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(*E*)-2-(3-Oxo-3-phenylprop-1-enyl)thiophene-3-carbaldehyde

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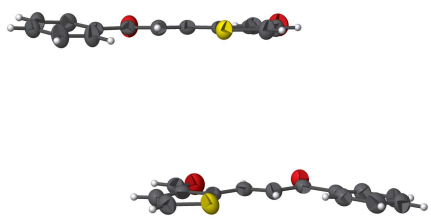
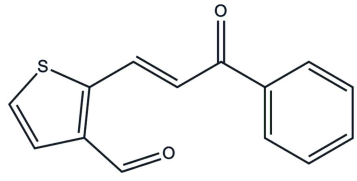
The title compound, $C_{14}H_{10}O_2S$, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. They have very similar conformations with the thiophene ring having an envelope conformation in both molecules. In molecule *A*, the benzene and thiophene rings makes a dihedral angle of 11.01 (9)°. The corresponding angle in molecule *B* is 9.58 (9)°. In the crystal, molecules are linked *via* pairs of C—H···O hydrogen bonds, forming dimers with an $R_2^2(18)$set-graph motif. The dimers are linked *via* C—H···O hydrogen bonds, forming slabs lying parallel to (100).

3D view



Chemical scheme



Structure description

Thiophenes are important heterocyclic compounds that are widely used as building blocks in many agrochemicals (Ansary & Omar, 2001). Thiophene possesses anti-microbial (Russel *et al.*, 1988), analgesic and anti-inflammatory (Chen *et al.*, 2008), antihypertensive (Mongevega *et al.*, 1980), anti diabetes mellitus (Abdelhamid *et al.*, 2009), gonadotropin releasing hormone antagonist (Sabins *et al.*, 1944) activities.

Fig. 1 shows the asymmertic unit consisting of the two independent molecules (*A* and *B*) of the title compound. The two molecules have the same geometrical parameters within the precision of the experiment. In molecule *A*, the benzene and thiophene rings make a dihedral angle of 11.01 (9)°, the corresponding angle in molecule *B* being 9.58 (9)°. In molecule *A*, the propane group assumes an extended conformation as can be seen from the C9—C8—C7—C6 torsion angle of 178.82 (15)° [in *B*, C19—C20—C21—C22 = 178.14 (15)°].

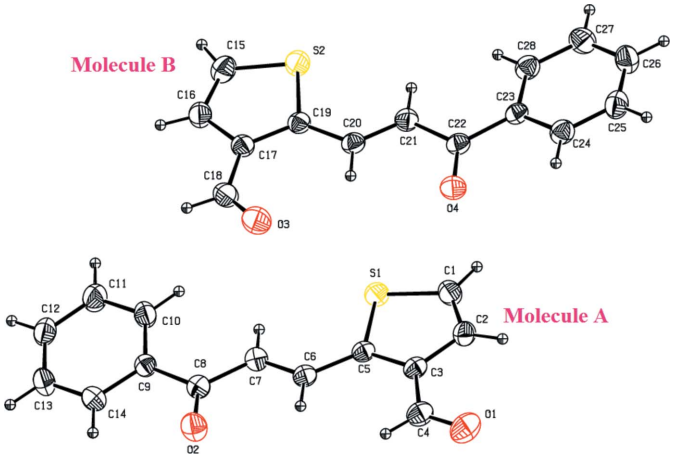


Figure 1
The molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

In the crystal, the *A* and *B* molecules are linked *via* pairs of C—H···O hydrogen bonds, forming dimers with an $R_2^2(18)$ ring motif. The dimers are linked *via* C—H···O hydrogen bonds, forming slabs lying parallel to (100) (Table 1, Fig. 2).

Synthesis and crystallization

To a stirred solution of (*E*)-3-(3-(bromomethyl)thiophen-2-yl)-1-phenylprop-2-en-1-one (1 g, 3.26 mmol) in dry DCM, *N*-methylmorpholine *N*-oxide (0.57 g, 4.87 mmol), was added and the reaction mixture was stirred at room temperature for 6 h. Removal of solvent followed by purification by column chromatographic (silica gel; 15% ethyl acetate in hexane) gave (*E*)-2-(3-oxo-3-phenylprop-1-enyl)-thiophene-3-carbaldehyde as a yellow solid (0.585 g, 74%). Crystals suitable for X-ray analysis were recrystallized by slow evaporation of a ethyl-acetate and methanol (1:1) solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

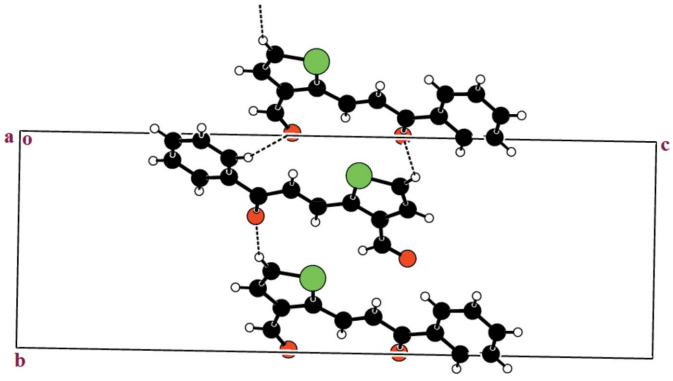


Figure 2
A view along the *b* axis of the partial crystal packing of the title compound. Hydrogen bonds are shown as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O4^{i}	0.93	2.49	3.125 (2)	126
C10—H1O···O3^{i}	0.93	2.59	3.466 (2)	158
C15—H15···O2^{ii}	0.93	2.44	3.287 (2)	152

Symmetry codes: (i) $x, y-1, z$; (ii) $x+1, y, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{10}O_2S$
M_r	242.28
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	273
a, b, c (Å)	10.4355 (4), 8.6955 (4), 25.7106 (9)
β (°)	95.420 (3)
V (Å^3)	2322.60 (16)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.26
Crystal size (mm)	0.23 × 0.17 × 0.11
Data collection	
Diffractometer	Bruker SMART APEXII area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.941, 0.971
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24652, 5662, 4287
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.688
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.116, 1.04
No. of reflections	5662
No. of parameters	307
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.21

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* and *SHELXTL* (Sheldrick 2008) and *SHELXL2014* (Sheldrick, 2015).

Acknowledgements

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full crystallographic data

IUCrData (2018). **3**, x180041 [https://doi.org/10.1107/S241431461800041X]

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(*E*)-2-(3-Oxo-3-phenylprop-1-enyl)thiophene-3-carbaldehyde

Crystal data

$C_{14}H_{10}O_2S$
M_r = 242.28
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 10.4355 (4) Å
b = 8.6955 (4) Å
c = 25.7106 (9) Å
β = 95.420 (3)°
V = 2322.60 (16) Å^3
Z = 8
$F(000)$ = 1008
D_x = 1.386 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5662 reflections
θ = 3.8–29.3°
μ = 0.26 mm^{-1}
T = 273 K
Colorless, yellow
0.23 × 0.17 × 0.11 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)
T_{min} = 0.941, T_{max} = 0.971
24652 measured reflections
5662 independent reflections
4287 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 29.3°, θ_{min} = 3.8°
h = −14→13
k = −11→11
l = −34→35

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.116
S = 1.04
5662 reflections
307 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.4625P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.
N and C-bound H atoms were positioned geometrically (C–H = 0.93–0.98 Å) and allowed to ride on their parent atoms, with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $1.2U_{eq}(C)$ for all other H atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.58222 (4)	0.17941 (5)	0.533986 (17)	0.05201 (13)
C7	0.41701 (15)	0.25005 (19)	0.42763 (6)	0.0456 (4)
H7	0.4819	0.1764	0.4300	0.055*
C5	0.45568 (14)	0.30548 (17)	0.52220 (6)	0.0406 (3)
C8	0.34529 (15)	0.28131 (18)	0.37647 (6)	0.0451 (4)
C6	0.39093 (15)	0.32474 (18)	0.47036 (6)	0.0439 (3)
H6	0.3246	0.3964	0.4666	0.053*
C9	0.38064 (14)	0.19583 (17)	0.32955 (6)	0.0424 (3)
O2	0.25734 (13)	0.37418 (15)	0.37253 (5)	0.0645 (3)
C3	0.43096 (14)	0.37960 (18)	0.56796 (6)	0.0432 (3)
O1	0.31113 (15)	0.55770 (17)	0.61230 (6)	0.0794 (4)
C1	0.60052 (17)	0.2255 (2)	0.59868 (7)	0.0564 (4)
H1	0.6627	0.1820	0.6225	0.068*
C4	0.33211 (17)	0.4959 (2)	0.57214 (8)	0.0555 (4)
H4	0.2820	0.5241	0.5418	0.067*
C2	0.51515 (16)	0.3316 (2)	0.61143 (7)	0.0516 (4)
H2	0.5117	0.3694	0.6451	0.062*
C14	0.29804 (17)	0.2032 (2)	0.28401 (7)	0.0561 (4)
H14	0.2242	0.2635	0.2831	0.067*
C12	0.43303 (19)	0.0341 (2)	0.24080 (7)	0.0599 (5)
H12	0.4499	−0.0218	0.2114	0.072*
C13	0.32441 (19)	0.1220 (3)	0.24013 (7)	0.0643 (5)
H13	0.2679	0.1272	0.2100	0.077*
C10	0.49070 (18)	0.1090 (2)	0.32932 (7)	0.0597 (5)
H10	0.5482	0.1041	0.3592	0.072*
C11	0.5166 (2)	0.0289 (3)	0.28494 (7)	0.0693 (6)
H11	0.5917	−0.0289	0.2852	0.083*
S2	1.06667 (4)	0.65651 (6)	0.463918 (18)	0.05982 (15)
O4	0.82888 (11)	0.99222 (14)	0.60156 (5)	0.0575 (3)
C19	0.93792 (14)	0.77858 (19)	0.46540 (6)	0.0434 (3)
C21	0.96631 (16)	0.8293 (2)	0.56034 (6)	0.0487 (4)
H21	1.0366	0.7632	0.5646	0.058*
C22	0.92485 (14)	0.91119 (18)	0.60602 (6)	0.0445 (4)
C20	0.90501 (15)	0.84822 (19)	0.51326 (6)	0.0450 (4)
H20	0.8337	0.9128	0.5109	0.054*
C23	1.00267 (14)	0.89828 (18)	0.65772 (6)	0.0428 (3)
C15	1.03801 (19)	0.6268 (2)	0.39857 (7)	0.0609 (5)
H15	1.0874	0.5631	0.3793	0.073*

C17	0.87663 (15)	0.79548 (19)	0.41555 (6)	0.0458 (4)
O3	0.71768 (14)	0.98696 (18)	0.42779 (6)	0.0736 (4)
C28	1.10468 (16)	0.7968 (2)	0.66730 (7)	0.0527 (4)
H28	1.1264	0.7309	0.6410	0.063*
C24	0.97212 (17)	0.9946 (2)	0.69792 (7)	0.0536 (4)
H24	0.9033	1.0624	0.6923	0.064*
C16	0.93469 (17)	0.7069 (2)	0.37799 (7)	0.0554 (4)
H16	0.9047	0.7042	0.3428	0.066*
C18	0.76643 (17)	0.8961 (2)	0.40051 (7)	0.0574 (4)
H18	0.7304	0.8888	0.3661	0.069*
C25	1.0425 (2)	0.9910 (2)	0.74601 (7)	0.0622 (5)
H25	1.0216	1.0571	0.7724	0.075*
C26	1.14275 (19)	0.8910 (3)	0.75513 (7)	0.0651 (5)
H26	1.1899	0.8884	0.7877	0.078*
C27	1.17403 (18)	0.7935 (2)	0.71576 (8)	0.0652 (5)
H27	1.2423	0.7251	0.7220	0.078*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0495 (2)	0.0542 (3)	0.0525 (2)	0.00988 (19)	0.00581 (18)	−0.00906 (19)
C7	0.0494 (8)	0.0405 (8)	0.0468 (8)	−0.0003 (7)	0.0038 (7)	0.0011 (7)
C5	0.0396 (7)	0.0359 (8)	0.0471 (8)	−0.0042 (6)	0.0088 (6)	−0.0017 (6)
C8	0.0483 (8)	0.0388 (8)	0.0483 (9)	−0.0022 (7)	0.0047 (7)	0.0037 (7)
C6	0.0429 (8)	0.0403 (8)	0.0489 (8)	−0.0021 (6)	0.0071 (6)	0.0000 (7)
C9	0.0455 (8)	0.0402 (8)	0.0413 (8)	−0.0055 (6)	0.0036 (6)	0.0057 (6)
O2	0.0710 (8)	0.0602 (8)	0.0610 (7)	0.0215 (7)	−0.0007 (6)	−0.0020 (6)
C3	0.0436 (8)	0.0388 (8)	0.0486 (8)	−0.0043 (6)	0.0114 (6)	−0.0043 (7)
O1	0.0856 (10)	0.0746 (10)	0.0820 (10)	0.0174 (8)	0.0291 (8)	−0.0217 (8)
C1	0.0542 (10)	0.0630 (11)	0.0507 (10)	0.0058 (9)	−0.0018 (8)	−0.0049 (8)
C4	0.0554 (10)	0.0504 (10)	0.0623 (11)	0.0028 (8)	0.0141 (8)	−0.0049 (8)
C2	0.0541 (9)	0.0555 (10)	0.0455 (9)	−0.0011 (8)	0.0065 (7)	−0.0081 (7)
C14	0.0516 (9)	0.0617 (11)	0.0535 (10)	0.0044 (8)	−0.0026 (8)	0.0039 (8)
C12	0.0702 (12)	0.0670 (12)	0.0436 (9)	−0.0065 (10)	0.0115 (8)	−0.0052 (8)
C13	0.0668 (12)	0.0818 (14)	0.0421 (9)	−0.0051 (10)	−0.0055 (8)	−0.0015 (9)
C10	0.0602 (11)	0.0753 (13)	0.0423 (9)	0.0153 (9)	−0.0015 (7)	−0.0011 (8)
C11	0.0700 (12)	0.0863 (15)	0.0523 (10)	0.0223 (11)	0.0089 (9)	−0.0025 (10)
S2	0.0575 (3)	0.0694 (3)	0.0529 (3)	0.0180 (2)	0.0068 (2)	0.0085 (2)
O4	0.0496 (7)	0.0635 (8)	0.0595 (7)	0.0141 (6)	0.0052 (5)	−0.0009 (6)
C19	0.0408 (8)	0.0437 (8)	0.0459 (8)	−0.0037 (6)	0.0059 (6)	0.0057 (7)
C21	0.0466 (8)	0.0512 (10)	0.0486 (9)	0.0057 (7)	0.0057 (7)	0.0009 (7)
C22	0.0415 (8)	0.0431 (9)	0.0498 (9)	−0.0017 (7)	0.0087 (6)	0.0036 (7)
C20	0.0403 (8)	0.0459 (9)	0.0497 (9)	−0.0028 (7)	0.0083 (6)	0.0043 (7)
C23	0.0411 (8)	0.0429 (9)	0.0457 (8)	−0.0023 (6)	0.0103 (6)	0.0035 (7)
C15	0.0667 (11)	0.0616 (12)	0.0563 (10)	0.0059 (9)	0.0152 (9)	−0.0034 (9)
C17	0.0431 (8)	0.0465 (9)	0.0477 (8)	−0.0064 (7)	0.0035 (7)	0.0042 (7)
O3	0.0663 (8)	0.0775 (10)	0.0759 (9)	0.0185 (7)	0.0006 (7)	0.0077 (8)
C28	0.0538 (9)	0.0519 (10)	0.0536 (10)	0.0064 (8)	0.0109 (8)	0.0027 (8)

C24	0.0546 (10)	0.0533 (10)	0.0538 (9)	0.0056 (8)	0.0097 (8)	−0.0010 (8)
C16	0.0587 (10)	0.0611 (11)	0.0462 (9)	−0.0068 (9)	0.0044 (8)	−0.0012 (8)
C18	0.0508 (10)	0.0638 (12)	0.0563 (10)	−0.0051 (9)	−0.0014 (8)	0.0083 (9)
C25	0.0721 (12)	0.0672 (12)	0.0479 (9)	−0.0041 (10)	0.0099 (9)	−0.0057 (9)
C26	0.0687 (12)	0.0758 (13)	0.0495 (10)	−0.0013 (10)	−0.0016 (8)	0.0077 (9)
C27	0.0587 (11)	0.0705 (13)	0.0653 (12)	0.0144 (9)	0.0009 (9)	0.0136 (10)

Geometric parameters (Å, º)

S1—C1	1.7040 (18)	S2—C15	1.6984 (19)
S1—C5	1.7209 (15)	S2—C19	1.7156 (16)
C7—C6	1.326 (2)	O4—C22	1.2211 (18)
C7—C8	1.476 (2)	C19—C17	1.385 (2)
C7—H7	0.9300	C19—C20	1.442 (2)
C5—C3	1.387 (2)	C21—C20	1.325 (2)
C5—C6	1.446 (2)	C21—C22	1.473 (2)
C8—O2	1.2195 (19)	C21—H21	0.9300
C8—C9	1.493 (2)	C22—C23	1.495 (2)
C6—H6	0.9300	C20—H20	0.9300
C9—C10	1.375 (2)	C23—C28	1.387 (2)
C9—C14	1.388 (2)	C23—C24	1.391 (2)
C3—C2	1.418 (2)	C15—C16	1.349 (3)
C3—C4	1.455 (2)	C15—H15	0.9300
O1—C4	1.203 (2)	C17—C16	1.416 (2)
C1—C2	1.345 (2)	C17—C18	1.468 (2)
C1—H1	0.9300	O3—C18	1.201 (2)
C4—H4	0.9300	C28—C27	1.381 (2)
C2—H2	0.9300	C28—H28	0.9300
C14—C13	1.380 (3)	C24—C25	1.378 (3)
C14—H14	0.9300	C24—H24	0.9300
C12—C11	1.365 (3)	C16—H16	0.9300
C12—C13	1.366 (3)	C18—H18	0.9300
C12—H12	0.9300	C25—C26	1.363 (3)
C13—H13	0.9300	C25—H25	0.9300
C10—C11	1.385 (3)	C26—C27	1.383 (3)
C10—H10	0.9300	C26—H26	0.9300
C11—H11	0.9300	C27—H27	0.9300
C1—S1—C5	92.04 (8)	C15—S2—C19	92.92 (9)
C6—C7—C8	121.44 (15)	C17—C19—C20	128.23 (15)
C6—C7—H7	119.3	C17—C19—S2	109.84 (12)
C8—C7—H7	119.3	C20—C19—S2	121.93 (12)
C3—C5—C6	128.31 (14)	C20—C21—C22	121.03 (15)
C3—C5—S1	110.35 (12)	C20—C21—H21	119.5
C6—C5—S1	121.34 (12)	C22—C21—H21	119.5
O2—C8—C7	120.67 (15)	O4—C22—C21	120.29 (15)
O2—C8—C9	120.28 (14)	O4—C22—C23	119.90 (14)
C7—C8—C9	119.04 (14)	C21—C22—C23	119.79 (14)

C7—C6—C5	126.31 (15)	C21—C20—C19	126.46 (15)
C7—C6—H6	116.8	C21—C20—H20	116.8
C5—C6—H6	116.8	C19—C20—H20	116.8
C10—C9—C14	118.31 (16)	C28—C23—C24	118.51 (15)
C10—C9—C8	123.18 (14)	C28—C23—C22	123.30 (15)
C14—C9—C8	118.52 (15)	C24—C23—C22	118.18 (14)
C5—C3—C2	112.39 (14)	C16—C15—S2	111.64 (14)
C5—C3—C4	125.12 (15)	C16—C15—H15	124.2
C2—C3—C4	122.48 (15)	S2—C15—H15	124.2
C2—C1—S1	112.55 (13)	C19—C17—C16	112.55 (15)
C2—C1—H1	123.7	C19—C17—C18	126.08 (16)
S1—C1—H1	123.7	C16—C17—C18	121.33 (16)
O1—C4—C3	124.18 (18)	C27—C28—C23	120.12 (17)
O1—C4—H4	117.9	C27—C28—H28	119.9
C3—C4—H4	117.9	C23—C28—H28	119.9
C1—C2—C3	112.67 (15)	C25—C24—C23	120.86 (17)
C1—C2—H2	123.7	C25—C24—H24	119.6
C3—C2—H2	123.7	C23—C24—H24	119.6
C13—C14—C9	120.65 (17)	C15—C16—C17	113.03 (16)
C13—C14—H14	119.7	C15—C16—H16	123.5
C9—C14—H14	119.7	C17—C16—H16	123.5
C11—C12—C13	119.55 (17)	O3—C18—C17	127.09 (17)
C11—C12—H12	120.2	O3—C18—H18	116.5
C13—C12—H12	120.2	C17—C18—H18	116.5
C12—C13—C14	120.35 (16)	C26—C25—C24	120.30 (18)
C12—C13—H13	119.8	C26—C25—H25	119.9
C14—C13—H13	119.8	C24—C25—H25	119.9
C9—C10—C11	120.53 (16)	C25—C26—C27	119.70 (17)
C9—C10—H10	119.7	C25—C26—H26	120.1
C11—C10—H10	119.7	C27—C26—H26	120.1
C12—C11—C10	120.59 (18)	C28—C27—C26	120.51 (17)
C12—C11—H11	119.7	C28—C27—H27	119.7
C10—C11—H11	119.7	C26—C27—H27	119.7

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O4^{i}	0.93	2.49	3.125 (2)	126
C10—H1O···O3^{i}	0.93	2.59	3.466 (2)	158
C15—H15···O2^{ii}	0.93	2.44	3.287 (2)	152

Symmetry codes: (i) x, $y-1$, z; (ii) $x+1$, y, z.