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1,5-Bis(3-bromo-2-thienyl)-3-(3-nitrophenyl)-pentane-1,5-dione

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.005 Å
R factor = 0.042
wR factor = 0.112
Data-to-parameter ratio = 17.4

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

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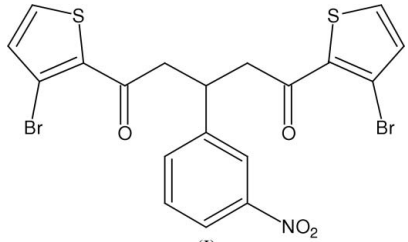
In the title compound, $C_{19}H_{13}Br_2NO_4S_2$, the two bromothienyl rings have different orientations with respect to the carbonyl groups. The nitro group is almost coplanar with the benzene ring to which it is attached.

Comment

Today, crystals play an important role in electronic and photonic industries, such as in the production of high-efficiency photovoltaic cells, fabrication of bright and long-lasting light emitting diodes (LEDs) and in liquid crystal displays (LCDs). Crystal growth is a multidisciplinary field, which demands collaboration of chemical and process engineers, electrical and mechanical engineers, instrumentation engineers, materials scientists, numerical simulation specialists, physicists and crystallographers (Tareen & Kutty, 2001). The present day demand is for large and high-quality ferroelectric, piezoelectric single crystals with minimum defects and inhomogeneities. The important goal of crystal growth is the improvement of microscopic and macroscopic homogeneity, which is a necessity for any application. The crystal structures of 3-hydroxy-1,3-bis(2-thienyl)prop-2-en-1-one (Baxter *et al.*, 1990) and 1-(4-chlorophenyl)-3-(2-thienyl)prop-2-en-1-one (Ng *et al.*, 2006) have been reported. In continuation of our work on crystal structures of new organic compounds and chalcones (Yathirajan *et al.*, 2006*a*,*b*), the title compound has been synthesized and its crystal structure is reported.



(I)

The molecular structure of the title compound is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.27, November 2005, updated August 2006; *Mogul*, Version 1.1; Allen, 2002). Whereas one of the carbonyl groups is *trans* to the nearest C—S bond, the other is *cis* configured (Table 1). The nitro group is almost coplanar with the benzene ring to which it is attached.

Experimental

2-Acetyl-3-bromothiophene (20 g, 0.096 mol) in methanol (50 ml) was mixed with 3-nitrobenzaldehyde (7.2 g, 0.048 mol) and the

mixture was treated with 10 ml of a 30% potassium hydroxide solution at 278 K. The reaction mixture was then brought to room temperature and stirred for 4 h. The solid that precipitated was filtered off, washed with water, dried and recrystallized from an acetone/methanol mixture (1:1) (yield 75%, m.p. 439–441 K). Analysis for $C_{19}H_{13}Br_2NO_4S_2$: found (calculated): C 41.91 (42.01), H 2.32 (2.41), N 2.46 (2.58), S 11.72 (11.80)%.

Crystal data

$C_{19}H_{13}Br_2NO_4S_2$
M_r = 543.24
Monoclinic, *Cc*
a = 17.5329 (13) Å
b = 15.6345 (9) Å
c = 7.4723 (6) Å
β = 96.932 (6)°
V = 2033.3 (3) Å^3
Z = 4
D_x = 1.775 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 4.22 mm^{-1}
T = 173 (2) K
Rod, colourless
0.26 × 0.13 × 0.12 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.407, T_{max} = 0.632
13028 measured reflections
4431 independent reflections
4195 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 27.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.112
S = 1.04
4431 reflections
254 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0814P)^2 + 0.7776P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0066 (6)
Absolute structure: Flack (1983), 2083 Friedel pair
Flack parameter: 0.002 (8)

Table 1
Selected torsion angles (°).

O1—N1—C3—C2	−3.8 (5)	S11—C11—C15—O15	170.7 (3)
O2—N1—C3—C4	−5.4 (5)	S21—C21—C25—O25	2.9 (4)

H atoms were found in a difference map, but placed geometrically and allowed to ride on their parent C atoms at distances ranging from 0.95 to 1.00 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

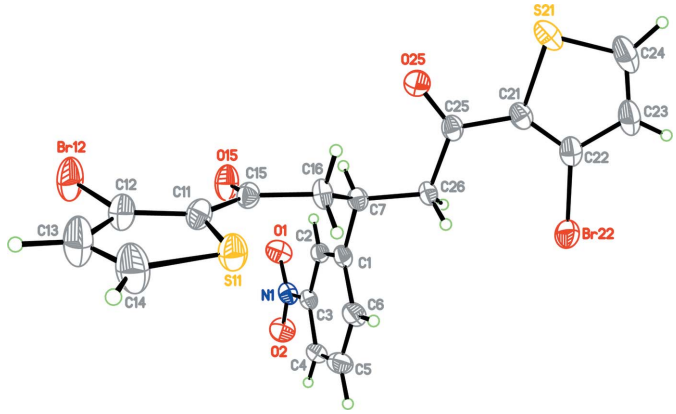


Figure 1
The molecular structure of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

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References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Baxter, L. A. M., Blake, A. J., Heath, G. A. & Stephenson, T. A. (1990). *Acta Cryst.* C**46**, 508–510.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Ng, S.-L., Patil, P. S., Razak, I. A., Fun, H.-K. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o3200–o3202.
Sheldrick, G. M. (1991). *SHELXTL-Plus*. Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Darmstadt, Germany.
Tareen, J. A. K. & Kutty, T. R. N. (2001). *A Basic Course in Crystallography*. Hyderabad, India: Universities Press (India) Limited.
Yathirajan, H. S., Sarojini, B. K., Narayana, B., Bindya, S. & Bolte, M. (2006*a*). *Acta Cryst.* E**62**, o3629–o3630.
Yathirajan, H. S., Sarojini, B. K., Narayana, B., Bindya, S. & Bolte, M. (2006*b*). *Acta Cryst.* E**62**, o3631–o3632.