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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.001$ Å
 R factor = 0.035
 wR factor = 0.096
Data-to-parameter ratio = 17.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

2,3-Bis[(pyrimidin-2-ylsulfanyl)methyl]quinoxaline

In the title compound, $\text{C}_{18}\text{H}_{14}\text{N}_6\text{S}_2$, the two terminal pyrimidine groups attached to the central quinoxaline system adopt an anti conformation, with the thiopyrimidine groups on opposite sides of the quinoxaline plane. The dihedral angles formed by each of the two terminal pyrimidine and the central quinoxaline planes are $81.1(3)$ and $82.0(3)^\circ$, while the two pyrimidine planes are almost parallel to each other, forming a dihedral angle of $6.0(3)^\circ$.

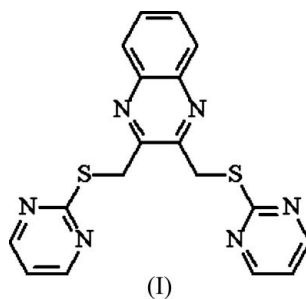
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Comment

The type of coordination architecture in complex compounds is mainly determined by a combination of two factors, namely the coordination preference of the metal ions and the nature of the ligands (Sun *et al.*, 2002). The purposeful design of specific ligands capable of controlling the assembly of supramolecular architectures has recently evolved as a popular and rapidly growing discipline (Zaworotko, 2000). In particular, multithioether ligands have been shown to exhibit high potential for structure control in inorganic chemistry, and many unusual crystal structures of complexes with multithioether ligands have been reported (Hartshorn & Steel, 1998). In this paper, we describe the crystal structure of a dithioether ligand, namely 2,3-bis[(pyrimidin-2-ylsulfanyl)methyl]quinoxaline, (I), which has already been used in the construction of silver(I) complexes (Wang *et al.*, 2001).



The molecular structure of (I) is shown in Fig. 1. Two terminal pyrimidine groups lie on the opposite sides of the planar quinoxaline system and their planes are almost orthogonal to the quinoxaline plane; the dihedral angles formed by the N3/N4/C6–C13 plane with the N1/N2/C1–C4 and N5/N6/C15–C18 planes are $81.1(3)$ and $82.0(3)^\circ$, respectively. The two pyrimidine planes are almost parallel to each other, the dihedral angle being $6.0(3)^\circ$.

Experimental

2,3-Bis[(pyrimidin-2-ylsulfanyl)methyl]quinoxaline, (I), was prepared by a procedure similar to that used for the synthesis of 1,4-bis-

(phenylsulfanyl)butane (Hartley *et al.*, 1979). A simple synthesis procedure has also been described by Wang *et al.* (2001), even though these authors did not isolate the free ligand. 2-Mercaptopyrimidine (1.12 g, 10 mmol) was added to a stirred solution of KOH (0.56 g, 10 mmol) in ethanol (20 ml). The mixture was heated to reflux, then an ethanol solution of 2,3-bis(bromomethyl)quinoxaline (1.57 g, 5 mmol) was added dropwise and the mixture was further refluxed for about 6 h. After adding more water (30 ml), the mixture was left to stand overnight. The precipitate was filtered off and washed with water, giving a fine white powder in 85% yield. ^1H NMR (CDCl_3): 5.00 (s, 4H, SCH₂), 6.95–8.37 (m, 10H, Ar-H); elemental analysis found: C 57.52, H 3.45, N 22.01%, calculated for C₁₈H₁₄N₆S₂: C 57.12, H 3.73, N 22.21%. Colorless single crystals of (I) were obtained by recrystallization from EtOH.

Crystal data

C₁₈H₁₄N₆S₂
M_r = 378.47
 Orthorhombic, *Pccn*
a = 22.485 (5) Å
b = 12.361 (3) Å
c = 12.560 (3) Å
V = 3490.9 (13) Å³
Z = 8
D_x = 1.440 Mg m⁻³

Mo *K*α radiation
 Cell parameters from 4783 reflections
 θ = 2.5–25.6°
 μ = 0.32 mm⁻¹
T = 293 (2) K
 Block, colorless
 0.22 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.933, *T_{max}* = 0.939
 21857 measured reflections

4126 independent reflections
 3069 reflections with *I* > 2σ(*I*)
R_{int} = 0.027
 θ_{max} = 27.9°
h = -29 → 29
k = -15 → 16
l = -16 → 14

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.035
wR (*F*²) = 0.096
S = 1.04
 4126 reflections
 235 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 0.5889P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.004$
 $\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.27 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

S1–C4	1.7465 (7)	S2–C14	1.8060 (7)
S1–C5	1.8052 (7)	S2–C15	1.7500 (6)
C4–S1–C5	101.88 (3)	C15–S2–C14	102.69 (3)

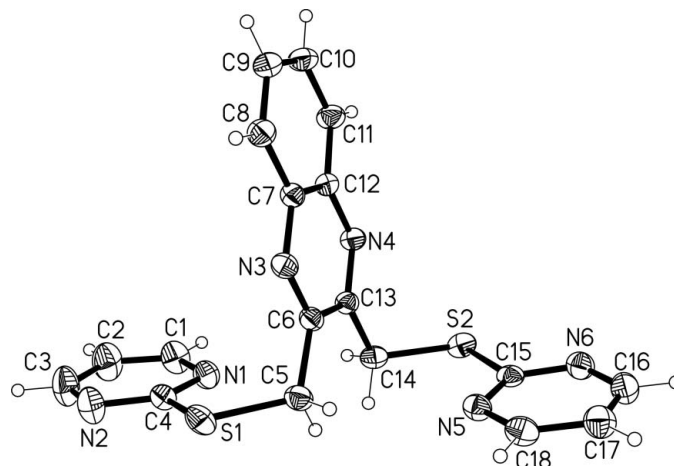


Figure 1

The molecular structure of the title compound, showing displacement ellipsoids drawn at the 30% probability level.

All H atoms were included in calculated positions and refined as riding atoms [C–H = 0.93 or 0.97 Å and *U_{iso}*(H) = 1.2*U_{eq}* of the carrier atom].

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT* and *SHELXTL* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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