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Crystal structure of (2*E*)-1-(1-benzofuran-2-yl)-3-(2-bromophenyl)prop-2-en-1-one monohydrate

S. Satheeshchandra* and Nandakumar Shetty

Department of Physics, S. D. M College (Autonomous), Ujire 574 240, India.
*Correspondence e-mail: ssatheeshchandra@rediffmail.com

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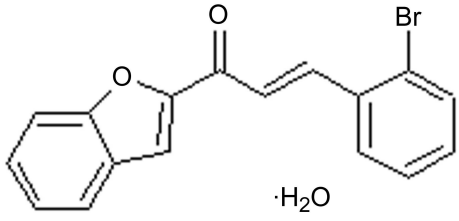
The title compound, $C_{17}H_{11}BrO_2\cdot H_2O$, crystallizes as a monohydrate in the chiral orthorhombic space group $P2_12_12_1$, and has non-linear optical (NLO) properties. The molecule has an *E* conformation about the C=C bond and is relatively planar with the benzofuran and bromophenyl rings being inclined to one another by 10.60 (14)°. In the crystal, the water molecule is linked to the organic molecule by O—H···O hydrogen bonds, forming an $R_2^2(7)$ ring motif while C—H···O hydrogen bonds lead to the formation of helices along the *b*-axis direction.

Keywords: crystal structure; benzofuran; chiral; NLO properties; hydrogen bonding.

CCDC reference: 1430039

1. Related literature

For background to chalcones and their biological and other properties, see: Choudary *et al.* (1999); Jayarama *et al.* (2013); Tomazela *et al.* (2000); Gu *et al.* (2008). For the crystal structure of a similar compound, see: Benmekhbi *et al.* (2009).



2. Experimental

2.1. Crystal data

$C_{17}H_{11}BrO_2\cdot H_2O$ M_r = 345.18
Orthorhombic, $P2_12_12_1$
a = 4.8614 (4) Å
b = 13.8220 (15) Å
c = 21.755 (2) Å
V = 1461.8 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.82 mm^{-1}
T = 296 K
0.40 × 0.30 × 0.25 mm

2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.399, T_{max} = 0.539
3636 measured reflections
3636 independent reflections
2134 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.102
S = 1.01
3636 reflections
196 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Absolute structure: Flack (1983), 1497 Friedel pairs
Absolute structure parameter: −0.011 (11)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*S*—H1*SA*···O1	0.96 (2)	2.37 (4)	3.181 (4)	142 (4)
O1*S*—H1*SB*···O2	0.95 (2)	2.11 (4)	2.928 (4)	143 (4)
C7—H7···O1*S*^{i}	0.93	2.32	3.229 (5)	164
C10—H10···O1*S*^{i}	0.93	2.45	3.375 (5)	174

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SU5214).

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supporting information

Acta Cryst. (2015). E**71**, o840–o841 [https://doi.org/10.1107/S2056989015018897]

Crystal structure of (2*E*)-1-(1-benzofuran-2-yl)-3-(2-bromophenyl)prop-2-en-1-one monohydrate

S. Satheeshchandra and Nandakumar Shetty

S1. Commentary

Chalcones are among the most abundant and ubiquitous group of natural products (Tomazela, *et al.*, 2000). Some of the chalcone derivatives shows high second-harmonic generation conversion efficiency (Gu *et al.*, 2008; Choudary *et al.*, 1999; Jayarama *et al.*, 2013). The title compound crystallizes in a non-centrosymmteric space group and exhibits interesting nonlinear optical properties.

In the title compound, Fig. 1, the benzofuran and bromophenyl groups are linked by a prop-2-en-1-one group. The benzofuran and bromophenyl rings are slightly non-planar with a dihedral angle of 10.60 (14) °. The torsion angle C7–C8–C9–O2 is 175.9 (4)° indicating that the O3 methoxy group is coplanar with the attached benzofuran ring. The C═C double bond shows an *E* conformation.

In the crystal, the water molecule is linked to the organic molecule by O—H···O hydrogen bonds forming an $R^2_2(7)$ ring motif (Table 1 and Fig. 2). The organic molecule is linked to the water molecule by C—H..O hydrogen bonds so forming helices along the *b*-axis direction (Table and Fig. 2).

S2. Synthesis and crystallization

2-Benzofuranyl methyl ketone (0.01 mol) and 2-bromobenzaldehyde (0.01 mol) were dissolved in methanol (60 ml). Sodium hydroxide (2 ml, 20%) was then added drop wise to the solution which was then stirred for 1.5 h. The contents of the flask were cooled using ice-cold water, and the resulting powder content was collected by filtration. The compound was dried and re-crystallized twice using acetone as solvent, yielding golden-yellow block-like crystals.

S3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The water H atoms were located in a difference Fourier map. They were refined with distance restraints: O—H = 0.88 (2) Å, H···H = 1.43 (2) Å with U_{iso}(H) = 1.5U_{eq}(O). The C-bound H atoms were placed in calculated positions and included in the refinement in the riding model approximation: C—H = 0.93 Å with U_{iso}(H) = 1.2U_{eq}(C).

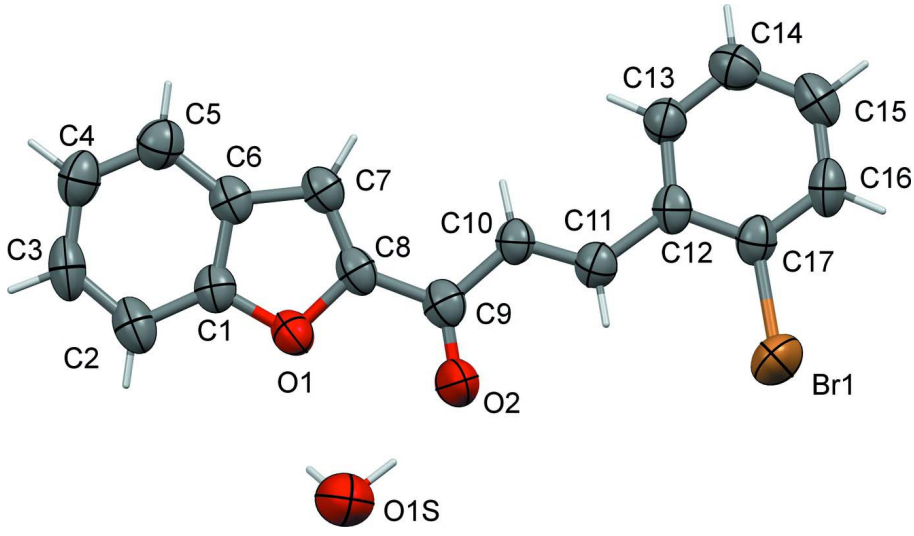

Figure 1

A view of the molecular structure of title compound, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

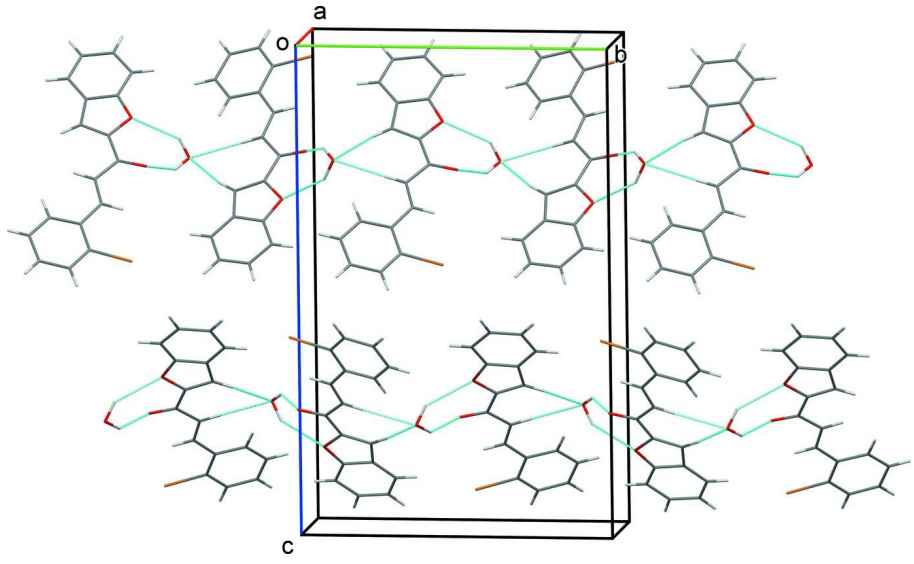

Figure 2

A view along the *a*-axis of the crystal packing of the title compound. The intermolecular interactions are represented by dashed lines (see Table 1).

(2*E*)-1-(1-Benzofuran-2-yl)-3-(2-bromophenyl)prop-2-en-1-one monohydrate

Crystal data

$C_{17}H_{11}BrO_2 \cdot H_2O$
$M_r = 345.18$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 4.8614$ (4) Å
$b = 13.8220$ (15) Å
$c = 21.755$ (2) Å
$V = 1461.8$ (2) Å^3
$Z = 4$
$F(000) = 696$
$D_x = 1.568$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2499 reflections
$\theta = 4.8$–41.6°

μ = 2.82 mm^{-1}
T = 296 K

Block, golden-yellow
0.40 × 0.30 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.399, T_{max} = 0.539

3636 measured reflections
3636 independent reflections
2134 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 28.4°, θ_{min} = 3.0°
h = −6→5
k = −18→18
l = −28→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.102
S = 1.01
3636 reflections
196 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 0.0197P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Absolute structure: Flack (1983), 1497 Friedel pairs
Absolute structure parameter: −0.011 (11)

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 $F^2 > 2$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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Br1	1.34723 (10)	0.98219 (3)	0.06738 (2)	0.0902 (2)
O1	0.3289 (4)	0.93267 (17)	0.32535 (10)	0.0513 (5)
O2	0.6697 (5)	0.99535 (19)	0.23842 (13)	0.0720 (7)
C1	0.1694 (7)	0.8801 (2)	0.36525 (14)	0.0463 (8)
C2	−0.0186 (7)	0.9171 (3)	0.40591 (16)	0.0593 (10)
H2	−0.0523	0.9831	0.4093	0.071*
C3	−0.1522 (7)	0.8509 (3)	0.44089 (16)	0.0634 (10)
H3	−0.2812	0.8724	0.4694	0.076*
C4	−0.1034 (7)	0.7519 (3)	0.43576 (17)	0.0607 (9)
H4	−0.2020	0.7091	0.4603	0.073*
C5	0.0860 (7)	0.7169 (3)	0.39547 (16)	0.0587 (10)
H5	0.1185	0.6507	0.3923	0.070*

C6	0.2301 (6)	0.7824 (3)	0.35908 (14)	0.0444 (8)
C7	0.4402 (6)	0.7757 (3)	0.31357 (15)	0.0468 (8)
H7	0.5256	0.7195	0.2997	0.056*
C8	0.4907 (6)	0.8671 (3)	0.29448 (15)	0.0463 (9)
C9	0.6756 (7)	0.9078 (3)	0.24929 (15)	0.0503 (8)
C10	0.8640 (6)	0.8424 (2)	0.21760 (14)	0.0446 (7)
H10	0.8712	0.7779	0.2297	0.054*
C11	1.0223 (6)	0.8713 (3)	0.17288 (16)	0.0480 (8)
H11	1.0081	0.9361	0.1619	0.058*
C12	1.2190 (6)	0.8136 (3)	0.13815 (14)	0.0439 (8)
C13	1.2629 (7)	0.7170 (3)	0.15197 (16)	0.0523 (9)
H13	1.1617	0.6892	0.1837	0.063*
C14	1.4478 (7)	0.6610 (3)	0.12115 (19)	0.0615 (10)
H14	1.4691	0.5961	0.1315	0.074*
C15	1.6028 (7)	0.7008 (3)	0.07476 (17)	0.0603 (10)
H15	1.7313	0.6633	0.0539	0.072*
C16	1.5667 (7)	0.7964 (3)	0.05931 (16)	0.0557 (9)
H16	1.6695	0.8239	0.0278	0.067*
C17	1.3787 (7)	0.8507 (3)	0.09068 (14)	0.0493 (8)
O1S	0.1601 (7)	1.1082 (2)	0.23870 (17)	0.0950 (10)
H1SA	0.179 (11)	1.078 (4)	0.2780 (12)	0.143*
H1SB	0.300 (9)	1.070 (3)	0.220 (2)	0.143*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1130 (4)	0.0695 (3)	0.0881 (3)	0.0070 (3)	0.0327 (3)	0.0255 (2)
O1	0.0458 (12)	0.0526 (14)	0.0555 (14)	0.0017 (11)	0.0037 (12)	−0.0104 (11)
O2	0.0594 (14)	0.0592 (19)	0.0974 (19)	0.0071 (14)	0.0271 (13)	0.0068 (15)
C1	0.0391 (17)	0.057 (2)	0.0426 (18)	−0.0028 (18)	−0.0028 (16)	−0.0049 (15)
C2	0.0461 (19)	0.079 (3)	0.053 (2)	0.0023 (19)	0.0023 (17)	−0.016 (2)
C3	0.0426 (18)	0.104 (3)	0.044 (2)	−0.003 (2)	0.0102 (19)	−0.009 (2)
C4	0.056 (2)	0.081 (3)	0.0447 (19)	−0.0068 (19)	0.002 (2)	0.008 (2)
C5	0.058 (2)	0.065 (2)	0.054 (2)	0.0003 (19)	−0.0023 (18)	0.0054 (19)
C6	0.0340 (17)	0.058 (2)	0.0408 (17)	0.0013 (15)	−0.0096 (14)	−0.0056 (16)
C7	0.0383 (17)	0.056 (2)	0.0460 (19)	0.0050 (15)	−0.0053 (15)	−0.0044 (17)
C8	0.0323 (16)	0.060 (2)	0.047 (2)	0.0051 (16)	−0.0044 (14)	−0.0082 (18)
C9	0.0368 (17)	0.060 (2)	0.054 (2)	−0.0001 (18)	−0.0042 (16)	−0.0041 (17)
C10	0.0346 (16)	0.052 (2)	0.0469 (18)	−0.0021 (17)	0.0011 (16)	0.0002 (15)
C11	0.0423 (16)	0.055 (2)	0.047 (2)	0.0008 (16)	−0.0021 (16)	0.0048 (16)
C12	0.0302 (16)	0.060 (2)	0.0419 (18)	−0.0028 (15)	−0.0042 (13)	−0.0007 (16)
C13	0.050 (2)	0.056 (2)	0.051 (2)	0.0004 (17)	0.0043 (15)	0.0046 (18)
C14	0.059 (2)	0.057 (2)	0.068 (3)	0.0079 (19)	−0.003 (2)	−0.001 (2)
C15	0.051 (2)	0.074 (3)	0.055 (2)	0.0128 (19)	0.0024 (18)	−0.014 (2)
C16	0.0437 (18)	0.085 (3)	0.0389 (19)	−0.0034 (18)	0.0069 (15)	0.0009 (19)
C17	0.0434 (18)	0.063 (2)	0.0418 (18)	−0.0013 (18)	−0.0009 (15)	0.0050 (15)
O1S	0.098 (2)	0.071 (2)	0.117 (3)	0.0067 (18)	0.019 (2)	0.0037 (18)

Geometric parameters (Å, º)

Br1—C17	1.893 (4)	C9—C10	1.460 (5)
O1—C1	1.372 (4)	C10—C11	1.303 (4)
O1—C8	1.375 (4)	C10—H10	0.9300
O2—C9	1.234 (4)	C11—C12	1.456 (4)
C1—C2	1.370 (5)	C11—H11	0.9300
C1—C6	1.390 (5)	C12—C13	1.385 (5)
C2—C3	1.356 (5)	C12—C17	1.390 (4)
C2—H2	0.9300	C13—C14	1.363 (5)
C3—C4	1.393 (5)	C13—H13	0.9300
C3—H3	0.9300	C14—C15	1.374 (5)
C4—C5	1.361 (5)	C14—H14	0.9300
C4—H4	0.9300	C15—C16	1.375 (5)
C5—C6	1.392 (5)	C15—H15	0.9300
C5—H5	0.9300	C16—C17	1.366 (5)
C6—C7	1.426 (4)	C16—H16	0.9300
C7—C8	1.353 (5)	O1S—H1SA	0.958 (19)
C7—H7	0.9300	O1S—H1SB	0.954 (19)
C8—C9	1.446 (5)		
C1—O1—C8	106.5 (3)	C8—C9—C10	118.1 (3)
C2—C1—O1	126.0 (3)	C11—C10—C9	122.2 (3)
C2—C1—C6	124.5 (3)	C11—C10—H10	118.9
O1—C1—C6	109.5 (3)	C9—C10—H10	118.9
C3—C2—C1	115.5 (4)	C10—C11—C12	127.4 (4)
C3—C2—H2	122.2	C10—C11—H11	116.3
C1—C2—H2	122.2	C12—C11—H11	116.3
C2—C3—C4	122.4 (3)	C13—C12—C17	115.6 (3)
C2—C3—H3	118.8	C13—C12—C11	121.1 (3)
C4—C3—H3	118.8	C17—C12—C11	123.4 (3)
C5—C4—C3	121.1 (3)	C14—C13—C12	122.8 (3)
C5—C4—H4	119.4	C14—C13—H13	118.6
C3—C4—H4	119.4	C12—C13—H13	118.6
C4—C5—C6	118.4 (4)	C13—C14—C15	119.7 (4)
C4—C5—H5	120.8	C13—C14—H14	120.2
C6—C5—H5	120.8	C15—C14—H14	120.2
C1—C6—C5	118.1 (3)	C14—C15—C16	119.7 (3)
C1—C6—C7	106.4 (3)	C14—C15—H15	120.2
C5—C6—C7	135.5 (4)	C16—C15—H15	120.2
C8—C7—C6	106.4 (3)	C17—C16—C15	119.4 (3)
C8—C7—H7	126.8	C17—C16—H16	120.3
C6—C7—H7	126.8	C15—C16—H16	120.3
C7—C8—O1	111.2 (3)	C16—C17—C12	122.8 (3)
C7—C8—C9	133.2 (3)	C16—C17—Br1	116.6 (3)
O1—C8—C9	115.6 (3)	C12—C17—Br1	120.6 (3)
O2—C9—C8	119.8 (3)	H1SA—O1S—H1SB	94 (2)
O2—C9—C10	122.1 (3)		

C8—O1—C1—C2	178.7 (3)	O1—C8—C9—O2	−3.8 (5)
C8—O1—C1—C6	−0.4 (3)	C7—C8—C9—C10	−3.6 (6)
O1—C1—C2—C3	−179.9 (3)	O1—C8—C9—C10	176.5 (3)
C6—C1—C2—C3	−1.0 (5)	O2—C9—C10—C11	−5.2 (5)
C1—C2—C3—C4	−0.3 (5)	C8—C9—C10—C11	174.5 (3)
C2—C3—C4—C5	1.0 (6)	C9—C10—C11—C12	179.5 (3)
C3—C4—C5—C6	−0.3 (5)	C10—C11—C12—C13	−2.0 (5)
C2—C1—C6—C5	1.6 (5)	C10—C11—C12—C17	179.6 (3)
O1—C1—C6—C5	−179.3 (3)	C17—C12—C13—C14	−0.5 (5)
C2—C1—C6—C7	−178.3 (3)	C11—C12—C13—C14	−179.0 (3)
O1—C1—C6—C7	0.8 (3)	C12—C13—C14—C15	1.0 (5)
C4—C5—C6—C1	−0.9 (5)	C13—C14—C15—C16	−1.0 (5)
C4—C5—C6—C7	179.0 (3)	C14—C15—C16—C17	0.5 (5)
C1—C6—C7—C8	−0.9 (3)	C15—C16—C17—C12	−0.1 (5)
C5—C6—C7—C8	179.1 (3)	C15—C16—C17—Br1	178.9 (3)
C6—C7—C8—O1	0.8 (4)	C13—C12—C17—C16	0.1 (5)
C6—C7—C8—C9	−179.1 (3)	C11—C12—C17—C16	178.6 (3)
C1—O1—C8—C7	−0.3 (4)	C13—C12—C17—Br1	−178.9 (2)
C1—O1—C8—C9	179.6 (3)	C11—C12—C17—Br1	−0.4 (4)
C7—C8—C9—O2	176.0 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*S*—H1*SA*···O1	0.96 (2)	2.37 (4)	3.181 (4)	142 (4)
O1*S*—H1*SB*···O2	0.95 (2)	2.11 (4)	2.928 (4)	143 (4)
C7—H7···O1*S*^{i}	0.93	2.32	3.229 (5)	164
C10—H10···O1*S*^{i}	0.93	2.45	3.375 (5)	174

Symmetry code: (i) −*x*+1, *y*−1/2, −*z*+1/2.