

2,3-Bis(1-methyl-1*H*-imidazol-2-ylsulfanylmethyl)-
quinoxalineNing-Ning Pan,^a Wei Wang^{a*}
and Bing Zhao^b^aSchool of Chemical Engineering, Anshan
University of Science and Technology, Anshan
114002, People's Republic of China, and^bSchool of Chemical Engineering and Tech-
nology, Tianjin University, Tianjin 300072,
People's Republic of China

Correspondence e-mail: panningning@163.com

Key indicators

Single-crystal X-ray study

 $T = 294$ KMean $\sigma(\text{C}-\text{C}) = 0.004$ Å R factor = 0.040 wR factor = 0.122

Data-to-parameter ratio = 13.7

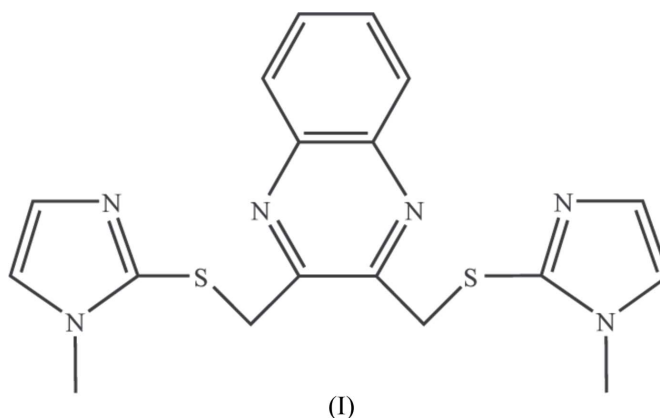
For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.The two terminal 1-methylimidazol-2-ylsulfanyl groups adopt
a *syn* conformation with respect to the central quinoxaline
ring system in the title compound, $\text{C}_{18}\text{H}_{18}\text{N}_6\text{S}_2$.

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Comment

To date, a large number of flexible or rigid chain-linked
dithioether ligands containing *N*-heterocyclic groups have
been synthesized and investigated, due to their diverse coor-
dination capabilities and to the important properties of their
metal complexes (Hester *et al.*, 1997; Yang *et al.*, 2000; Bu *et al.*,
2002; Hong *et al.*, 2000; Tong *et al.*, 1998). In this context, a new
imidazole derivative, *viz.* 2,3-bis(1-methyl-1*H*-imidazol-2-
ylsulfanylmethyl)quinoxaline, (I), has been synthesized.

In the molecular structure of (I) (Fig. 1 and Table 1), the two terminal 1-methylimidazol-2-ylsulfanyl groups adopt a *syn* conformation with respect to the central quinoxaline ring system and the dihedral angle formed between the imidazole rings is $128.7(3)^\circ$. The central quinoxaline ring system is practically planar, forming dihedral angles of $130.9(3)$ and $27.7(3)^\circ$ with the imidazoles attached to S2 and S1, respectively, with the imidazole rings. In one imidazole ring, atom C10 attached to the sulfanyl group has a distorted trigonal geometry, with the $\text{N3}-\text{C10}-\text{N4}$ [$112.0(2)^\circ$] and $\text{N4}-\text{C10}-\text{S1}$ [$126.74(19)^\circ$] angles deviating significantly from the ideal sp^2 -hybridized values; the comparable values for the other imidazole ring are $111.8(2)^\circ$ for $\text{N5}-\text{C15}-\text{N6}$ and $125.0(2)^\circ$ for $\text{N6}-\text{C15}-\text{S2}$. Owing to $p-\pi$ conjugation, the $\text{C}sp^2-\text{S}$ bonds, *i.e.* $\text{S1}-\text{C10}$ and $\text{S2}-\text{C15}$, are significantly shorter, as expected, than the $\text{C}sp^3-\text{S}$ bonds, *i.e.* $\text{S1}-\text{C9}$ and $\text{S2}-\text{C14}$ (see Table 1). The average lengths for the $\text{C}sp^2-\text{S}$ and $\text{C}sp^3-\text{S}$ bonds are $1.745(3)$ and $1.814(3)$ Å, respectively, which are comparable to those reported in the literature (Zhang *et al.*, 2003; Zheng & Liu, 2003).

Experimental

A solution of 2,3-bis(bromomethyl)quinoxaline (1.58 g, 5 mmol) in ethanol (10 ml) was added dropwise to a mixture of 1-methyl-2-thioimidazole (1.26 g, 11 mmol), KOH (0.62 g, 11 mmol) and ethanol (10 ml). The reaction mixture was stirred for 24 h at room temperature. Water (30 ml) was gradually added after which a yellow precipitate appeared. This was filtered off and recrystallized from an ethanol and water (1:1 v/v) mixture (yield 70%, m.p. 374–375 K). Analysis found: C 56.48, H 4.69, N 22.05%; C₁₈H₁₈N₆S₂ requires C 56.52, H 4.74, N 21.97%. IR (KBr): ν 3103, 2940, 1484, 1460, 1410, 1372, 1272, 1118, 1014, 760, 676 cm⁻¹. ¹H NMR (CDCl₃): δ 3.45 (s, 3H), 4.61 (s, 2H), 6.86 (d, 1H, *J* = 1.5 Hz), 7.00 (d, 1H, *J* = 2.5 Hz), 7.70 (d, 1H, *J* = 4 Hz), 7.91 (d, 1H, *J* = 3.5 Hz). Crystals of (I) suitable for single-crystal X-ray analysis were obtained by slow evaporation of a mixture of ethanol and water (1:2 v/v).

Crystal data

C₁₈H₁₈N₆S₂ *Z* = 2
M_r = 382.50 *D_x* = 1.383 Mg m⁻³
 Triclinic, *P* $\bar{1}$ Mo *K* α radiation
 Cell parameters from 1798 reflections
a = 6.8978 (14) Å θ = 2.9–26.1°
b = 9.953 (2) Å μ = 0.31 mm⁻¹
c = 14.556 (3) Å *T* = 294 (2) K
 α = 96.495 (4)° Block, yellow
 β = 97.418 (3)° 0.28 × 0.24 × 0.14 mm
 γ = 109.863 (3)°

Data collection

Bruker SMART CCD area-detector 3244 independent reflections
 diffractometer 2350 reflections with *I* > 2σ(*I*)
 φ and ω scans *R*_{int} = 0.021
 Absorption correction: multi-scan θ_{max} = 25.0°
 (SADABS; Sheldrick, 1996) *h* = -7 → 8
*T*_{min} = 0.923, *T*_{max} = 0.958 *k* = -9 → 11
 4713 measured reflections *l* = -17 → 16

Refinement

Refinement on *F*² $w = 1/[\sigma^2(F_o^2) + (0.067P)^2 + 0.146P]$
 $R[F^2 > 2\sigma(F^2)] = 0.040$ where $P = (F_o^2 + 2F_c^2)/3$
 $wR(F^2) = 0.122$ (Δ/σ)_{max} = 0.002
 3244 reflections $\Delta\rho_{max} = 0.24 \text{ e \AA}^{-3}$
 237 parameters $\Delta\rho_{min} = -0.24 \text{ e \AA}^{-3}$
 H-atom parameters constrained

Table 1

Selected geometric parameters (Å, °).

S1–C9	1.803 (3)	S2–C14	1.825 (3)
S1–C10	1.754 (2)	S2–C15	1.736 (3)
S1–C10–N3	121.20 (18)	S2–C15–N5	123.13 (19)
S1–C10–N4	126.74 (19)	S2–C15–N6	125.0 (2)
N3–C10–N4	112.0 (2)	N5–C15–N6	111.8 (2)

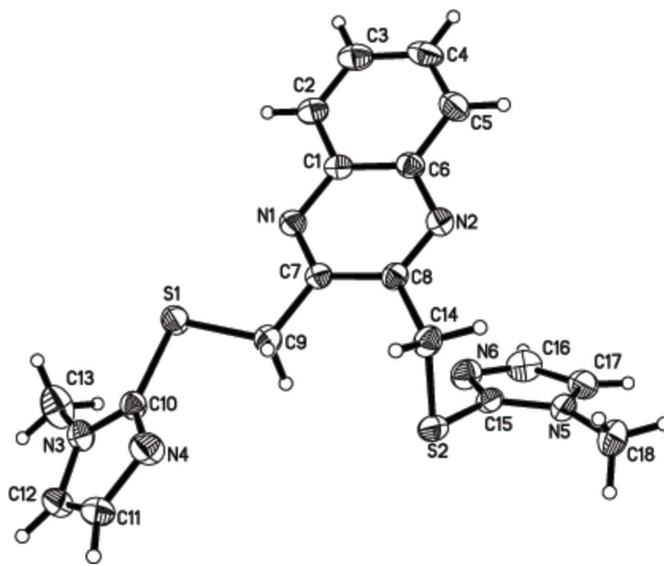


Figure 1 View of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

H atoms were included in the riding-model approximation, with aromatic C–H = 0.93 Å, methylene C–H = 0.97 Å and methyl C–H = 0.96 Å, and with *U*_{iso}(H) = 1.2*U*_{eq}(aromatic and methylene C) and *U*_{iso}(H) = 1.5*U*_{eq}(methyl C).

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

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