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2,3-Dithien-2-ylquinoxaline

Guy Crundwell,[a]* David Sayers,[a] Steven R. Herron[b] and Katherine A. Kantardjieff[b]

[a]Department of Chemistry, Central Connecticut State University, New Britain, CT 06053, USA, and [b]W.M. Keck Foundation Center for Molecular Structure, Department of Chemistry and Biochemistry, California State University Fullerton, 800 State College Boulevard, Fullerton, CA 92834, USA

Correspondence e-mail: crundwellg@mail.ccsu.edu

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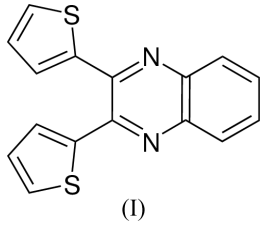
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–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, $C_{16}H_{10}N_2S_2$, (I), which was synthesized *via* the reaction of 2,2′-thenil 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*. C**58**, m50–m52].



(I)

Experimental

The title compound, (I), was prepared in adequate yields by heating equimolar amounts of 2,2′-thenil 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 ^{1}H and ^{13}C NMR data on (I) were in agreement with published values (Lukes *et al.*, 2001).

Crystal data

$C_{16}H_{10}N_2S_2$
M_r = 294.38
Monoclinic, $P2_1/c$
a = 11.521 (3) Å
b = 5.2071 (14) Å
c = 22.745 (7) Å
β = 103.681 (4)°
V = 1325.8 (6) Å^3
Z = 4
D_x = 1.475 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 11758 reflections
θ = 2.1–28.3°
μ = 0.39 mm^{-1}
T = 293 (2) K
Needle, yellow
0.36 × 0.23 × 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_{int} = 0.049
θ_{max} = 26.0°
$h = -14 \rightarrow 14$
$k = -6 \rightarrow 6$
$l = -27 \rightarrow 28$

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 $U_{iso} = 1.2U_{eq}$ of the carrier atom.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* (Bruker, 2001) and *SHELXTL* (Bruker, 2001); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXL*97; software used to prepare material for publication: *SHELXL*97.

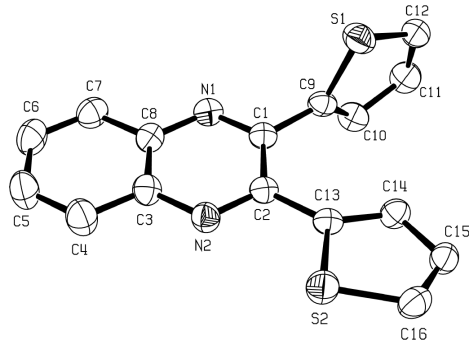


Figure 1
A view of (I) (Farrugia, 1997). Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

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