by a mixture of independent and constrained refinement

w = 1/[σ^{2}(F_{o}^{2}) + (0.0832 P)^{2} + 0.0828 P]
where P = (F_{o}^{2} + 2F_{c}^{2})/3
Δρ_{min} = 0.47 e A^{−3}
Δρ_{max} = 0.001

Selected geometric parameters (Å, °).

Table 1

Cu1—O1 1.932 (3) Cu1—O2 2.229 (3)
Cu1—N1 2.077 (4) O1—Cu1—O2 86.3 (1)
O1—Cu1—O2i 93.7 (1) O1—Cu1—O2 180
O1—Cu1—N1 90.8 (1) O1—Cu1—N1i 89.2 (1)
O1—Cu1—N1i 91.4 (1) O1—Cu1—N1 180
O2—Cu1—O2i 180 O2—Cu1—N1 91.4 (1)
O2—Cu1—N1i 88.6 (1) O2—Cu1—N1i 180
N1—Cu1—N1i 180 N1—Cu1—N1 180

Symmetry code: (i) 1/2 x, 1/2 y, 1/2 z.

Table 2

Hydrogen-bond geometry (Å, °).

Table 2

D—H—A D—H H—A D—A D—H—A
O1w—H1w1—O1 0.86 (1) 2.23 (4) 2.948 (5) 142 (6)
O1w—H1w2—O3a 0.86 (1) 2.25 (4) 3.018 (6) 149 (6)

Symmetry code: (ii) 1/2 x, 1/2 y, 1/2 z.

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References

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