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Crystal structure and Hirshfeld surface analysis of (*E*)-3-(2-chlorophenyl)-1-(2,5-dichlorothiophen-3-yl)prop-2-en-1-one

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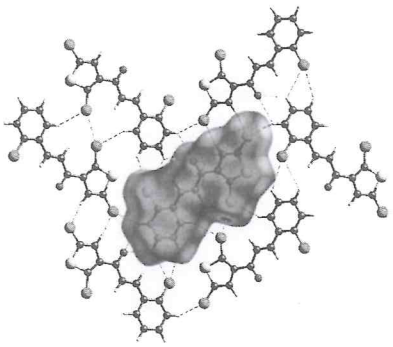
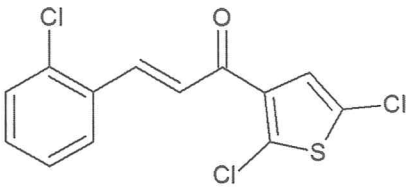
The molecular structure of the title compound, $C_{13}H_7Cl_3OS$, consists of a 2,5-dichlorothiophene ring and a 2-chlorophenyl ring linked *via* a prop-2-en-1-one spacer. The dihedral angle between the 2,5-dichlorothiophene and 2-chlorophenyl rings is 9.69 (12)°. The molecule has an *E* configuration about the C=C bond and the carbonyl group is *syn* with respect to the C=C bond. The molecular conformation is stabilized by two intramolecular C—H···Cl contacts and one intramolecular C—H···O contact, forming *S*(5)*S*(5)*S*(6) ring motifs. In the crystal, the molecules are linked along the *a*-axis direction through van der Waals forces and along the *b* axis by face-to-face π-stacking between the thiophene rings and between the benzene rings of neighbouring molecules, forming corrugated sheets lying parallel to the *bc* plane. The intermolecular interactions in the crystal packing were further analysed using Hirshfeld surface analysis, which indicates that the most significant contacts are Cl···H/ H···Cl (28.6%), followed by C···H/H···C (11.9%), C···C (11.1%), H···H (11.0%), Cl···Cl (8.1%), O···H/H···O (8.0%) and S···H/H···S (6.6%).

1. Chemical context

Chalcone is an aromatic ketone that forms a central core for a variety of biological compounds, which are collectively known as chalcones. Chalcones, considered to be the precursors of flavonoids and isoflavonoids, are abundant in edible plants. They consist of open-chain flavonoids in which the two aromatic rings are joined by a three-carbon α,β-unsaturated carbonyl system. Chalcone was first isolated from Chinese liquorice (Glycyrrhizae inflata) (Rao *et al.*, 2004). It has a 1,3-diaryl-1-one skeletal system, which was recognized as the main pharmacophore for chalcones. The introduction of various substituents into the two aryl rings is also an area of interest for investigating structure–activity relationships. Chalcones are coloured compounds because of the presence of the –CO—CH=CH– chromophore. Different methods have been reported for the preparation of chalcones, the most convenient method being the Claisen-Schimdt condensation of equimolar quantities of an aryl methylketone with an aryl aldehyde in the presence of alcoholic alkali. The synthesis and antimicrobial evaluation of new chalcones containing a



2,5-dichlorothiophene moiety have been reported (Tomar *et al.*, 2007). Recently, chalcones have been used in the field of materials science as non-linear optical devices (Raghavendra *et al.*, 2017; Chandra Shekhara Shetty *et al.*, 2016). The crystal structures of (*E*)-1-(2,5-dichloro-3-thienyl)-3-[4-(dimethylamino)phenyl]prop-2-en-1-one (Dutkiewicz *et al.*, 2010), (2*E*)-1-(2,5-dichloro-3-thienyl)-3-(6-methoxy-2-naphthyl)prop-2-en-1-one (Jasinski *et al.*, 2010), (*E*)-1-(2,5-dichloro-3-thienyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (Harrison *et al.*, 2010*a*), (*E*)-3-(2-chloro-4-fluorophenyl)-1-(2,5-dichlorothiophen-3-yl)prop-2-en-1-one (Sanjeeva Murthy *et al.*, 2018) and (2*E*)-3-(2,4-dichlorophenyl)-1-(2,5-dichlorothiophen-3-yl)-prop-2-en-1-one (Murthy *et al.*, 2018) have previously been reported.



As part of our studies in this area, we report the crystal and molecular structures of the title compound.

2. Structural commentary

As shown in Fig. 1, the title compound is constructed from two aromatic rings (2,5-dichlorothiophene and terminal 2-chlorophenyl rings), which are linked by a C=C—C(=O)—C enone bridge. The C3—C4—C5—O1 and O1—C5—C6—C7 torsion angles about the enone bridge are 6.7 (4) and 4.3 (4)°, respectively, probably as a result of steric repulsion between the chlorine atoms of adjacent molecules. The dihedral angle between the 2-chlorothiophene and 2,4-dichlorophenyl rings is 9.69 (12)°. The bond lengths and angles in the title compound are comparable with those in the related compounds (2*E*)-3-(2,4-dichlorophenyl)-1-(2,5-dichlorothiophen-3-yl)prop-2-en-1-one (Sanjeeva Murthy *et al.*, 2018), (*E*)-3-(3,4-dimethoxyphenyl)-1-(1-hydroxynaphthalen-2yl)prop-2-en-1-one (Ezhilarasi *et al.*, 2015), (*E*)-1-(3-bromophenyl)-3-(3,4-dimethoxyphenyl)-prop-2-en-1-one (Escobar *et al.*, 2012) and (*E*)-3-(2-bromophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one (Li *et al.*, 2012). The molecular conformation is stabilized by two intramolecular C—H···Cl contacts and one intramolecular C—H···O contact (Table 1), forming *S*(5)*S*(5)*S*(6) ring motifs.

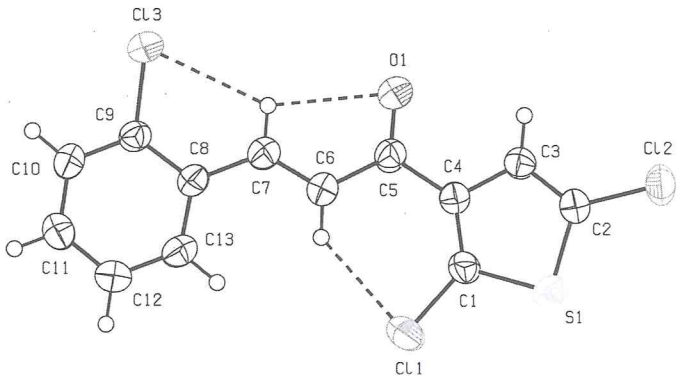


Figure 1
The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level. Intramolecular hydrogen bonds (Table 1) are shown as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6*A*···Cl1	0.93	2.54	3.245 (3)	133
C7—H7*A*···Cl3	0.93	2.59	3.043 (3)	110
C7—H7*A*···O1	0.93	2.46	2.790 (3)	101

Table 2
Summary of short interatomic contacts (Å) in the title compound.

Contact	distance	Symmetry operation
Cl1···Cl1	3.2876 (11)	$2-x, 1-y, 1-z$
Cl2···C10	3.618 (3)	$2-x, \frac{1}{2}+y, \frac{3}{2}-z$
Cl2···H10*A*	3.06	$1-x, \frac{1}{2}+y, \frac{3}{2}-z$
H3*A*···Cl2	3.01	$2-x, 1-y, 2-z$
H3*A*···Cl2	2.98	$3-x, 1-y, 2-z$
Cl3···H12*A*	3.11	$x, \frac{1}{2}-y, \frac{1}{2}+z$
C6···C7	3.504 (4)	$1+x, y, z$
O1···H10*A*	2.85	$1+x, \frac{1}{2}-y, \frac{1}{2}+z$

3. Supramolecular features

In the crystal, conventional hydrogen bonds are not observed. Molecules are linked along the *a*-axis direction through van der Waals forces. π-stacking is observed between thiophene rings (S1/C1–C4, centroid *Cg*1) of adjacent molecules in alternating sheets along the [100] direction [$Cg1\cdots Cg1^{i,ii}$: centroid–centroid distance = 3.902 (2) Å, shortest perpendicular distance for the centroid of one ring to the plane of the other = 3.597 (1) Å, ring-centroid offset = 1.512 Å; symmetry codes: (i) $-1+x, y, z$; (ii) $1+x, y, z$] and between the benzene rings (C8–C13, centroid *Cg*2) of the same molecules [$Cg2\cdots Cg2^{i,ii}$: centroid–centroid distance = 3.902 (2) Å,

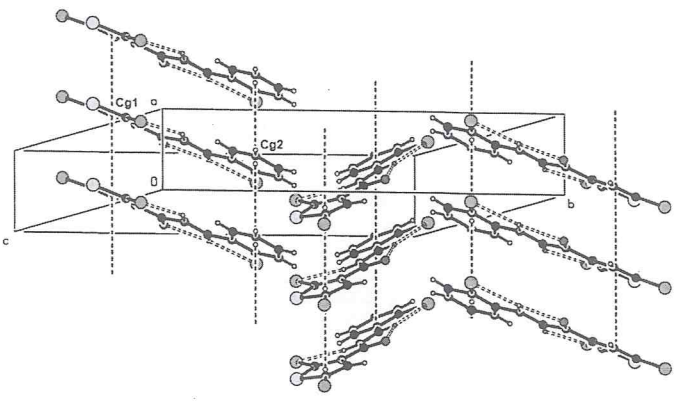


Figure 2
View along the *b*-axis direction of the zigzag sheets lying parallel to (011). π-stacking is observed between the thiophene rings (centroid *Cg*1) of adjacent molecules in alternating sheets along the [100] direction and between the benzene rings (centroid *Cg*2) of the same molecules.

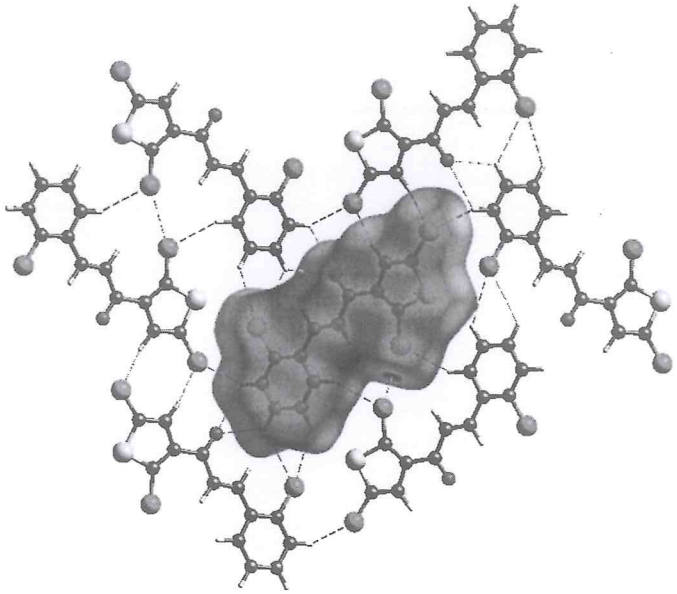


Figure 3
Hirshfeld surface mapped d_{norm} showing the intra- and intermolecular C—H···Cl and C—H···O hydrogen-bonded contacts.

shortest perpendicular distance = 3.482 (1) Å, offset = 1.760 Å]. The molecules are packed into corrugated sheets lying parallel to (011) (Figs. 2 and 3). Details of Cl···H and O···H contacts are given in Table 2.

4. Hirshfeld surface analysis

Hirshfeld surfaces and fingerprint plots were generated for the title compound using *CrystalExplorer* (McKinnon *et al.*, 2007). Hirshfeld surfaces enable the visualization of intermolecular interactions by using different colours and colour intensity to represent short or long contacts and indicate the relative strength of the interactions. The overall two-dimensional fingerprint plot for the title compound and those delineated into Cl···H/H···Cl, C···H/H···C, C···C, H···H, Cl···Cl, O···H/H···O and S···H/H···S contacts are illustrated in Fig. 4; the percentage contributions from the different interatomic contacts to the Hirshfeld surfaces are as follows: Cl···H/H···Cl (28.6%), C···H/H···C (11.9%), C···C (11.1%), H···H (11.0%), Cl···Cl (8.1%), O···H/H···O (8.0%) and S···H/H···S (6.6%). The contributions of the other weak intermolecular contacts to the Hirshfeld surfaces are listed in Table 3.

The C—H···Cl interactions appear as two distinct spikes in the fingerprint plot [Fig. 4(*b*)] with $d_e + d_i \simeq 2.85$ Å [d_e and d_i represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively]. The C···H/H···C interactions are shown in Fig. 4(*c*). The scattered points show the van der Waals contacts and π–π stacking interactions. The interatomic C···C contacts appear as an arrow-shaped distribution of points in Fig. 4(*d*), with the vertex at $d_e = d_i = 1.75$ Å. The C···C contacts reflect π–π interactions between the aromatic rings. The H···H interactions are reflected in Fig. 4(*e*) as

Table 3
Percentage contributions of interatomic contacts to the Hirshfeld surface for the compound.

Contact	Percentage contribution
Cl···H/H···Cl	28.6
C···H/H···C	11.9
C···C	11.1
H···H	11.0
Cl···Cl	8.1
O···H/H···O	8.0
S···H/H···S	6.6
C···Cl/Cl···C	4.7
S···Cl/Cl···S	4.1
S···C/C···S	2.1
O···C/C···O	1.6
O···Cl/Cl···O	1.0
S···S	0.8
O···O	0.3

widely scattered points of high density due to the large hydrogen content of the molecule. The split spike with the tip at $d_e = d_i \simeq 1.3$ Å is due to the short interatomic H···H contacts. Cl···Cl contacts [Fig. 4(*f*)] are disfavoured when the number of H atoms on the molecular surface is large because of competition with the more attractive H···Cl contacts. Cl···Cl contacts from a parallel alignment of C—Cl bonds

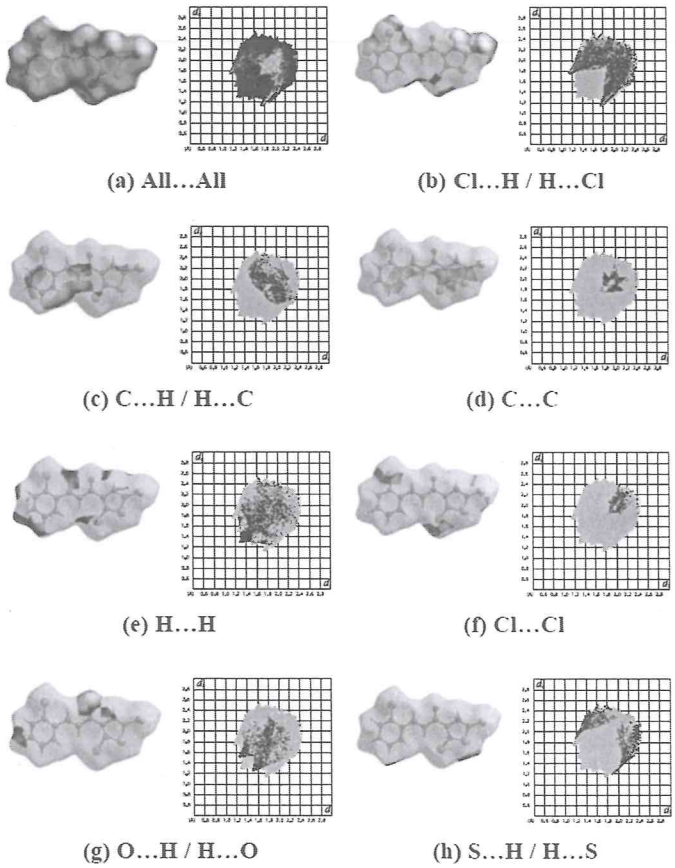


Figure 4
The two-dimensional fingerprint plots for the title compound, showing (*a*) all interactions, and delineated into (*b*) Cl···H/H···Cl, (*c*) C···H/H···C, (*d*) C···C, (*e*) H···H, (*f*) Cl···Cl, (*g*) O···H/H···O and (*h*) S···H/H···S interactions.

[C1—Cl1···Cl1^{iii}, and C2—Cl2···C10^{iv}; symmetry codes: (iii) $2-x, 1-y, 1-z$; (iv) $2-x, \frac{1}{2}+y, \frac{3}{2}-z$] may be indicated. They are known in the literature as type-I halogen–halogen interactions (Bui *et al.*, 2009), with both C—Cl···Cl angles equal to one another. In the present case, these angles are close to 165°. The H···O/O···H contacts [Fig. 4(*g*)] also have a symmetrical distribution of points, with two pairs of thin and thick edges at $d_e + d_i \simeq 2.75$ Å. The S···H contacts shown in Fig. 4(*h*) are contracted to a much lesser degree.

The large number of Cl···H/H···Cl, C···H/H···C, C···C, H···H, Cl···Cl, O···H/H···O and S···H/H···S interactions suggest that van der Waals interactions and hydrogen bonding play the major roles in the crystal packing (Hathwar *et al.*, 2015).

5. Database survey

The closest related compounds with the same skeleton and containing a similar bis-chalcone moiety to the title compound but with different substituents on the aromatic rings are: (2*E*)-1-(5-chlorothiophen-2-yl)-3-(4-ethylphenyl)prop-2-en-1-one [(I); Naik *et al.*, 2015], (2*E*)-1-(5-bromothiophen-2-yl)-3-(4-ethylphenyl)prop- 2-en-1-one [(II); Naik *et al.*, 2015], (2*E*)-1-(5-chlorothiophen-2-yl)-3-(4-ethoxyphenyl)prop-2-en-1-one [(III); Naik *et al.*, 2015], (2*E*)-1-(5-bromothiophen-2-yl)-3-(4-ethoxyphenyl)prop-2-en-1-one [(IV); Naik *et al.*, 2015], (2*E*)-3-(4-bromophenyl)-1-(5-chlorothiophen-2-yl)prop-2-en-1-one [(V); Naik *et al.*, 2015], (2*E*)-1-(5-bromothiophen-2-yl)-3-(3-methoxyphenyl)prop-2-en-1-one [(VI); Naik *et al.*, 2015], (*E*)-1-(5-chlorothiophen-2-yl)-3-(*p*-tolyl)prop-2-en-1-one [(VII); Kumara *et al.*, 2017], (*E*)-1-(5-chlorothiophen-2-yl)-3-(2,4-dimethylphenyl) prop-2-en-1-one [(VIII); Naveen *et al.*, 2016], (2*E*)-1-(5-bromothiophen- 2-yl)-3-(2-chlorophenyl)prop-2-en-1-one [(IX); Anitha *et al.*, 2015], (2*E*)-1-[4-hydroxy-3-(morpholin-4-ylmethyl)phenyl]-3-(thiophen-2-yl)prop-2-en-1-one [(X); Yesilyurt *et al.*, 2018], (*E*)-1-(2-aminophenyl)-3-(thiophen-2-yl)prop-2-en-1-one [(XI); Chantrapromma *et al.*, 2013] and (2E)-3-(2,4-dichlorophenyl)-1-(2,5-dichlorothiophen- 3-yl)prop-2-en-1-one [(XII); Sanjeeva Murthy *et al.*, 2018]. In (I) and (II), the structures are isostructural in space group *P*1, while (III) and (IV) are isostructural in space group $P2_1/c$. There are no hydrogen bonds of any kind in the structures of compounds (I) and (II), but in the structures of compounds (III) and (IV), the molecules are linked into *C*(7) chains by means of C—H···O hydrogen bonds. In (V), there are again no hydrogen bonds nor any π–π stacking interactions but in (VI), the molecules are linked into *C*(5) chains by C—H···O hydrogen bonds. In each of compounds (I)–(VI), the molecular skeletons are close to planarity, and there are short halogen–halogen contacts in the structures of compounds (II) and (V) and a short Br···O contact in the structure of compound (VI). In (VII), the molecule is non-planar, with a dihedral angle of 22.6 (2)° between the aromatic rings. The molecules are linked by pairs of C—H···π interactions, forming inversion dimers. There are no other significant intermolecular interactions present. In (VIII), the molecule is nearly planar, the dihedral angle between the thiophene and phenyl rings being 9.07 (8)°. The molecules are linked via weak C—H···O and C—H···S hydrogen bonds, forming chains propagating along the *c*-axis direction. In (IX), the thienyl ring is not coplanar with the benzene ring, their planes forming a dihedral angle of 13.2 (4)°. In the crystal, molecules stack along the *a*-axis direction, with the interplanar separation between the thienyl rings and between the benzene rings being 3.925 (6) Å. In (X), the thiophene ring forms a dihedral angle of 26.04 (9)° with the benzene ring. The molecular conformation is stabilized by an O—H···N hydrogen bond. The molecules are connected through C—H···O hydrogen bonds, forming wave-like layers parallel to the *ab* plane, which are further linked into a three-dimensional network by C—H···π interactions. In (XI), the molecule is almost planar with a dihedral angle of 3.73 (8)° between the phenyl and thiophene rings. An intramolecular N—H···O hydrogen bond generates an *S*(6) ring motif. Adjacent molecules are linked into dimers in an anti-parallel face-to-face manner by pairs of C—H···O interactions. Neighbouring dimers are further linked into chains along the *c*-axis direction by N—H···N hydrogen bonds. In (XII), the dihedral angle between the thiophene and benzene rings increases to12.24 (15)°. The molecular conformation is stabilized by intramolecular C—H···Cl contacts, forming *S*(6) and *S*(5) ring motifs. In the crystal, the molecules are linked through face-to-face π-stacking between the thiophene rings and the benzene rings of the molecules into zigzag sheets lying parallel to the *bc* plane.

6. Synthesis and crystallization

The title compound was synthesized by a reported procedure (Kumar *et al.*, 2013*a*,*b*). 1-(2,5-Dichlorothiophen-3-yl)ethanone (0.01 mol) (Harrison *et al.*, 2010*b*) and 2-chlorobenzaldehyde (0.01 mol) were dissolved in 20 ml of methanol. A catalytic amount of NaOH was added to the solution dropwise with vigorous stirring. The reaction mixture was stirred for about 4 h at room temperature. The formed crude products were filtered, washed successively with distilled water and recrystallized from methanol. The melting point (352–363 K) was determined using a Stuart Scientific (UK) apparatus.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. H atoms were positioned geometrically and refined using riding model, with C—H = 0.93–0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C-methyl).

Acknowledgements

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Table 4
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_7Cl_3OS$
M_r	317.60
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	294
a, b, c (Å)	3.9017 (6), 22.038 (3), 15.127 (2)
β (°)	96.998 (3)
V (Å^3)	1291.0 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.85
Crystal size (mm)	0.56 × 0.10 × 0.06
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 2007)
T_{min}, T_{max}	0.907, 0.953
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10683, 2669, 1977
R_{int}	0.039
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.630
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.099, 1.08
No. of reflections	2669
No. of parameters	163
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.32

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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Crystal structure and Hirshfeld surface analysis of (*E*)-3-(2-chlorophenyl)-1-(2,5-dichlorothiophen-3-yl)prop-2-en-1-one

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Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

(*E*)-3-(2-chlorophenyl)-1-(2,5-dichlorothiophen-3-yl)prop-2-en-1-one

Crystal data

$C_{13}H_7Cl_3OS$
$M_r = 317.60$
Monoclinic, $P2_1/c$
$a = 3.9017$ (6) Å
$b = 22.038$ (3) Å
$c = 15.127$ (2) Å
$\beta = 96.998$ (3)°
$V = 1291.0$ (3) Å^3
$Z = 4$
$F(000) = 640$
$D_x = 1.634$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2207 reflections
$\theta = 2.7$–$23.3°$
$\mu = 0.85$ mm^{-1}
$T = 294$ K
Needle, colourless
0.56 × 0.10 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2007)
$T_{min} = 0.907$, $T_{max} = 0.953$
10683 measured reflections
2669 independent reflections
1977 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 26.6°$, $\theta_{min} = 1.6°$
$h = -4 \rightarrow 4$
$k = -25 \rightarrow 27$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.099$
$S = 1.08$
2669 reflections
163 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0397P)^2 + 0.3125P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	1.19136 (18)	0.57814 (3)	0.76052 (4)	0.0475 (2)
O1	0.7421 (6)	0.37898 (9)	0.81944 (13)	0.0729 (7)
Cl1	0.8918 (3)	0.51901 (4)	0.59796 (4)	0.0767 (3)
Cl2	1.37875 (18)	0.58175 (3)	0.95615 (4)	0.0553 (2)
Cl3	0.18192 (19)	0.21002 (3)	0.65287 (4)	0.0547 (2)
C1	1.0021 (6)	0.51465 (11)	0.71070 (15)	0.0419 (6)
C2	1.2074 (6)	0.54379 (11)	0.86299 (15)	0.0405 (6)
C3	1.0742 (6)	0.48785 (11)	0.85791 (16)	0.0409 (6)
H3A	1.062770	0.463252	0.907420	0.049*
C4	0.9511 (6)	0.46945 (11)	0.76907 (15)	0.0368 (5)
C5	0.7905 (7)	0.40836 (12)	0.75452 (17)	0.0432 (6)
C6	0.6952 (7)	0.38479 (12)	0.66419 (17)	0.0498 (7)
H6A	0.750113	0.407394	0.615933	0.060*
C7	0.5354 (7)	0.33292 (12)	0.64948 (16)	0.0442 (6)
H7A	0.484449	0.311865	0.699544	0.053*
C8	0.4278 (6)	0.30426 (11)	0.56358 (16)	0.0383 (5)
C9	0.2658 (6)	0.24794 (11)	0.55730 (16)	0.0389 (6)
C10	0.1648 (7)	0.22027 (12)	0.47628 (17)	0.0478 (6)
H10A	0.058424	0.182449	0.474158	0.057*
C11	0.2228 (8)	0.24897 (13)	0.39919 (17)	0.0548 (7)
H11A	0.153881	0.230816	0.344393	0.066*
C12	0.3828 (8)	0.30463 (13)	0.40288 (18)	0.0568 (7)
H12A	0.423175	0.324019	0.350527	0.068*
C13	0.4827 (7)	0.33156 (12)	0.48330 (17)	0.0503 (7)
H13A	0.590560	0.369228	0.484531	0.060*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0609 (4)	0.0364 (4)	0.0465 (4)	−0.0055 (3)	0.0117 (3)	−0.0010 (3)
O1	0.1185 (19)	0.0477 (12)	0.0502 (11)	−0.0279 (12)	0.0013 (12)	0.0062 (10)
Cl1	0.1343 (8)	0.0581 (5)	0.0363 (4)	−0.0125 (5)	0.0043 (4)	0.0020 (3)
Cl2	0.0611 (4)	0.0495 (4)	0.0514 (4)	−0.0053 (3)	−0.0085 (3)	−0.0104 (3)
Cl3	0.0722 (5)	0.0451 (4)	0.0472 (4)	−0.0141 (3)	0.0086 (3)	0.0062 (3)
C1	0.0527 (15)	0.0377 (15)	0.0357 (12)	0.0016 (12)	0.0069 (11)	−0.0030 (10)
C2	0.0395 (13)	0.0417 (15)	0.0395 (13)	0.0005 (11)	0.0013 (10)	−0.0045 (11)
C3	0.0456 (14)	0.0375 (14)	0.0382 (12)	−0.0001 (11)	0.0001 (11)	0.0019 (11)
C4	0.0366 (12)	0.0349 (14)	0.0387 (12)	0.0033 (10)	0.0029 (10)	−0.0009 (10)
C5	0.0476 (14)	0.0356 (14)	0.0452 (14)	0.0002 (11)	0.0010 (11)	0.0000 (11)

C6	0.0636 (17)	0.0416 (16)	0.0434 (14)	−0.0111 (13)	0.0028 (12)	−0.0013 (12)
C7	0.0496 (15)	0.0376 (15)	0.0448 (13)	−0.0028 (12)	0.0031 (11)	0.0013 (11)
C8	0.0373 (13)	0.0332 (14)	0.0440 (13)	−0.0011 (10)	0.0037 (10)	0.0006 (10)
C9	0.0414 (13)	0.0340 (14)	0.0412 (13)	0.0004 (11)	0.0042 (10)	0.0023 (10)
C10	0.0518 (15)	0.0399 (15)	0.0508 (15)	−0.0081 (12)	0.0023 (12)	−0.0030 (12)
C11	0.0685 (19)	0.0525 (18)	0.0419 (14)	−0.0038 (15)	0.0011 (13)	−0.0041 (13)
C12	0.0710 (19)	0.0553 (19)	0.0434 (15)	−0.0100 (15)	0.0043 (13)	0.0090 (13)
C13	0.0586 (17)	0.0383 (15)	0.0532 (15)	−0.0082 (13)	0.0041 (13)	0.0068 (12)

Geometric parameters (Å, º)

S1—C1	1.713 (3)	C6—H6A	0.9300
S1—C2	1.719 (2)	C7—C8	1.460 (3)
O1—C5	1.210 (3)	C7—H7A	0.9300
Cl1—C1	1.710 (2)	C8—C9	1.391 (3)
Cl2—C2	1.704 (2)	C8—C13	1.395 (3)
Cl3—C9	1.735 (2)	C9—C10	1.382 (3)
C1—C4	1.362 (3)	C10—C11	1.369 (4)
C2—C3	1.336 (3)	C10—H10A	0.9300
C3—C4	1.430 (3)	C11—C12	1.374 (4)
C3—H3A	0.9300	C11—H11A	0.9300
C4—C5	1.490 (3)	C12—C13	1.367 (4)
C5—C6	1.467 (3)	C12—H12A	0.9300
C6—C7	1.308 (3)	C13—H13A	0.9300
C1—S1—C2	90.19 (12)	C6—C7—H7A	116.2
C4—C1—Cl1	130.5 (2)	C8—C7—H7A	116.2
C4—C1—S1	113.67 (18)	C9—C8—C13	116.2 (2)
Cl1—C1—S1	115.81 (14)	C9—C8—C7	121.7 (2)
C3—C2—Cl2	127.67 (19)	C13—C8—C7	122.0 (2)
C3—C2—S1	112.53 (18)	C10—C9—C8	122.2 (2)
Cl2—C2—S1	119.80 (15)	C10—C9—Cl3	117.64 (19)
C2—C3—C4	113.5 (2)	C8—C9—Cl3	120.21 (18)
C2—C3—H3A	123.2	C11—C10—C9	119.5 (2)
C4—C3—H3A	123.2	C11—C10—H10A	120.2
C1—C4—C3	110.1 (2)	C9—C10—H10A	120.2
C1—C4—C5	131.1 (2)	C10—C11—C12	119.9 (2)
C3—C4—C5	118.8 (2)	C10—C11—H11A	120.0
O1—C5—C6	121.3 (2)	C12—C11—H11A	120.0
O1—C5—C4	117.9 (2)	C13—C12—C11	120.2 (3)
C6—C5—C4	120.8 (2)	C13—C12—H12A	119.9
C7—C6—C5	122.0 (2)	C11—C12—H12A	119.9
C7—C6—H6A	119.0	C12—C13—C8	122.0 (2)
C5—C6—H6A	119.0	C12—C13—H13A	119.0
C6—C7—C8	127.5 (2)	C8—C13—H13A	119.0
C2—S1—C1—C4	0.4 (2)	O1—C5—C6—C7	4.3 (4)
C2—S1—C1—Cl1	177.73 (16)	C4—C5—C6—C7	−175.9 (2)

C1—S1—C2—C3	−0.3 (2)	C5—C6—C7—C8	−179.7 (2)
C1—S1—C2—Cl2	179.98 (16)	C6—C7—C8—C9	178.5 (3)
Cl2—C2—C3—C4	179.88 (19)	C6—C7—C8—C13	−1.2 (4)
S1—C2—C3—C4	0.2 (3)	C13—C8—C9—C10	0.1 (4)
Cl1—C1—C4—C3	−177.2 (2)	C7—C8—C9—C10	−179.6 (2)
S1—C1—C4—C3	−0.3 (3)	C13—C8—C9—Cl3	−179.60 (19)
Cl1—C1—C4—C5	1.6 (4)	C7—C8—C9—Cl3	0.7 (3)
S1—C1—C4—C5	178.5 (2)	C8—C9—C10—C11	−0.4 (4)
C2—C3—C4—C1	0.0 (3)	Cl3—C9—C10—C11	179.3 (2)
C2—C3—C4—C5	−178.9 (2)	C9—C10—C11—C12	0.5 (4)
C1—C4—C5—O1	−172.0 (3)	C10—C11—C12—C13	−0.3 (5)
C3—C4—C5—O1	6.7 (4)	C11—C12—C13—C8	0.0 (5)
C1—C4—C5—C6	8.1 (4)	C9—C8—C13—C12	0.1 (4)
C3—C4—C5—C6	−173.2 (2)	C7—C8—C13—C12	179.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6*A*···Cl1	0.93	2.54	3.245 (3)	133
C7—H7*A*···Cl3	0.93	2.59	3.043 (3)	110
C7—H7*A*···O1	0.93	2.46	2.790 (3)	101

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