

2,3-Dithien-2-ylquinoxaline

Guy Crundwell *et al.*

Synopsis

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Subject index

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2,3-Dithien-2-ylquinoxaline

Organic formula index

All residues containing organic carbon are included in this index.

$C_{16}H_{10}N_2S_2$

Author index

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2,3-Dithien-2-ylquinoxaline

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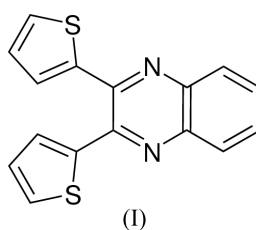
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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.061
 wR factor = 0.122
Data-to-parameter ratio = 14.5

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title compound, $\text{C}_{16}\text{H}_{10}\text{N}_2\text{S}_2$, (I), which was synthesized *via* the reaction of 2,2'-thienil and 1,2-phenylenediamine, the thienyl rings display ideal geometries, with no evidence of ring-flip disorders often found with unsubstituted terminal 2-thienyl rings [Zheng, Wang, Liu, Carducci, Peyghambarian & Jabbourb (2002). *Acta Cryst. C58*, m50–m52].



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Experimental

The title compound, (I), was prepared in adequate yields by heating equimolar amounts of 2,2'-thienil and 1,2-phenylenediamine in absolute ethanol for 30 min (Lukes *et al.*, 2001). Recrystallization from acetonitrile yielded yellow needles with a melting point of 418 K, which along with ^1H and ^{13}C NMR data on (I) were in agreement with published values (Lukes *et al.*, 2001).

Crystal data

$\text{C}_{16}\text{H}_{10}\text{N}_2\text{S}_2$
 $M_r = 294.38$
Monoclinic, $P2_1/c$
 $a = 11.521$ (3) Å
 $b = 5.2071$ (14) Å
 $c = 22.745$ (7) Å
 $\beta = 103.681$ (4)°
 $V = 1325.8$ (6) Å³
 $Z = 4$

$D_x = 1.475$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 11758 reflections
 $\theta = 2.1$ – 28.3°
 $\mu = 0.39$ mm⁻¹
 $T = 293$ (2) K
Needle, yellow
 $0.36 \times 0.23 \times 0.12$ mm

Data collection

Bruker SMART $P3/512$ CCD diffractometer
 ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.867$, $T_{\max} = 0.954$
10027 measured reflections

2617 independent reflections
2103 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.049$
 $\theta_{\max} = 26.0^\circ$
 $h = -14 \rightarrow 14$
 $k = -6 \rightarrow 6$
 $l = -27 \rightarrow 28$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.061$
 $wR(F^2) = 0.122$
 $S = 1.19$
2617 reflections
181 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0403P)^2 + 1.0471P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.24$ e Å⁻³
 $\Delta\rho_{\min} = -0.29$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

N1—C1	1.314 (4)	C7—C8	1.406 (4)
N1—C8	1.366 (4)	C9—C10	1.353 (4)
C1—C2	1.440 (4)	C9—S1	1.712 (3)
C1—C9	1.476 (4)	C10—C11	1.417 (4)
N2—C2	1.317 (4)	C11—C12	1.338 (5)
N2—C3	1.361 (4)	C12—S1	1.700 (3)
C2—C13	1.468 (4)	C13—C14	1.370 (4)
C3—C8	1.400 (4)	C13—S2	1.726 (3)
C3—C4	1.407 (4)	C14—C15	1.404 (4)
C4—C5	1.356 (5)	C15—C16	1.346 (4)
C5—C6	1.406 (5)	C16—S2	1.705 (3)
C6—C7	1.356 (4)		
C1—N1—C8	117.8 (2)	N1—C8—C7	119.5 (3)
N1—C1—C2	121.4 (3)	C3—C8—C7	119.8 (3)
N1—C1—C9	115.4 (2)	C10—C9—C1	129.5 (3)
C2—C1—C9	123.1 (3)	C10—C9—S1	110.9 (2)
C2—N2—C3	117.8 (2)	C1—C9—S1	119.6 (2)
N2—C2—C1	121.0 (3)	C9—C10—C11	112.5 (3)
N2—C2—C13	115.7 (2)	C12—C11—C10	112.8 (3)
C1—C2—C13	123.3 (3)	C11—C12—S1	111.8 (2)
N2—C3—C8	121.3 (3)	C12—S1—C9	91.96 (16)
N2—C3—C4	119.6 (3)	C14—C13—C2	133.0 (3)
C8—C3—C4	119.1 (3)	C14—C13—S2	110.0 (2)
C5—C4—C3	120.3 (3)	C2—C13—S2	117.0 (2)
C4—C5—C6	120.4 (3)	C13—C14—C15	113.2 (3)
C7—C6—C5	120.6 (3)	C16—C15—C14	113.0 (3)
C6—C7—C8	119.8 (3)	C15—C16—S2	111.8 (2)
N1—C8—C3	120.7 (3)	C16—S2—C13	92.06 (15)

All H atoms were placed in calculated positions, with C—H distances of 0.93 Å, and were included in the refinement in riding-motion approximation with $U_{\text{iso}} = 1.2U_{\text{eq}}$ of the carrier atom.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE* (Bruker, 2001) and *SHELXTL* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure:

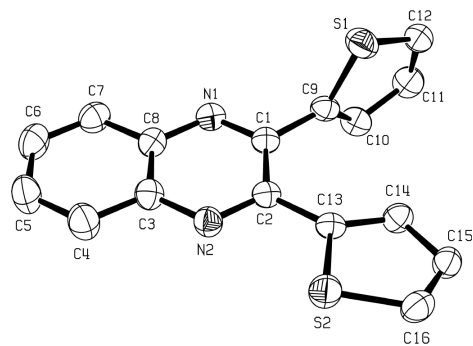


Figure 1

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

SHELXL97 (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *SHELXL97*.

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