

{Bis[4-(2-pyridyl)pyrimidin-2-yl] sulfide}-dibromidocobalt(II)

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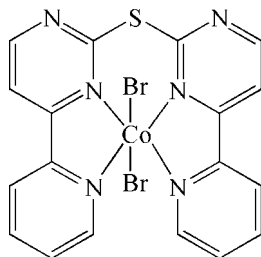
Received 15 May 2008; accepted 26 May 2008

Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.028; wR factor = 0.062; data-to-parameter ratio = 15.4.

The title compound, $[\text{CoBr}_2(\text{C}_{18}\text{H}_{12}\text{N}_6\text{S})]$, is a mononuclear complex in which a twofold rotation axis passes through the Co and S atoms. The Co^{II} center is six-coordinated by four N atoms from one bis[4-(2-pyridyl)pyrimidin-2-yl] sulfide (*L*) ligand and two bromide anions, forming an octahedral coordination geometry, where the four donor N atoms are located in the equatorial plane and the Br atoms occupy the axial positions. The sum of the bond angles around the Co atom in the equatorial plane is 360.5° , with the four N atoms and the central Co atom almost coplanar. In the crystal structure, the mononuclear units are linked by π - π stacking interactions (the interplanar distances are 3.469 and 3.533 Å, and the corresponding centroid-centroid distances are 3.791 and 3.896 Å) into a three-dimensional supramolecular network.

Related literature

For related literature, see: de Faria *et al.* (2007); Teles *et al.* (2006); Li & Bu (2008); Bridson & Walker (1970).



Experimental

Crystal data

$[\text{CoBr}_2(\text{C}_{18}\text{H}_{12}\text{N}_6\text{S})]$
 $M_r = 563.15$

 Monoclinic, $C2/c$
 $a = 15.191$ (5) Å

 $b = 10.350$ (4) Å

 $c = 13.338$ (5) Å

 $\beta = 112.312$ (5) $^\circ$
 $V = 1940.0$ (12) Å³
 $Z = 4$

 Mo $K\alpha$ radiation

 $\mu = 5.13$ mm⁻¹
 $T = 294$ (2) K

 $0.20 \times 0.18 \times 0.14$ mm

Data collection

Bruker SMART 1000 CCD diffractometer

 Absorption correction: multi-scan (*SADABS*; Bruker, 1998)

 $T_{\text{min}} = 0.375$, $T_{\text{max}} = 0.489$

5288 measured reflections

1970 independent reflections

 1456 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.036$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.061$
 $S = 1.04$

1970 reflections

128 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.39$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.36$ e Å⁻³

Table 1

 Selected geometric parameters (Å, $^\circ$).

Br1—Co1	2.6178 (10)	Co1—N1	2.125 (2)
Co1—N2	2.099 (2)		
N2 ⁱ —Co1—N2	96.18 (13)	N2—Co1—Br1	86.87 (7)
N2—Co1—N1	78.04 (9)	N1—Co1—Br1	92.90 (7)
N1—Co1—N1 ⁱ	108.24 (13)		

 Symmetry code: (i) $-x + 1, y, -z + \frac{1}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1998); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank Nankai University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2083).

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