Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-1-(2-Thienyl)ethanone 8-quinolylhydrozone

Daniel E. Lynch[a]* and Ian McClenaghan[b]†

[a]School of Natural and Environmental Sciences, Coventry University, Coventry CV1 5FB, England, and [b]Spa Contract Synthesis, School of Natural and Environmental Sciences, Coventry University, Coventry CV1 5FB, England

† E-mail: 106355.1670@CompuServe.com.

Correspondence e-mail: apx106@coventry.ac.uk

Received 21 November 2000
Accepted 4 December 2000
Online 14 December 2000

Key indicators

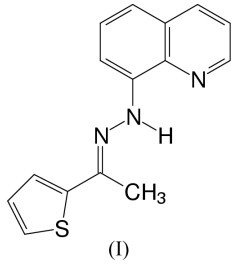
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
R factor = 0.061
wR factor = 0.170
Data-to-parameter ratio = 16.6

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

The structure of the title compound, $C_{15}H_{13}N_3S$, comprises planar molecules. The dihedral angle between the quinoline and thiophene rings is 2.6 (2)°.

Comment

Two distinct crystal colours (orange and yellow) were observed in the bulk following crystallization of the title compound, (I). The molecular structures from both crystal types were determined and proved to be identical, as were the melting points. Both structures refined to approximately the same R value and the structure obtained from the orange crystals is reported here. The cell for the yellow crystals was determined as a = 10.1194 (9), b = 14.251 (1), c = 18.136 (2) Å and V = 2615.4 (4) Å^3. The origin of the difference in colour is currently unknown and cannot be simply explained by crystal morphology because both crystal types were indistinguishable in size and shape. However, we cannot discard the possibility of two different rates of crystallization, which we are currently investigating.



(I)

Experimental

The title compound, (I), was prepared by Spa Contract Synthesis. Crystals were grown from an aqueous solution.

Crystal data

$C_{15}H_{13}N_3S$
M_r = 267.34
Orthorhombic, *Pbca*
a = 10.148 (2) Å
b = 14.251 (3) Å
c = 18.103 (4) Å
V = 2618.1 (9) Å^3
Z = 8
D_x = 1.357 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 46446 reflections
θ = 1.0–27.5°
μ = 0.24 mm^{-1}
T = 150 (2) K
Plate, orange
0.30 × 0.24 × 0.02 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.933, T_{max} = 0.995
20 334 measured reflections
2947 independent reflections
1498 reflections with $I > 2\sigma(I)$
R_{int} = 0.121
θ_{max} = 27.5°
$h = -11 \rightarrow 13$
$k = -18 \rightarrow 18$
$l = -23 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.170$
$S = 0.98$
2947 reflections
177 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0867P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N11—H11···N1	0.97 (4)	2.36 (3)	2.675 (4)	98 (2)

All H atoms were included in the refinement at calculated positions as riding models with C—H set to 0.95 (Ar-H) and 0.98 Å (CH_3), except for the amine H atom, which was located on difference syntheses and for which both positional and displacement parameters were refined. The higher than expected R_{int} value (>0.10) may be due to a slight misalignment of the crystal plate on the diffractometer with respect to the beam.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

The authors thank the EPSRC National Crystallography Service (Southampton).

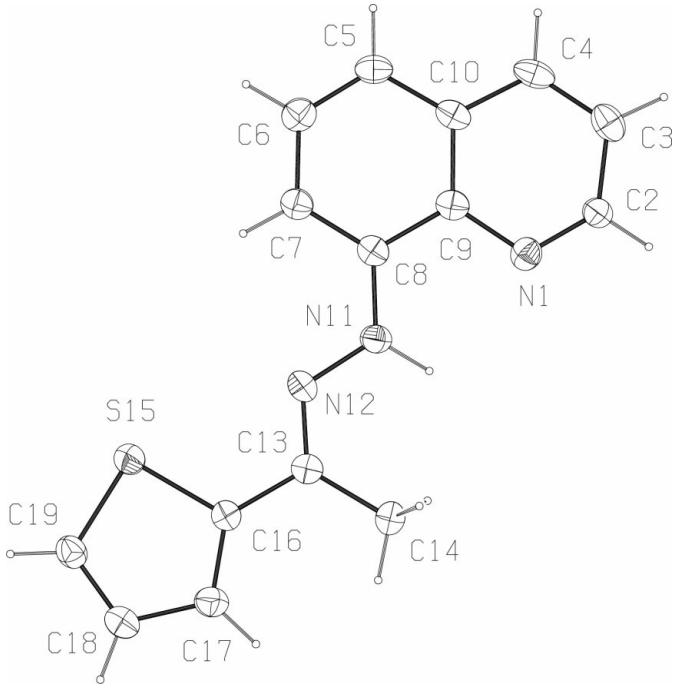


Figure 1
The molecular configuration and atom numbering scheme for (I), showing 30% probability ellipsoids.

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–37.
Hooft, R. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods Enzymol.* **276**, 307–326.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.