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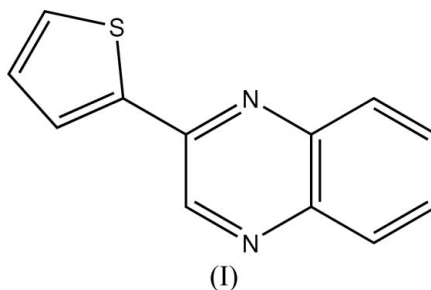
Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.045
 wR factor = 0.112
Data-to-parameter ratio = 34.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

2-(2-Thienyl)quinoxaline

The crystal structure of the title compound, $\text{C}_{12}\text{H}_8\text{N}_2\text{S}$, was determined at 293 K. The molecule is planar and packs in a herring-bone pattern.Received 3 August 2005
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Comment

We have previously investigated the crystal structures of 2,3-dithienylquinoxalines (Crundwell, Sayers *et al.*, 2003) and bromo-substituted 2,3-dithienylquinoxalines (Crundwell *et al.*, 2004). Quinoxalines, in general, have shown versatility in binding a wide variety of metals. We have now expanded our studies to the monosubstituted thienylquinoxalines.

The title compound, (I), sits on a general position. All bond lengths and angles are in agreement with those of other published quinoxalines and thienyl-containing compounds. Thienyl ring geometries and difference maps show no evidence of thienyl ring flip disorders, which are common in molecules with unsubstituted thienyl rings (Crundwell, Sullivan *et al.*, 2003). Like 2-phenylquinoxaline (Yeng & Li, 1989) and 2-(2'-pyridyl)quinoxaline (Kasselouri *et al.*, 1994), the molecule is planar and packs in a herring-bone motif. The interplanar spacing for layers in (I) is 3.537 Å, whereas the interplanar spacings for 2-phenyl and 2-(2'-pyridyl)quinoxalines are 3.428 and 3.490 Å, respectively.

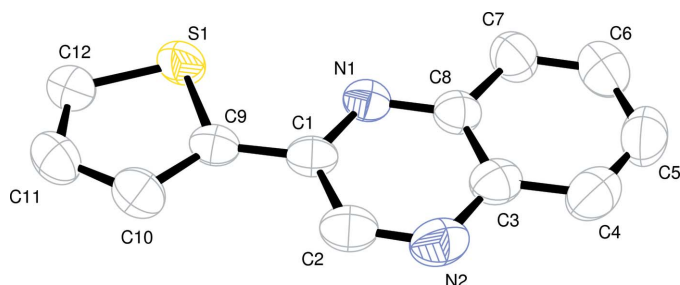


Figure 1
A view of (I) (Farrugia, 1997). Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

Experimental

Equimolar amounts of thiophen-2-ylglyoxal and 1,2-phenylenediamine were refluxed in 95% ethanol for 2 h. The resulting mixture was filtered and washed with ice-cold ethanol. The precipitate was recrystallized from a boiling ethanol–toluene mixture and crystals were grown from slowly evaporated solutions of ethanol. A light-brown plate that displayed homogeneous birefringence was mounted for diffraction studies. ¹H NMR and UV–vis spectroscopies, as well as melting points of the title compound, agree with literature values (Peter *et al.*, 2004).

Crystal data

C₁₂H₈N₂S
M_r = 212.27
 Monoclinic, *P*2₁/*c*
a = 5.5062 (13) Å
b = 16.119 (3) Å
c = 11.939 (3) Å
 β = 101.77 (2)°
V = 1037.4 (4) Å³
Z = 4

D_x = 1.359 Mg m⁻³
 Mo Kα radiation
 Cell parameters from 1179 reflections
 θ = 3.8–29.7°
 μ = 0.28 mm⁻¹
T = 293 K
 Plate, light brown
 0.32 × 0.16 × 0.09 mm

Data collection

Oxford Diffraction Sapphire3 diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
T_{min} = 0.891, *T_{max}* = 0.989
 8510 measured reflections

4739 independent reflections
 2529 reflections with *I* > 3σ(*I*)
R_{int} = 0.032
 θ_{max} = 29.7°
h = -6 → 7
k = -22 → 22
l = -16 → 12

Refinement

Refinement on *F*
R[*F*² > 2σ(*F*²)] = 0.045
wR(*F*²) = 0.112
S = 1.00
 4739 reflections
 136 parameters
 Only H-atom coordinates refined

Weighting scheme: Prince modified Chebychev polynomial (Watkin, 1994; Prince, 1982) [weight] = 1.0/[3.05*T*₀(*x*) + 3.88*T*₁(*x*) + 0.969*T*₃(*x*)], where *x* = *F_{calc}*/*F_{max}*
 (Δ/σ)_{max} = 0.001
 Δρ_{max} = 0.58 e Å⁻³
 Δρ_{min} = -0.80 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

C1–N1	1.3361 (17)	C5–C6	1.401 (3)
C1–C2	1.436 (2)	C6–C7	1.372 (3)
C1–C9	1.457 (2)	C7–C8	1.426 (2)
N1–C8	1.3658 (19)	S1–C9	1.7226 (15)
C2–N2	1.301 (2)	S1–C12	1.7091 (16)
N2–C3	1.381 (2)	C9–C10	1.3893 (19)
C3–C4	1.413 (2)	C10–C11	1.403 (2)
C3–C8	1.414 (2)	C11–C12	1.361 (2)
C4–C5	1.361 (3)		
N1–C1–C2	120.36 (14)	C6–C7–C8	119.95 (16)
N1–C1–C9	118.09 (13)	C7–C8–C3	119.08 (15)
C2–C1–C9	121.55 (12)	C7–C8–N1	119.43 (14)
C1–N1–C8	117.23 (13)	C3–C8–N1	121.50 (13)
C1–C2–N2	123.57 (14)	C9–S1–C12	91.56 (8)
C2–N2–C3	116.69 (14)	C1–C9–S1	119.14 (9)
N2–C3–C4	120.04 (15)	C1–C9–C10	129.99 (13)
N2–C3–C8	120.63 (15)	S1–C9–C10	110.84 (12)
C4–C3–C8	119.30 (15)	C9–C10–C11	112.52 (14)
C3–C4–C5	120.13 (17)	C10–C11–C12	112.66 (14)
C4–C5–C6	121.30 (17)	S1–C12–C11	112.42 (13)
C5–C6–C7	120.21 (16)		

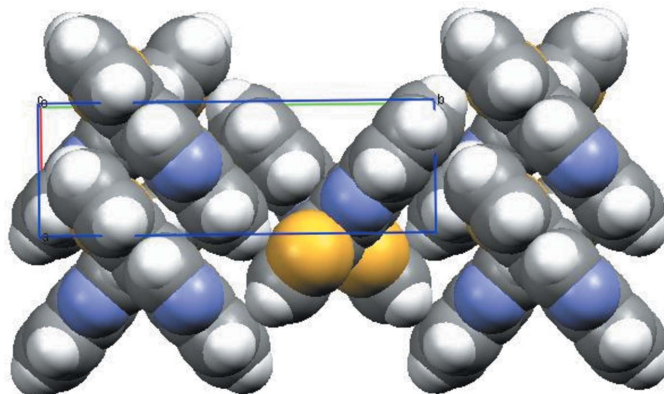


Figure 2

Packing diagram for (I) (Bruno *et al.*, 2002), showing the herringbone motif as viewed along the [001] direction.

H atoms were found in difference maps and their positional parameters were refined. The *U*_{iso}(H) values were set at 0.05 Å².

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2005); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2005); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *MERCURY* (Bruno *et al.*, 2002); software used to prepare material for publication: *CRYSTALS*.

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