

Crystal structure and Hirshfeld surface analysis of 3-(2,6-dichlorophenyl)-1,5-bis(thiophen-2-yl)-pentane-1,5-dione

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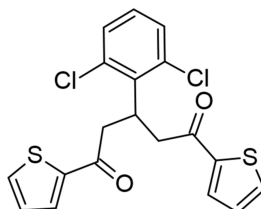
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In the crystal of the title compound, C₁₉H₁₄Cl₂O₂S₂, molecules are linked by intermolecular C—H···O hydrogen bonds, forming a square-ring around a fourfold rotation axis parallel to the *c*-axis. In addition, C—H··· π and π – π interactions [centroid-to-centroid distances = 3.759 (3) and 3.760 (3) Å] connect molecules, forming a three-dimensional network. Two thiophene rings are disordered with a 180° rotation over two positions; the first in a 0.686 (2)(3):0.314 (2) ratio and the second in a 0.787 (2):0.213 (2) ratio. The major contributions to the Hirshfeld surface are from H···H (32.4%), C···H/H···C (25.6%), Cl···H/H···Cl (17.2%) and O···H/H···O (14.4%) contacts.

1. Chemical context

Thiophenes with a five-membered planar ring are a family of sulfur-containing chemical compounds that are highly important in synthesis, crystal engineering, medicine and materials science (Nuralieva *et al.*, 2025, 2026; Torambetov *et al.*, 2026; Peng *et al.*, 2024). Selective functionalization of a thiophene ring in homogeneous or heterogeneous catalytic systems (Makhmudova *et al.*, 2022; Mahmudov *et al.*, 2023) can be a powerful synthetic strategy towards new materials. In fact, substituted thiophene drugs have been approved by the Food and Drug Administration (FDA), such as Cefoxitin, Raloxifene and Suprofen (Schweizer *et al.*, 2011), and these derivatives were used as multidentate ligands in coordination chemistry (Javadzade *et al.*, 2026; Mahmudov *et al.*, 2021). Halogenated derivatives of thiophene are essential building blocks for synthesizing advanced functional materials like catalysts, organic solar cells, sensitizers and drugs (Guseinov *et al.*, 2025; Huseynov *et al.*, 2021; Mamedov *et al.*, 2024). Similarly to the fluorine analogue (Gurbanov *et al.*, 2025), attachment of a chlorine atom-containing residue to the thiophene can lead to a new type of intermolecular interactions. Thus, in the current work, we have synthesized the new title thiophene derivative, (I), which presents multiple intermolecular non-covalent interactions in the crystal packing.



2. Structural commentary

The intramolecular C10—H10A···C11 contact forms an *S*(6) ring motif (Bernstein *et al.*, 1995) with atoms C10, C9, C14, and C15, the intramolecular C9—H9···C12 contact forms a *S*(5) ring motif with atoms C9, C14, and C19, the intramolecular C12—H12A···C11 contact forms an *S*(6) ring motif with atoms C12, C9, C14, and C15, and the intramolecular C9—H9···O1 contact forms an *S*(5) ring motif with atoms C9, C10, and C11 (Fig. 1, Table 1). The planes described by the dichlorophenyl (C14—C19) and the thiophene rings (S1/C1—C4 and S2/C5—C8) are rotated by 45.5 (3) and 82.8 (2)°, respectively. The angle between these two thiophene rings is 48.5 (3)°. The C14—C9—C10—C11, C9—C10—C11—C1, C9—C10—C11—O1, C14—C9—C12—C13, C9—C12—C13—O2 and C9—C12—C13—C5 torsion angles are 154.89 (12), 169.19 (12), −12.0 (2), −55.14 (16), −38.13 (19) and 143.98 (13)°, respectively. These interactions maintain the molecular conformation. The geometric properties of the title compound are normal and consistent with those of similar compounds listed in the *Database survey* section.

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, molecules are connected by C—H···O hydrogen bonds, which involve atoms O2, C1, C2, C9, C11, C10, C12, and C13, forming a square-ring around a fourfold rotation axis with graph set $R_4^4(40)$ (Fig. 2*a,b,c*; Table 1). Furthermore, C—H··· π and π — π interactions [$Cg1\cdots Cg5^b = 3.759$ (3) Å, slippage = 1.317 Å and $Cg5\cdots Cg1^c = 3.760$ (3) Å, slippage = 1.572 Å; symmetry codes (b) $y, \frac{1}{2} - x, \frac{1}{2} - z$; (c) $\frac{1}{2} - y, x, \frac{1}{2} - z$; Cg1 and Cg5 are the centroids of the (S1/C1—C4) thiophene and (C14—C19) dichlorophenyl rings, respectively] connect molecules, forming a three-dimensional network (Fig. 3*a,b,c*; Table 1).

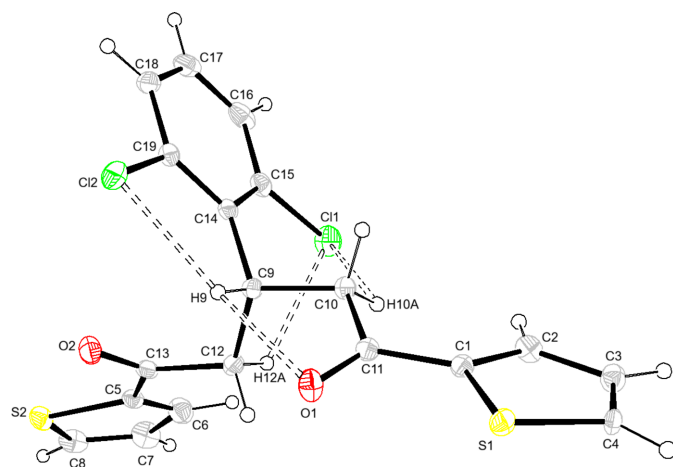


Figure 1

Molecular structure showing the atomic labelling. Displacement ellipsoids are drawn at the 30% probability level. Minor disorder components have been omitted for clarity.

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C3—H3···O2 ⁱ	0.95	2.48	3.238 (8)	136
C9—H9···C12	1.00	2.47	3.0884 (18)	120
C9—H9···O1	1.00	2.44	2.819 (2)	102
C10—H10A···C11	0.99	2.75	3.3095 (19)	116
C12—H12A···C11	0.99	2.64	3.317 (2)	126
C4—H4···Cg5 ⁱⁱ	0.95	2.83	3.431 (7)	122
C10—H10B···Cg1 ⁱⁱ	0.99	2.72	3.704 (4)	171

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

Table 2

Summary of short interatomic contacts (Å).

Contact	Distance	Symmetry operation
*H3···O2	2.48	$y, \frac{1}{2} - x, \frac{1}{2} - z$
*H4···C18	2.83	$1 - x, 1 - y, -z$
*H2X···*H8	2.42	$1 - y, \frac{1}{2} + x, -\frac{1}{2} + z$
*H2X···C13	2.94	$1 - x, 1 - y, 1 - z$
H9···H17	2.56	$1 - y, \frac{1}{2} + x, \frac{1}{2} + z$
*C7···*H7	2.93	$y, \frac{1}{2} - x, \frac{3}{2} - z$

The prefix * indicates an atom of a disordered component.

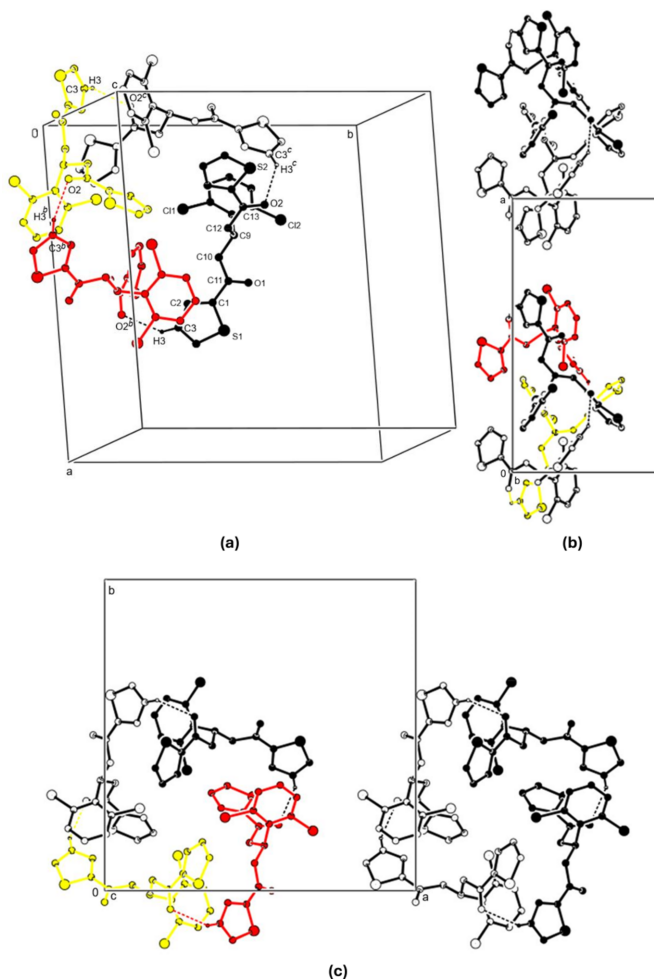


Figure 2

(a) A partial view of the C—H···O interactions in the unit cell. (b) A view down the *b* axis of the C—H···O interactions. (c) Crystal packing viewed along the *c* axis showing the C—H···O interactions (dashed lines) for the situation shown in Fig. 2*b*. Minor disorder components and hydrogen atoms not involved in hydrogen bonding have been omitted for clarity. Symmetry codes: (b) $y, \frac{1}{2} - x, \frac{1}{2} - z$; (c) $\frac{1}{2} - y, x, \frac{1}{2} - z$.

A Hirshfeld surface analysis was performed with *Crystal-Explorer* (Spackman *et al.*, 2021) to explore the intermolecular interactions (Tables 1 and 2). In this analysis, the major and minor components of the disordered thiophene rings in the refined CIF were considered together in the calculations. The Hirshfeld surface was mapped over d_{norm} in the range of -0.1652 to $+1.4465$ a.u. The red and blue areas of the Hirshfeld surface plotted over the d_{norm} (Fig. 4) indicate connections that are shorter or longer than the van der Waals radii, respectively, whereas the white surface shows contacts that are equal to the sum of the van der Waals radii. The most important interactions are $\text{H}\cdots\text{H}$, $\text{C}\cdots\text{H}$, $\text{Cl}\cdots\text{H}$ and $\text{O}\cdots\text{H}$ interactions (Tables 1 and 2).

Two-dimensional fingerprint plots together with their percentage contributions are shown in Fig. 5. The crystal packing is dominated by $\text{H}\cdots\text{H}$ contacts, which represent van der Waals interactions (32.4% of the entire surface), followed

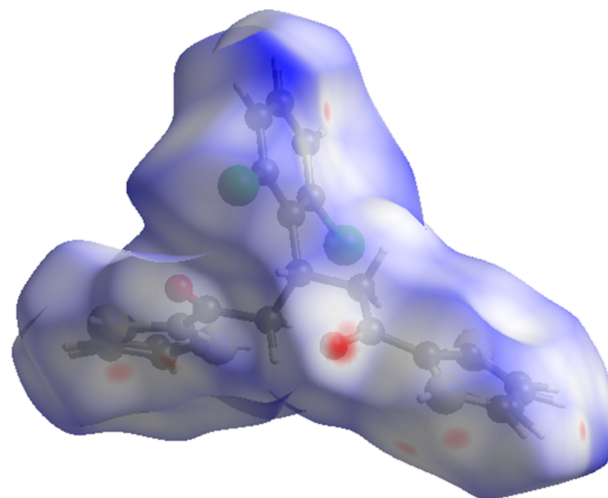


Figure 4
Three-dimensional Hirshfeld surface analysis mapped over d_{norm} .

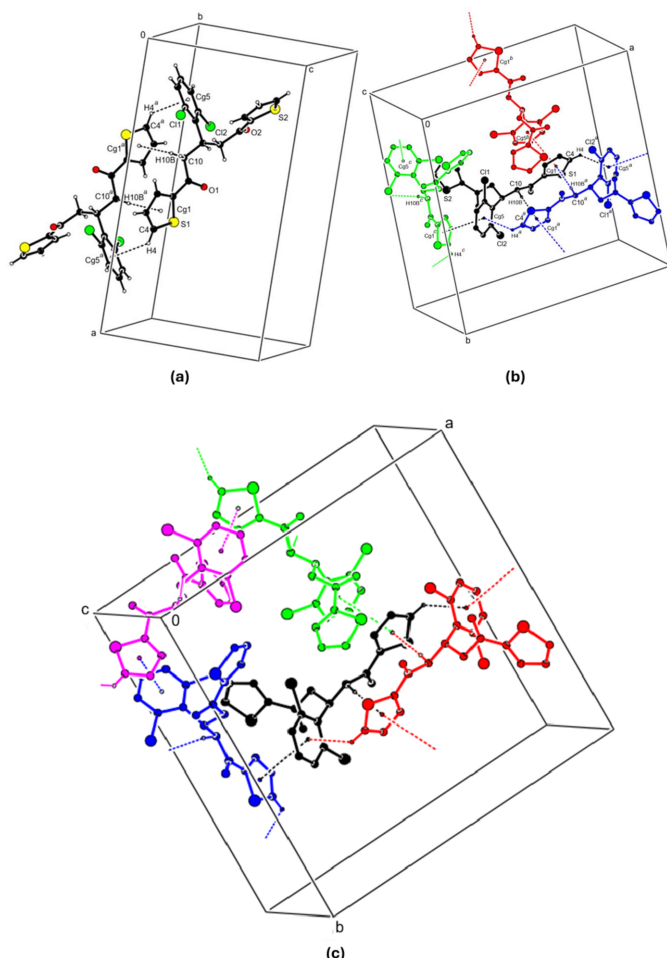


Figure 3
(a) A view of the $\text{C}-\text{H}\cdots\pi$ interactions between two adjacent molecules in the unit cell (dashed lines). (b) A partial view of the $\text{C}-\text{H}\cdots\pi$ and $\pi-\pi$ interactions (dashed lines) in the unit cell. (c) Partial view of $\text{C}-\text{H}\cdots\pi$ and $\pi-\pi$ interactions and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds (dashed lines) in the unit cell. For clarity, minor disorder components have been removed in all of them, and in (b) and (c) hydrogen atoms not involved in hydrogen bonding have been removed. Symmetry codes: (a) $1-x, 1-y, -z$; (b) $y, \frac{1}{2}-x, \frac{1}{2}-z$; (c) $\frac{1}{2}-y, x, \frac{1}{2}-z$.

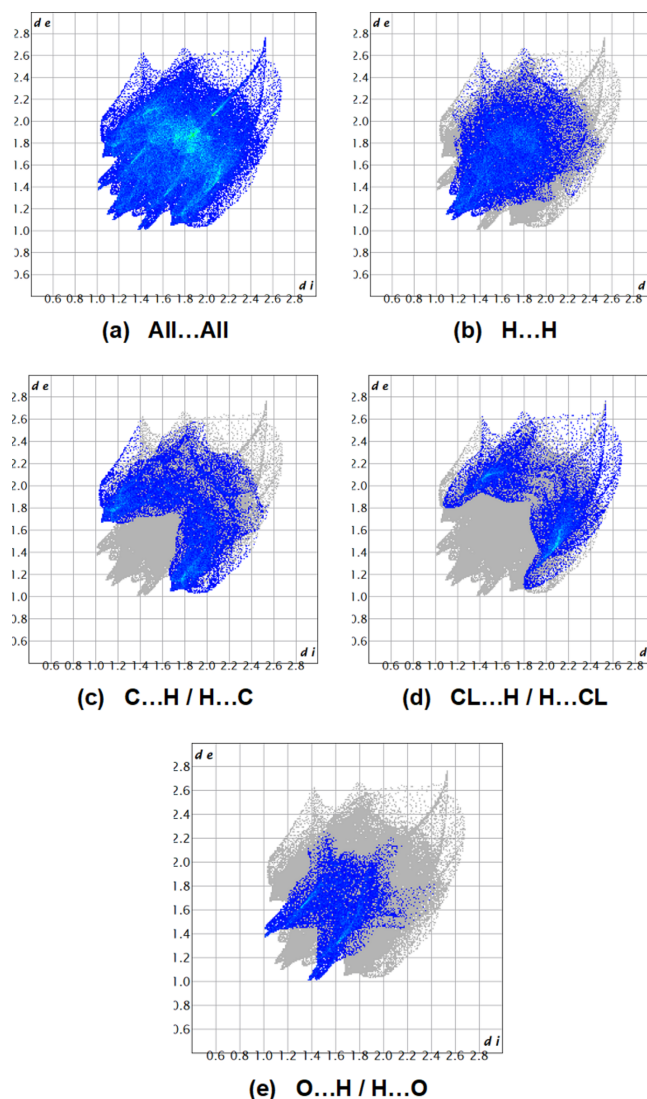


Figure 5
The two-dimensional fingerprint plots showing (a) all interactions, and those delineated into (b) $\text{H}\cdots\text{H}$, (c) $\text{C}\cdots\text{H}/\text{H}\cdots\text{C}$, (d) $\text{Cl}\cdots\text{H}/\text{H}\cdots\text{Cl}$ and (e) $\text{O}\cdots\text{H}/\text{H}\cdots\text{O}$ interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

by C...H/H...C (25.6%), Cl...H/H...Cl (17.2%) and O...H/H...O (14.4%) interactions. Smaller contributions are observed for the S...H/H...S (3.5%), C...C (3.4%), Cl...Cl (1.7%), S...C/C...S (0.7%), S...O/O...S (0.5%), Cl...S/S...Cl (0.4%), O...O (0.1%), S...S (0.1%), O...C/C...O (0.1%) and Cl...C/C...Cl (0.1%) contacts.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 6.00, update of April 2025; Groom *et al.*, 2016) for closely related 3-aryl-1,5-bis(thiophen-2-yl)pentane-1,5-dione structures found 3-(2-chloro-6-fluorophenyl)-1,5-bis(thiophen-2-yl)pentane-1,5-dione (AQILEV: Gurbanov *et al.*, 2025), 1,5-bis(3-bromothien-2-yl)-3-(2,3,5-trichlorophenyl)pentane-1,5-dione (MIGVEE: Butcher *et al.*, 2007), 1,5-bis(3-bromothien-2-yl)-3-(3-nitrophenyl)pentane-1,5-dione (WEPJOR: Yathirajan *et al.*, 2006), 3-[4-(dimethylamino)phenyl]-1,5-bis(thiophen-2-yl)pentane-1,5-dione (XUJRAZ: Sharmoukh *et al.*, 2025) and 1,5-bis(thiophen-2-yl)-3-(2,4,5-trimethoxyphenyl)pentane-1,5-dione (OCAXAT: Fun *et al.*, 2011).

The angles between the plane of the benzene ring and those of the two thiophene rings are 40.9 (1) and 51.6 (1)° for AQILEV, 89.7 (5) and 63.7 (1)° for MIGVEE, 84.9 (2) and 68.8 (2)° for WEPJOR, 75.27 (5) and 83.8 (2)° for XUJRAZ, and 41.51 (6) and 25.83 (6)° for OCAXAT.

In the crystal of AQILEV, the molecules are linked into [010] chains by C—H...O hydrogen bonds, forming a C(6) motif; weak C—H...F and C—H...Cl interactions link these chains into sheets parallel to the (100) plane. In MIGVEE, the molecules are linked by C—Br... π and C—Cl... π interactions and there are no classical hydrogen bonds. In WEPJOR, the molecules form layers parallel to (200) through C—H...O hydrogen bonds. C—H... π , C—Br... π , and C—O... π interactions formed between the layers strengthen the molecular packing. In the crystal of XUJRAZ, C—H...O hydrogen bonds form chains of molecules extending along the *c*-axis direction. These are linked by C—H...S hydrogen bonds and C—H... π interactions into corrugated layers parallel to the *bc* plane. In OCAXAT, molecules are linked into a three-dimensional network by weak C—H...O and C—H... π interactions, and a π — π stacking with a centroid-centroid distance of 3.6527 (8) Å. The respective observed pattern in the crystal of the title compound is, hence, also notably uncommon.

5. Synthesis and crystallization

2,6-Dichlorobenzaldehyde (10 mmol) was added to a solution of 1-(thiophen-2-yl)ethan-1-one (20 mmol) in EtOH (60 ml). KOH pellets (25 mmol) were then added to the solution (Fig. 6). The solution was stirred at room temperature for 8 h. The off-white solid was collected by filtration and washed with EtOH (3 × 10 ml). Recrystallization from CHCl₃–MeOH afforded a white crystalline solid of the title compound (yield, 64%). Analysis calculated for C₁₉H₁₄Cl₂O₂S₂: C 55.75, H 3.45.

Table 3

Experimental details.

Crystal data	
Chemical formula	C ₁₉ H ₁₄ Cl ₂ O ₂ S ₂
<i>M</i> _r	409.32
Crystal system, space group	Tetragonal, <i>P</i> ₄ ₂ / <i>n</i>
Temperature (K)	150
<i>a</i> , <i>c</i> (Å)	18.853 (3), 10.235 (4)
<i>V</i> (Å ³)	3637.9 (18)
<i>Z</i>	8
Radiation type	Mo <i>K</i> α
μ (mm ^{−1})	0.60
Crystal size (mm)	0.36 × 0.23 × 0.23
Data collection	
Diffraction	—
Absorption correction	—
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	34717, 3693, 3195
<i>R</i> _{int}	0.026
(sin θ /λ) _{max} (Å ^{−1})	0.624
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.027, 0.074, 1.04
No. of reflections	3693
No. of parameters	300
No. of restraints	608
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ^{−3})	0.29, −0.20

Computer programs: APEX2 and SAINT (Bruker, 2012), SHELXT (Sheldrick, 2015a), SHELXL (Sheldrick, 2015b), ORTEP-3 for Windows (Farrugia, 2012) and PLATON (Spek, 2020).

Found: C 55.72, H 3.43. ¹H NMR (400 MHz, CDCl₃): δ = 4.12–4.16 (1H, CH), 3.36–3.52 (4H, 2CH₂), 7.14–8.26 (9H, Ar and thiophen-2-yl) ppm. ¹³C NMR (100 MHz, CDCl₃): δ = 196.4, 160.0, 142.2, 136.8, 135.8, 133.4, 132.2, 129.8, 128.0, 46.8, 34.9 ppm.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were positioned geometrically (C—H = 0.95–1.00 Å) and refined as riding with *U*_{iso}(H) = 1.2–1.5*U*_{eq}(C). Two thiophene rings (S1/C1–C4 and S2/C5–C8) are disordered with a 180° rotation over two positions; the first around the C1–C11 bond with a 0.686 (2)(3):0.314 (2) ratio and the second around the C5–C13 bond with a 0.787 (2):0.213 (2) ratio. The restraints on bond lengths and atomic displacement parameters on each pair of disorder fragments (SADI and SAME instructions of

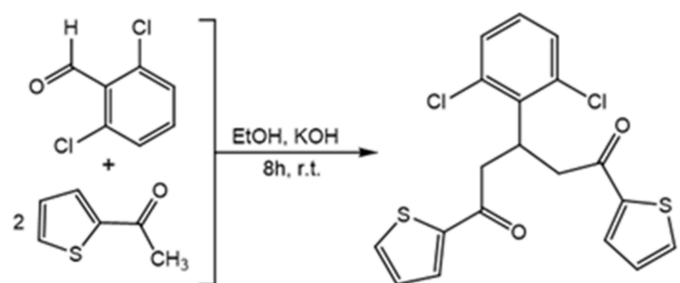


Figure 6

The reaction scheme of the title compound.

SHELXL) as well as the restraints of the atomic displacement parameters (SIMU/RIGU instructions of *SHELXL*) were applied for the atoms of the two disorder thiophene rings (S1/C1–C4 and S2/C5–C8). Five outlier reflections (110, 020, 011, 021 and 121), affected by the incident beam-stop were omitted in the last cycles of the refinement.

Acknowledgements

The author's contributions are as follows. Conceptualization, AVG, MA and GMM; synthesis and X-ray analysis AVG; writing (review and editing of the manuscript) AVG and MA; funding acquisition, AVG; supervision, MA.

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supporting information

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Computing details

3-(2,6-Dichlorophenyl)-1,5-bis(thiophen-2-yl)pentane-1,5-dione

Crystal data

$C_{19}H_{14}Cl_2O_2S_2$

$M_r = 409.32$

Tetragonal, $P4_2/n$

$a = 18.853(3) \text{ \AA}$

$c = 10.235(4) \text{ \AA}$

$V = 3637.9(18) \text{ \AA}^3$

$Z = 8$

$F(000) = 1680$

$D_x = 1.495 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 9964 reflections

$\theta = 2.5\text{--}26.4^\circ$

$\mu = 0.60 \text{ mm}^{-1}$

$T = 150 \text{ K}$

Plate, yellow

$0.36 \times 0.23 \times 0.23 \text{ mm}$

Data collection

Bruker APEXII CCD

diffractometer

φ and ω scans

34717 measured reflections

3693 independent reflections

3195 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\text{max}} = 26.3^\circ$, $\theta_{\text{min}} = 3.1^\circ$

$h = -23 \rightarrow 23$

$k = -23 \rightarrow 23$

$l = -7 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.074$

$S = 1.04$

3693 reflections

300 parameters

608 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0383P)^2 + 1.3968P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.54327 (7)	0.45619 (7)	0.17318 (14)	0.0213 (3)	
C2	0.5388 (3)	0.3969 (4)	0.0932 (9)	0.0290 (13)	0.686 (2)
H2	0.495095	0.375484	0.069437	0.035*	0.686 (2)
C3	0.6049 (2)	0.3716 (4)	0.0506 (10)	0.0286 (9)	0.686 (2)
H3	0.611278	0.331904	−0.005434	0.034*	0.686 (2)
C4	0.6592 (2)	0.4118 (4)	0.1008 (8)	0.0250 (9)	0.686 (2)
H4	0.708035	0.402763	0.084738	0.030*	0.686 (2)
S1	0.62866 (5)	0.48026 (8)	0.19615 (17)	0.0256 (2)	0.686 (2)
C2X	0.6159 (4)	0.4696 (6)	0.1882 (14)	0.0295 (19)	0.314 (2)
H2X	0.634291	0.506938	0.240594	0.035*	0.314 (2)
C3X	0.6587 (4)	0.4224 (8)	0.1180 (17)	0.0252 (18)	0.314 (2)
H3X	0.708972	0.424644	0.114403	0.030*	0.314 (2)
C4X	0.6185 (4)	0.3724 (9)	0.055 (2)	0.0264 (19)	0.314 (2)
H4X	0.637537	0.334632	0.004448	0.032*	0.314 (2)
S1X	0.52868 (18)	0.3865 (2)	0.0791 (5)	0.0254 (6)	0.314 (2)
C5	0.24771 (7)	0.44532 (8)	0.57830 (13)	0.0235 (3)	
C6	0.2346 (4)	0.3742 (2)	0.5597 (6)	0.0396 (11)	0.787 (2)
H6	0.256125	0.347344	0.491950	0.048*	0.787 (2)
C7	0.1870 (3)	0.3451 (2)	0.6494 (6)	0.0408 (10)	0.787 (2)
H7	0.173350	0.296622	0.650717	0.049*	0.787 (2)
C8	0.1625 (4)	0.3950 (2)	0.7348 (7)	0.0349 (9)	0.787 (2)
H8	0.129320	0.385120	0.802326	0.042*	0.787 (2)
S2	0.19795 (5)	0.47731 (4)	0.70732 (9)	0.0295 (2)	0.787 (2)
C6X	0.2054 (8)	0.4615 (5)	0.6847 (12)	0.036 (2)	0.213 (2)
H6X	0.204915	0.506882	0.724860	0.043*	0.213 (2)
C7X	0.1634 (15)	0.4052 (8)	0.728 (2)	0.035 (2)	0.213 (2)
H7X	0.132681	0.407117	0.801252	0.043*	0.213 (2)
C8X	0.1725 (10)	0.3468 (7)	0.650 (2)	0.033 (2)	0.213 (2)
H8X	0.145785	0.304283	0.657880	0.040*	0.213 (2)
S2X	0.2382 (4)	0.3595 (2)	0.5347 (6)	0.0376 (10)	0.213 (2)
C9	0.35448 (7)	0.51320 (7)	0.28580 (13)	0.0212 (3)	
H9	0.373277	0.559825	0.316950	0.025*	
C10	0.41125 (7)	0.48186 (8)	0.19393 (14)	0.0244 (3)	
H10A	0.403534	0.430095	0.186030	0.029*	
H10B	0.405555	0.502934	0.105964	0.029*	
C11	0.48646 (7)	0.49511 (7)	0.24127 (14)	0.0220 (3)	
C12	0.34579 (7)	0.46603 (8)	0.40816 (14)	0.0245 (3)	
H12A	0.330170	0.418175	0.380605	0.029*	
H12B	0.392426	0.461014	0.451647	0.029*	
C13	0.29274 (7)	0.49555 (7)	0.50549 (13)	0.0226 (3)	
C14	0.28523 (7)	0.52898 (8)	0.21384 (13)	0.0218 (3)	
C15	0.24264 (8)	0.47786 (8)	0.15209 (15)	0.0277 (3)	
C16	0.18201 (8)	0.49449 (10)	0.08089 (16)	0.0355 (4)	
H16	0.155454	0.457985	0.039652	0.043*	
C17	0.16059 (8)	0.56445 (10)	0.07042 (16)	0.0376 (4)	

H17	0.119155	0.576165	0.022198	0.045*
C18	0.19967 (8)	0.61723 (10)	0.13036 (15)	0.0332 (4)
H18	0.185163	0.665370	0.124235	0.040*
C19	0.26051 (8)	0.59915 (8)	0.19980 (14)	0.0259 (3)
O1	0.50021 (5)	0.53666 (6)	0.32983 (11)	0.0315 (3)
O2	0.28861 (6)	0.55928 (5)	0.52630 (10)	0.0312 (2)
Cl1	0.26457 (2)	0.38719 (2)	0.16007 (5)	0.04004 (12)
Cl2	0.30752 (2)	0.66987 (2)	0.26885 (4)	0.03587 (11)

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0217 (7)	0.0211 (7)	0.0212 (7)	0.0004 (5)	0.0025 (5)	0.0041 (5)
C2	0.027 (2)	0.031 (3)	0.028 (2)	−0.0061 (16)	0.0004 (16)	−0.0019 (16)
C3	0.0314 (17)	0.0242 (15)	0.0302 (18)	0.0018 (17)	0.005 (2)	0.0001 (13)
C4	0.0243 (16)	0.027 (2)	0.023 (2)	0.0107 (13)	0.0073 (13)	0.0000 (13)
S1	0.0162 (3)	0.0319 (5)	0.0287 (4)	−0.0003 (3)	−0.0004 (3)	−0.0022 (3)
C2X	0.033 (3)	0.029 (4)	0.027 (3)	−0.003 (3)	−0.002 (3)	0.005 (3)
C3X	0.024 (3)	0.026 (4)	0.026 (4)	−0.004 (2)	−0.003 (3)	0.005 (3)
C4X	0.021 (3)	0.028 (3)	0.030 (4)	0.007 (3)	0.012 (3)	−0.002 (3)
S1X	0.0266 (11)	0.0230 (10)	0.0266 (11)	−0.0035 (8)	0.0053 (8)	−0.0080 (7)
C5	0.0199 (7)	0.0310 (7)	0.0197 (7)	−0.0003 (5)	−0.0027 (5)	0.0011 (6)
C6	0.0379 (17)	0.048 (2)	0.033 (2)	0.0014 (17)	0.0022 (15)	−0.0013 (15)
C7	0.035 (2)	0.0426 (14)	0.0445 (17)	−0.0132 (13)	−0.0007 (15)	0.0033 (13)
C8	0.0265 (14)	0.0465 (18)	0.0317 (16)	−0.0119 (16)	0.0020 (12)	0.0101 (15)
S2	0.0254 (3)	0.0393 (4)	0.0238 (4)	−0.0022 (3)	0.0062 (2)	0.0010 (3)
C6X	0.035 (4)	0.046 (4)	0.027 (4)	0.004 (3)	−0.005 (3)	0.001 (3)
C7X	0.030 (4)	0.050 (4)	0.027 (4)	0.006 (4)	0.003 (4)	0.002 (4)
C8X	0.025 (5)	0.045 (4)	0.030 (4)	−0.010 (3)	0.004 (4)	0.006 (3)
S2X	0.0422 (16)	0.0377 (17)	0.033 (2)	−0.0115 (14)	0.0100 (13)	0.0022 (14)
C9	0.0193 (7)	0.0245 (7)	0.0198 (7)	0.0027 (5)	0.0013 (5)	0.0008 (6)
C10	0.0223 (7)	0.0292 (7)	0.0218 (7)	0.0038 (6)	0.0024 (6)	0.0007 (6)
C11	0.0243 (7)	0.0200 (7)	0.0218 (7)	0.0002 (5)	0.0040 (6)	0.0048 (6)
C12	0.0239 (7)	0.0263 (7)	0.0234 (7)	0.0054 (6)	0.0027 (6)	0.0036 (6)
C13	0.0212 (7)	0.0289 (7)	0.0176 (7)	0.0014 (6)	−0.0026 (5)	0.0015 (6)
C14	0.0199 (7)	0.0286 (7)	0.0169 (6)	0.0028 (6)	0.0038 (5)	0.0010 (6)
C15	0.0258 (7)	0.0347 (8)	0.0227 (7)	−0.0008 (6)	0.0053 (6)	−0.0018 (6)
C16	0.0231 (8)	0.0603 (11)	0.0230 (8)	−0.0085 (7)	0.0019 (6)	−0.0035 (8)
C17	0.0202 (7)	0.0684 (12)	0.0240 (8)	0.0082 (8)	0.0010 (6)	0.0069 (8)
C18	0.0276 (8)	0.0478 (10)	0.0242 (8)	0.0153 (7)	0.0052 (6)	0.0068 (7)
C19	0.0258 (7)	0.0316 (8)	0.0202 (7)	0.0054 (6)	0.0042 (6)	0.0003 (6)
O1	0.0285 (5)	0.0316 (6)	0.0345 (6)	−0.0019 (4)	0.0045 (5)	−0.0096 (5)
O2	0.0393 (6)	0.0266 (6)	0.0276 (6)	0.0004 (5)	0.0070 (5)	−0.0022 (4)
Cl1	0.0426 (2)	0.0314 (2)	0.0462 (3)	−0.00663 (16)	0.00020 (19)	−0.00862 (18)
Cl2	0.0449 (2)	0.02447 (19)	0.0383 (2)	0.00821 (16)	−0.00231 (18)	−0.00167 (16)

Geometric parameters (Å, °)

C1—C2	1.388 (5)	C6X—H6X	0.9500
C1—C2X	1.402 (7)	C7X—C8X	1.373 (7)
C1—C11	1.4734 (19)	C7X—H7X	0.9500
C1—S1X	1.652 (3)	C8X—S2X	1.725 (8)
C1—S1	1.6891 (16)	C8X—H8X	0.9500
C2—C3	1.404 (7)	C9—C14	1.5283 (19)
C2—H2	0.9500	C9—C10	1.5423 (19)
C3—C4	1.373 (4)	C9—C12	1.545 (2)
C3—H3	0.9500	C9—H9	1.0000
C4—S1	1.718 (4)	C10—C11	1.519 (2)
C4—H4	0.9500	C10—H10A	0.9900
C2X—C3X	1.400 (9)	C10—H10B	0.9900
C2X—H2X	0.9500	C11—O1	1.2257 (18)
C3X—C4X	1.370 (6)	C12—C13	1.517 (2)
C3X—H3X	0.9500	C12—H12A	0.9900
C4X—S1X	1.732 (7)	C12—H12B	0.9900
C4X—H4X	0.9500	C13—O2	1.2228 (17)
C5—C6	1.376 (5)	C14—C15	1.405 (2)
C5—C6X	1.384 (7)	C14—C19	1.410 (2)
C5—C13	1.4740 (19)	C15—C16	1.391 (2)
C5—S2X	1.688 (4)	C15—C11	1.7605 (16)
C5—S2	1.7285 (16)	C16—C17	1.384 (3)
C6—C7	1.396 (6)	C16—H16	0.9500
C6—H6	0.9500	C17—C18	1.382 (3)
C7—C8	1.365 (4)	C17—H17	0.9500
C7—H7	0.9500	C18—C19	1.392 (2)
C8—S2	1.713 (3)	C18—H18	0.9500
C8—H8	0.9500	C19—C12	1.7500 (16)
C6X—C7X	1.394 (9)		
C2—C1—C11	129.5 (3)	C6X—C7X—H7X	124.6
C2X—C1—C11	124.7 (4)	C7X—C8X—S2X	112.1 (6)
C2X—C1—S1X	111.7 (3)	C7X—C8X—H8X	124.0
C11—C1—S1X	123.42 (15)	S2X—C8X—H8X	124.0
C2—C1—S1	110.8 (3)	C5—S2X—C8X	91.7 (4)
C11—C1—S1	119.55 (11)	C14—C9—C10	111.94 (11)
C1—C2—C3	113.8 (4)	C14—C9—C12	114.34 (11)
C1—C2—H2	123.1	C10—C9—C12	110.33 (11)
C3—C2—H2	123.1	C14—C9—H9	106.6
C4—C3—C2	110.9 (4)	C10—C9—H9	106.6
C4—C3—H3	124.5	C12—C9—H9	106.6
C2—C3—H3	124.5	C11—C10—C9	112.97 (12)
C3—C4—S1	112.2 (3)	C11—C10—H10A	109.0
C3—C4—H4	123.9	C9—C10—H10A	109.0
S1—C4—H4	123.9	C11—C10—H10B	109.0
C1—S1—C4	92.23 (16)	C9—C10—H10B	109.0

C3X—C2X—C1	113.0 (5)	H10A—C10—H10B	107.8
C3X—C2X—H2X	123.5	O1—C11—C1	120.95 (13)
C1—C2X—H2X	123.5	O1—C11—C10	122.57 (13)
C4X—C3X—C2X	111.2 (6)	C1—C11—C10	116.47 (12)
C4X—C3X—H3X	124.4	C13—C12—C9	113.02 (11)
C2X—C3X—H3X	124.4	C13—C12—H12A	109.0
C3X—C4X—S1X	111.6 (6)	C9—C12—H12A	109.0
C3X—C4X—H4X	124.2	C13—C12—H12B	109.0
S1X—C4X—H4X	124.2	C9—C12—H12B	109.0
C1—S1X—C4X	92.4 (3)	H12A—C12—H12B	107.8
C6—C5—C13	131.2 (2)	O2—C13—C5	120.43 (13)
C6X—C5—C13	126.1 (4)	O2—C13—C12	121.12 (13)
C6X—C5—S2X	110.9 (4)	C5—C13—C12	118.42 (12)
C13—C5—S2X	122.91 (19)	C15—C14—C19	114.14 (13)
C6—C5—S2	110.4 (2)	C15—C14—C9	124.86 (13)
C13—C5—S2	118.34 (11)	C19—C14—C9	120.94 (13)
C5—C6—C7	114.0 (4)	C16—C15—C14	123.41 (15)
C5—C6—H6	123.0	C16—C15—C11	115.85 (12)
C7—C6—H6	123.0	C14—C15—C11	120.74 (11)
C8—C7—C6	111.6 (3)	C17—C16—C15	119.69 (15)
C8—C7—H7	124.2	C17—C16—H16	120.2
C6—C7—H7	124.2	C15—C16—H16	120.2
C7—C8—S2	112.7 (3)	C18—C17—C16	119.76 (14)
C7—C8—H8	123.6	C18—C17—H17	120.1
S2—C8—H8	123.6	C16—C17—H17	120.1
C8—S2—C5	91.23 (13)	C17—C18—C19	119.33 (16)
C5—C6X—C7X	114.1 (6)	C17—C18—H18	120.3
C5—C6X—H6X	122.9	C19—C18—H18	120.3
C7X—C6X—H6X	122.9	C18—C19—C14	123.66 (15)
C8X—C7X—C6X	110.8 (7)	C18—C19—C12	115.91 (12)
C8X—C7X—H7X	124.6	C14—C19—C12	120.42 (11)
C11—C1—C2—C3	−176.6 (6)	C2X—C1—C11—C10	169.3 (8)
S1—C1—C2—C3	−0.2 (10)	S1X—C1—C11—C10	−16.2 (3)
C1—C2—C3—C4	0.8 (13)	S1—C1—C11—C10	166.87 (13)
C2—C3—C4—S1	−1.1 (12)	C9—C10—C11—O1	−12.0 (2)
C2—C1—S1—C4	−0.3 (6)	C9—C10—C11—C1	169.19 (12)
C11—C1—S1—C4	176.5 (3)	C14—C9—C12—C13	−55.14 (16)
C3—C4—S1—C1	0.8 (8)	C10—C9—C12—C13	177.64 (12)
C11—C1—C2X—C3X	176.6 (11)	C6—C5—C13—O2	168.8 (4)
S1X—C1—C2X—C3X	1.5 (17)	C6X—C5—C13—O2	−9.2 (9)
C1—C2X—C3X—C4X	−2 (2)	S2X—C5—C13—O2	167.2 (3)
C2X—C3X—C4X—S1X	2 (2)	S2—C5—C13—O2	−8.30 (19)
C2X—C1—S1X—C4X	−0.2 (13)	C6—C5—C13—C12	−13.3 (5)
C11—C1—S1X—C4X	−175.4 (9)	C6X—C5—C13—C12	168.7 (9)
C3X—C4X—S1X—C1	−1.1 (19)	S2X—C5—C13—C12	−14.9 (4)
C13—C5—C6—C7	−178.8 (4)	S2—C5—C13—C12	169.61 (11)
S2—C5—C6—C7	−1.6 (7)	C9—C12—C13—O2	−38.13 (19)

C5—C6—C7—C8	1.4 (9)	C9—C12—C13—C5	143.98 (13)
C6—C7—C8—S2	−0.6 (9)	C10—C9—C14—C15	62.28 (18)
C7—C8—S2—C5	−0.3 (7)	C12—C9—C14—C15	−64.11 (18)
C6—C5—S2—C8	1.1 (5)	C10—C9—C14—C19	−114.87 (14)
C13—C5—S2—C8	178.7 (3)	C12—C9—C14—C19	118.75 (14)
C13—C5—C6X—C7X	174.6 (19)	C19—C14—C15—C16	1.2 (2)
S2X—C5—C6X—C7X	−2 (2)	C9—C14—C15—C16	−176.13 (13)
C5—C6X—C7X—C8X	−2 (4)	C19—C14—C15—C11	−179.44 (10)
C6X—C7X—C8X—S2X	6 (4)	C9—C14—C15—C11	3.24 (19)
C6X—C5—S2X—C8X	4.5 (13)	C14—C15—C16—C17	−1.1 (2)
C13—C5—S2X—C8X	−172.4 (9)	C11—C15—C16—C17	179.50 (12)
C7X—C8X—S2X—C5	−6 (2)	C15—C16—C17—C18	0.2 (2)
C14—C9—C10—C11	154.89 (12)	C16—C17—C18—C19	0.5 (2)
C12—C9—C10—C11	−76.57 (15)	C17—C18—C19—C14	−0.3 (2)
C2—C1—C11—O1	164.1 (6)	C17—C18—C19—C12	178.53 (12)
C2X—C1—C11—O1	−9.6 (8)	C15—C14—C19—C18	−0.5 (2)
S1X—C1—C11—O1	164.9 (3)	C9—C14—C19—C18	176.96 (13)
S1—C1—C11—O1	−12.0 (2)	C15—C14—C19—C12	−179.27 (10)
C2—C1—C11—C10	−17.0 (6)	C9—C14—C19—C12	−1.84 (18)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C3—H3 $\cdots$ O2 ⁱ	0.95	2.48	3.238 (8)	136
C9—H9 $\cdots$ Cl2	1.00	2.47	3.0884 (18)	120
C9—H9 $\cdots$ O1	1.00	2.44	2.819 (2)	102
C10—H10 <i>A</i> $\cdots$ Cl1	0.99	2.75	3.3095 (19)	116
C10—H10 <i>A</i> $\cdots$ S1X	0.99	2.73	3.085 (4)	102
C12—H12 <i>A</i> $\cdots$ Cl1	0.99	2.64	3.317 (2)	126
C12—H12 <i>A</i> $\cdots$ S2X	0.99	2.59	3.135 (6)	114
C4—H4 $\cdots$ Cg5 ⁱⁱ	0.95	2.83	3.431 (7)	122
C10—H10 <i>B</i> $\cdots$ Cg1 ⁱⁱ	0.99	2.72	3.704 (4)	171
C10—H10 <i>B</i> $\cdots$ Cg3 ⁱⁱ	0.99	2.74	3.720 (6)	170
C3X—H3X $\cdots$ Cg5 ⁱⁱ	0.95	2.97	3.528 (14)	119
C8X—H8X $\cdots$ Cg2 ⁱⁱⁱ	0.95	2.91	3.699 (17)	141
C8X—H8X $\cdots$ Cg4 ⁱⁱⁱ	0.95	2.97	3.743 (18)	139

Symmetry codes: (i) *y*, −*x*+1/2, −*z*+1/2; (ii) −*x*+1, −*y*+1, −*z*; (iii) *x*−1/2, *y*−1/2, −*z*+1.