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5-Nitrothiophene-2-carbaldehyde

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In the crystal structure of the title compound, $C_5H_3NO_3S$, determined at 100 K, the nitro group and the aldehyde group make angles of 8.37 (16) and 8.5 (4)°, respectively, with the plane of the thiophene ring.

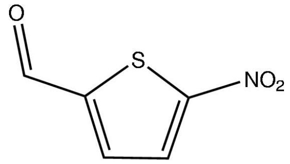
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.027
wR factor = 0.075
Data-to-parameter ratio = 9.2

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

Comment

In the title compound, (I), all bond distances and angles fall within the normal ranges. The molecule is essentially planar; however, the nitro group and the aldehyde group are at angles of 8.37 (16) and of 8.5 (4)°, respectively, with plane of the thiophene ring. In the crystal structure, molecules are connected by weak C—H···O hydrogen bonds (see Table 1).



(I)

Experimental

The title compound was purchased from Aldrich (98% purity) and was recrystallized from ethanol prior to its use as a reactant in the Adler synthesis for porphyrins (Adler *et al.*, 1967). White crystals of the title compound were grown from the slow evaporation of ethanol solutions at 278 K.

Crystal data

$C_5H_3NO_3S$
$M_r = 157.14$
Orthorhombic, $Pna2_1$
$a = 11.4180\ (7)$ Å
$b = 13.9536\ (8)$ Å
$c = 3.8525\ (2)$ Å
$V = 613.79\ (6)$ Å^3
$Z = 4$
$D_x = 1.701$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5184 reflections
$\theta = 2.3–28.3°$
$\mu = 0.46$ mm^{-1}
$T = 100\ (2)$ K
Needle, white
0.50 × 0.05 × 0.05 mm

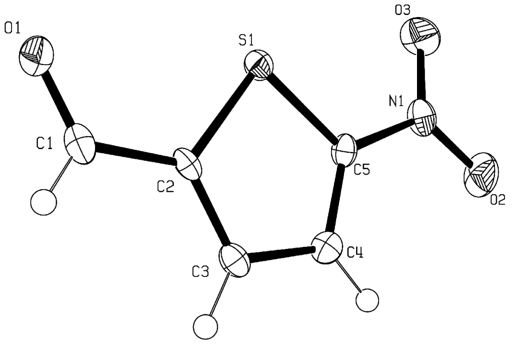


Figure 1
A view of (I) (Farrugia, 1997). Displacement ellipsoids are drawn at the 50% probability level.

Data collection

Bruker SMART APEX diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{\min} = 0.921$, $T_{\max} = 0.980$
5572 measured reflections
872 independent reflections
871 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.025$
$\theta_{\max} = 28.3°$
$h = -15 \rightarrow 15$
$k = -18 \rightarrow 18$
$l = -5 \rightarrow 5$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.075$
$S = 1.18$
872 reflections
95 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 0.2249P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.37$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O1$^{\rm i}$	0.93 (3)	2.52 (3)	3.373 (3)	152 (2)
C4—H4*A*···O1$^{\rm ii}$	0.93	2.46	3.364 (3)	163

Symmetry codes: (i) $1 - x, -y, z - \frac{1}{2}$; (ii) $x - \frac{1}{2}, \frac{1}{2} - y, z - 1$.

Thienyl H atoms were included in calculated positions with a C—H distance of 0.95 Å and were included in the refinement in riding-model approximation with $U_{\rm iso} = 1.2U_{\rm eq}$ of the carrier atom. The aldehyde H atom was found in a difference map during the inital stages of refinement and was refined independently with an isotropic displacement parameter. Refinements to determine the absolute structure gave inconclusive results [yielding a Flack (1983) parameter of 0.15 (9)] and the Friedel equivalents were therefore merged before the final refinement cycles.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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