Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-[(4-Chlorophenyl)sulfinyl]-2,4,6,7-tetramethyl-1-benzofuran

Hong Dae Choi,[a] Pil Ja Seo,[a] Byeng Wha Son[b] and Uk Lee[b]*

[a]Department of Chemistry, Dongeui University, San 24 Kaya-dong Busanjin-gu, Busan 614-714, Republic of Korea, and [b]Department of Chemistry, Pukyong National University, 599-1 Daeyeon 3-dong Nam-gu, Busan 608-737, Republic of Korea
Correspondence e-mail: uklee@pknu.ac.kr

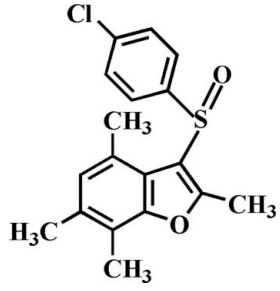
Received 6 October 2010; accepted 19 October 2010

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.038; wR factor = 0.090; data-to-parameter ratio = 16.7.

In the title compound, $C_{18}H_{17}ClO_2S$, the 4-chlorophenyl ring is oriented approximately perpendicular to the mean plane of the benzofuran ring [dihedral angle = 87.49 (5)°]. In the crystal, molecules are linked through weak intermolecular C—H$\cdots\pi$ interactions, forming left- and right-handed pseudo-helices along the a axis.

Related literature

For the biological activity of benzofuran compounds, see: Aslam *et al.* (2006); Galal *et al.* (2009); Khan *et al.* (2005). For natural products with benzofuran rings, see: Akgul & Anil (2003); Soekamto *et al.* (2003). For the structures of related 3-(4–chlorophenylsulfinyl)-2-methyl-1-benzofuran derivatives, see: Choi *et al.* (2010*a*,*b*,*c*).



Experimental

Crystal data

$C_{18}H_{17}ClO_2S$
M_r = 332.83
Orthorhombic, $Pna2_1$
a = 12.2329 (4) Å
b = 20.1499 (7) Å
c = 6.4840 (2) Å
V = 1598.25 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 173 K
0.33 × 0.16 × 0.10 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.651, T_{max} = 0.746
8651 measured reflections
3392 independent reflections
2809 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.090
S = 1.05
3392 reflections
203 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983), 1382 Friedel pairs
Flack parameter: −0.03 (6)

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

*Cg*1 and *Cg*2 are the centroids of the C13–C18 4-chlorophenyl ring and the C2–C7 benzene ring, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C11—H11$A\cdots Cg1^{i}$	0.96	2.76	3.613 (3)	148
C12—H12$B\cdots Cg2^{ii}$	0.96	2.83	3.653 (3)	144

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, z$; (ii) $x, y, z-1$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2316).

References

Akgul, Y. Y. & Anil, H. (2003). *Phytochemistry*, **63**, 939–943.
Aslam, S. N., Stevenson, P. C., Phythian, S. J., Veitch, N. C. & Hall, D. R. (2006). *Tetrahedron*, **62**, 4214–4226.
Brandenburg, K. (1998). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2009). *APEX2*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2010*a*). *Acta Cryst.* E**66**, o2325.
Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2010*b*). *Acta Cryst.* E**66**, o2551.
Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2010*c*). *Acta Cryst.* E**66**, o2702.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Galal, S. A., Abd El-All, A. S., Abdallah, M. M. & El-Diwani, H. I. (2009). *Bioorg. Med. Chem. Lett.* **19**, 2420–2428.
Khan, M. W., Alam, M. J., Rashid, M. A. & Chowdhury, R. (2005). *Bioorg. Med. Chem.* **13**, 4796–4805.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Soekamto, N. H., Achmad, S. A., Ghisalberti, E. L., Hakim, E. H. & Syah, Y. M. (2003). *Phytochemistry*, **64**, 831–834.

supporting information

Acta Cryst. (2010). E**66**, o3087 [https://doi.org/10.1107/S1600536810042339]

3-[(4-Chlorophenyl)sulfinyl]-2,4,6,7-tetramethyl-1-benzofuran

Hong Dae Choi, Pil Ja Seo, Byeng Wha Son and Uk Lee

S1. Comment

A series of benzofuran ring system have received much attention in view of their interesting pharmacological properties such as antifungal, antimicrobial, antitumor and antiviral activities (Aslam *et al.*, 2006; Galal *et al.*, 2009; Khan *et al.*, 2005). These compounds widely occur in nature (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our study of the substituent effect on the solid state structures of 3-(4-chlorophenylsulfinyl)-2-methyl-1-benzofuran analogues (Choi *et al.*, 2010*a,b,c*), we report herein on the crystal structure of the title compound.

In the title molecule (Fig. 1), the benzofuran unit is essentially planar, with a mean deviation of 0.011 (2) Å from the least-squares plane defined by the nine constituent atoms. The 4-chlorophenyl ring makes a dihedral angle of 87.49 (5)° with the mean plane of the benzofuran fragment. The crystal packing (Fig. 2) is stabilized by weak intermolecular C—H···π interactions; the first one between a methyl H atom and the 4-chlorophenyl ring (C11—H11A···Cg1^{i}; Table 1, Cg1 is the centroid of the C13···C18 4–chlorophenyl ring), and the second one between a methyl H atom and the benzene ring (C12—H12B···Cg2^{ii}; Table 1, Cg2 is the centroid of the C2···C7 benzene ring). The title compound crystallizes in the non-centrosymmetric space group *Pna*2$_1$ in spite of having no asymmetric C atoms. The space group is caused by a right-hand pseudo-helix along the *a* axis (Fig. 2).

S2. Experimental

77% 3-chloroperoxybenzoic acid (269 mg, 1.2 mmol) was added in small portions to a stirred solution of 3-(4-chlorophenylsulfanyl)-2,4,6,7-tetramethyl-1-benzofuran (348 mg, 1.0 mmol) in dichloromethane (40 mL) at 273 K. After being stirred at room temperature for 4h, the mixture was washed with saturated sodium bicarbonate solution and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated at reduced pressure. The residue was purified by column chromatography (hexane-ethyl acetate, 2:1 *v*/*v*) to afford the title compound as a colorless solid [yield 76%, m.p. 442–443 K; R_f = 0.67 (hexane-ethyl acetate, 2:1 *v*/*v*)]. Single crystals suitable for X–ray diffraction were prepared by slow evaporation of a solution of the title compound in ethyl acetate at room temperature.

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å for aryl and 0.96 Å for methyl H atoms. U_{iso}(H) = 1.2U_{eq}(C) for aryl and 1.5U_{eq}(C) for methyl H atoms.

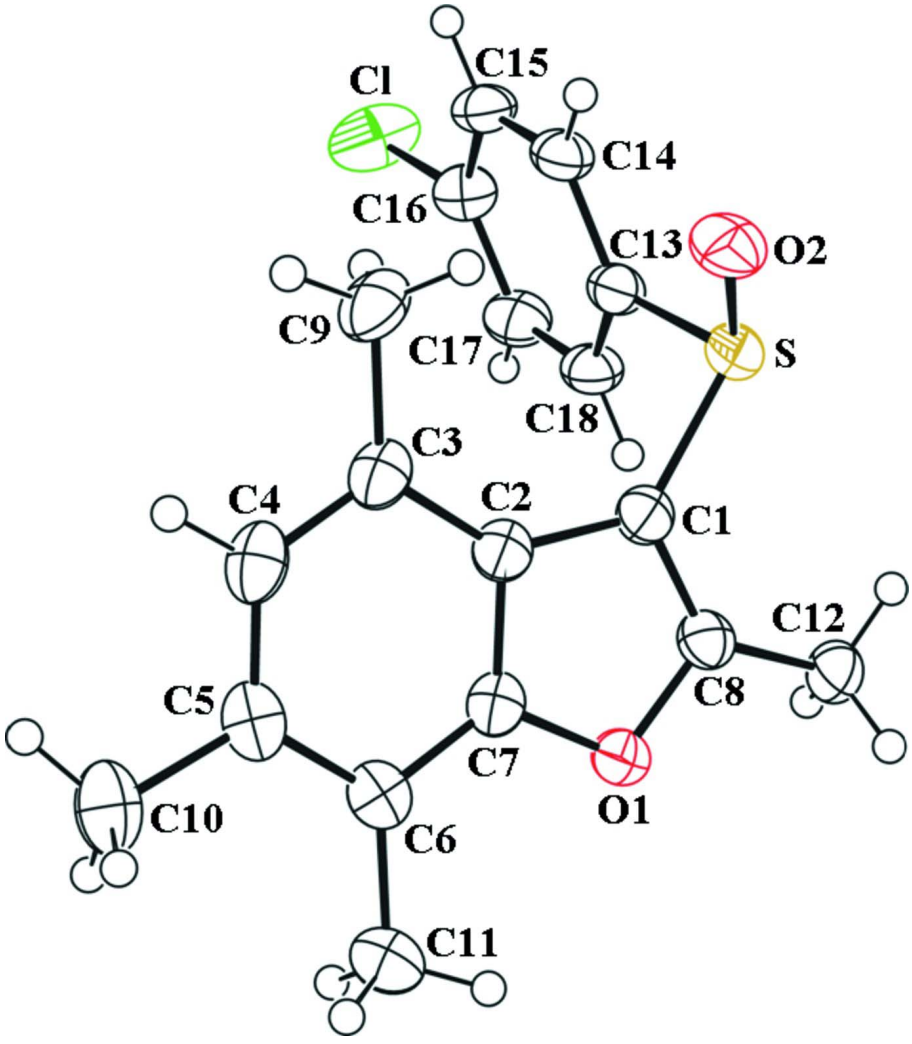


Figure 1

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.

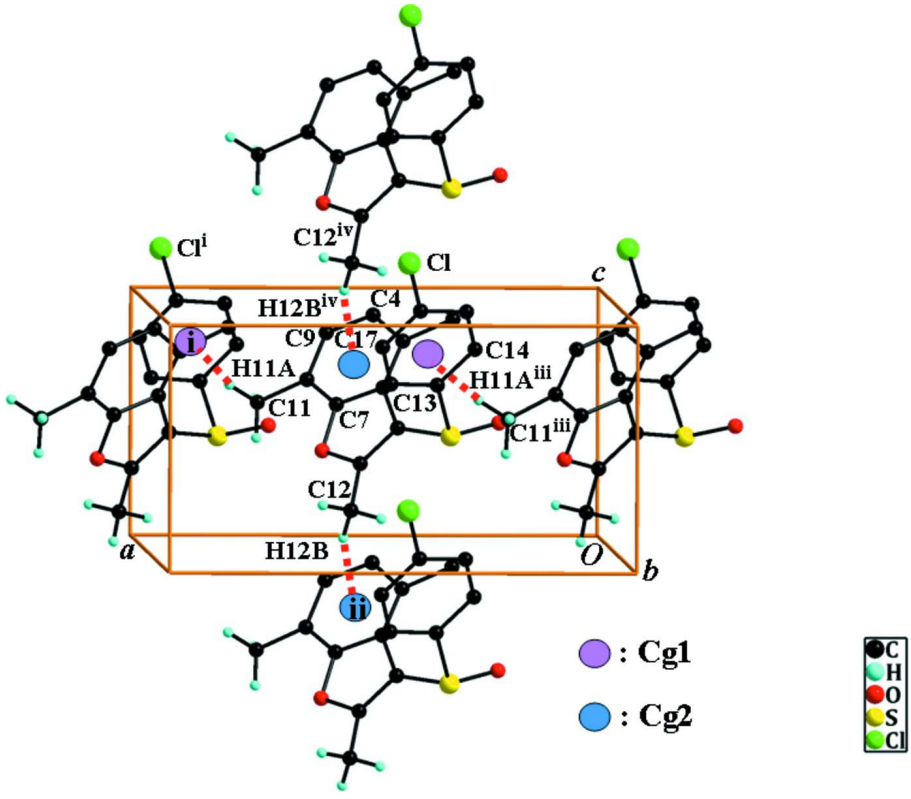


Figure 2

A view of the C—H···π interactions (dotted lines) in the crystal structure of the title compound. Cg1 and Cg2 denote the centroids of the C13···C18 4-chlorophenyl ring and the C2···C7 benzene ring, respectively. [Symmetry codes: (*i*) *x*-1/2, -*y*+3/2, *z*; (*ii*) *x*, *y*, *z*-1; (*iii*) *x*-1/2, -*y*+3/2, *z*; (*iv*) *x*, *y*, *z*+1].

3-[(4-Chlorophenyl)sulfinyl]-2,4,6,7-tetramethyl-1-benzofuran

Crystal data

$C_{18}H_{17}ClO_2S$
M_r = 332.83
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
a = 12.2329 (4) Å
b = 20.1499 (7) Å
c = 6.4840 (2) Å
V = 1598.25 (9) Å^3
Z = 4
F(000) = 696
D_x = 1.383 Mg m^{-3}
Melting point: 442 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2945 reflections
θ = 2.6–26.8°
μ = 0.37 mm^{-1}
T = 173 K
Block, colourless
0.33 × 0.16 × 0.10 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: rotating anode
Graphite multilayer monochromator
Detector resolution: 10.0 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.651, T_{max} = 0.746
8651 measured reflections
3392 independent reflections
2809 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

θ_{max} = 27.6°, θ_{min} = 2.0°
h = −15→11
k = −26→20
l = −8→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.090
S = 1.05
3392 reflections
203 parameters
1 restraint
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2 + 0.1096P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983), 1382 Friedel pairs
Absolute structure parameter: −0.03 (6)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl	0.48480 (5)	0.93993 (4)	1.24227 (15)	0.0644 (2)
S	0.37852 (4)	0.74513 (3)	0.51507 (13)	0.03587 (15)
O1	0.64405 (11)	0.64000 (7)	0.4393 (2)	0.0317 (4)
O2	0.27233 (11)	0.71240 (9)	0.5638 (3)	0.0462 (5)
C1	0.48689 (15)	0.68792 (10)	0.5388 (4)	0.0304 (5)
C2	0.51433 (16)	0.63782 (11)	0.6943 (4)	0.0308 (5)
C3	0.47011 (16)	0.61312 (12)	0.8785 (4)	0.0350 (5)
C4	0.52973 (19)	0.56352 (12)	0.9760 (4)	0.0394 (6)
H4	0.5030	0.5469	1.1000	0.047*
C5	0.62780 (17)	0.53683 (12)	0.8996 (4)	0.0368 (6)
C6	0.67069 (16)	0.55999 (10)	0.7143 (4)	0.0331 (5)
C7	0.61165 (16)	0.61008 (11)	0.6216 (4)	0.0301 (5)
C8	0.56685 (15)	0.68753 (11)	0.3949 (4)	0.0312 (5)
C9	0.36522 (17)	0.63876 (14)	0.9713 (4)	0.0443 (7)
H9A	0.3772	0.6823	1.0272	0.066*
H9B	0.3418	0.6094	1.0791	0.066*
H9C	0.3099	0.6409	0.8665	0.066*
C10	0.6861 (2)	0.48422 (12)	1.0225 (5)	0.0506 (7)
H10A	0.7622	0.4953	1.0329	0.076*
H10B	0.6783	0.4421	0.9548	0.076*
H10C	0.6549	0.4817	1.1581	0.076*
C11	0.77427 (18)	0.53408 (12)	0.6181 (4)	0.0423 (6)
H11A	0.8362	0.5515	0.6912	0.063*
H11B	0.7777	0.5477	0.4764	0.063*
H11C	0.7750	0.4865	0.6255	0.063*
C12	0.58942 (18)	0.72823 (11)	0.2117 (4)	0.0370 (5)
H12A	0.6521	0.7557	0.2370	0.055*
H12B	0.5273	0.7557	0.1824	0.055*
H12C	0.6036	0.6998	0.0959	0.055*
C13	0.41185 (16)	0.79762 (10)	0.7289 (4)	0.0322 (5)

C14	0.33260 (16)	0.81193 (11)	0.8759 (4)	0.0353 (5)
H14	0.2642	0.7920	0.8672	0.042*
C15	0.35484 (16)	0.85543 (11)	1.0343 (5)	0.0361 (5)
H15	0.3025	0.8644	1.1346	0.043*
C16	0.45579 (17)	0.88545 (11)	1.0414 (4)	0.0381 (6)
C17	0.53552 (17)	0.87296 (12)	0.8939 (4)	0.0405 (6)
H17	0.6029	0.8942	0.9008	0.049*
C18	0.51360 (16)	0.82887 (11)	0.7378 (4)	0.0367 (6)
H18	0.5663	0.8199	0.6384	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0533 (4)	0.0701 (5)	0.0699 (5)	−0.0190 (3)	0.0152 (4)	−0.0291 (4)
S	0.0257 (2)	0.0485 (3)	0.0334 (3)	0.0036 (2)	−0.0013 (3)	0.0026 (3)
O1	0.0293 (6)	0.0334 (8)	0.0324 (9)	0.0032 (6)	0.0014 (7)	0.0023 (7)
O2	0.0239 (7)	0.0632 (11)	0.0516 (12)	−0.0027 (7)	−0.0036 (8)	−0.0053 (9)
C1	0.0256 (9)	0.0357 (12)	0.0299 (12)	−0.0028 (8)	−0.0019 (11)	−0.0005 (11)
C2	0.0251 (9)	0.0363 (13)	0.0310 (13)	−0.0064 (8)	−0.0011 (10)	0.0004 (10)
C3	0.0307 (10)	0.0434 (14)	0.0310 (13)	−0.0115 (10)	0.0007 (11)	0.0016 (11)
C4	0.0425 (12)	0.0428 (14)	0.0330 (15)	−0.0160 (10)	−0.0024 (11)	0.0065 (11)
C5	0.0388 (11)	0.0315 (13)	0.0401 (14)	−0.0094 (9)	−0.0084 (12)	0.0049 (12)
C6	0.0318 (10)	0.0291 (12)	0.0384 (14)	−0.0052 (9)	−0.0054 (11)	0.0002 (11)
C7	0.0288 (10)	0.0324 (12)	0.0292 (13)	−0.0075 (9)	−0.0007 (10)	0.0017 (10)
C8	0.0268 (10)	0.0343 (12)	0.0324 (12)	−0.0009 (9)	−0.0042 (11)	−0.0024 (10)
C9	0.0385 (11)	0.0578 (16)	0.0366 (17)	−0.0109 (11)	0.0089 (12)	0.0031 (12)
C10	0.0594 (14)	0.0451 (15)	0.0472 (15)	−0.0088 (12)	−0.0102 (16)	0.0129 (14)
C11	0.0396 (12)	0.0361 (13)	0.0513 (17)	0.0052 (10)	−0.0004 (13)	0.0006 (12)
C12	0.0341 (11)	0.0457 (14)	0.0312 (13)	−0.0004 (10)	0.0025 (12)	0.0069 (12)
C13	0.0268 (9)	0.0334 (12)	0.0363 (13)	0.0047 (9)	0.0039 (11)	0.0074 (12)
C14	0.0238 (9)	0.0403 (13)	0.0419 (14)	0.0029 (9)	0.0036 (12)	0.0044 (12)
C15	0.0297 (10)	0.0376 (12)	0.0410 (15)	0.0037 (9)	0.0109 (13)	0.0020 (13)
C16	0.0355 (10)	0.0360 (13)	0.0426 (15)	−0.0007 (9)	0.0038 (12)	−0.0022 (12)
C17	0.0282 (10)	0.0423 (14)	0.0510 (16)	−0.0048 (10)	0.0047 (12)	0.0017 (13)
C18	0.0275 (10)	0.0405 (13)	0.0421 (14)	0.0035 (9)	0.0086 (12)	0.0070 (13)

Geometric parameters (Å, º)

Cl—C16	1.740 (3)	C9—H9C	0.9600
S—O2	1.4907 (15)	C10—H10A	0.9600
S—C1	1.763 (2)	C10—H10B	0.9600
S—C13	1.791 (3)	C10—H10C	0.9600
O1—C8	1.375 (2)	C11—H11A	0.9600
O1—C7	1.385 (3)	C11—H11B	0.9600
C1—C8	1.352 (3)	C11—H11C	0.9600
C1—C2	1.466 (3)	C12—H12A	0.9600
C2—C7	1.397 (3)	C12—H12B	0.9600
C2—C3	1.402 (3)	C12—H12C	0.9600

C3—C4	1.389 (3)	C13—C14	1.390 (3)
C3—C9	1.508 (3)	C13—C18	1.396 (3)
C4—C5	1.405 (3)	C14—C15	1.377 (4)
C4—H4	0.9300	C14—H14	0.9300
C5—C6	1.391 (4)	C15—C16	1.376 (3)
C5—C10	1.506 (3)	C15—H15	0.9300
C6—C7	1.379 (3)	C16—C17	1.389 (3)
C6—C11	1.506 (3)	C17—C18	1.373 (4)
C8—C12	1.470 (3)	C17—H17	0.9300
C9—H9A	0.9600	C18—H18	0.9300
C9—H9B	0.9600		

O2—S—C1	110.33 (10)	C5—C10—H10B	109.5
O2—S—C13	107.20 (11)	H10A—C10—H10B	109.5
C1—S—C13	98.48 (10)	C5—C10—H10C	109.5
C8—O1—C7	106.57 (16)	H10A—C10—H10C	109.5
C8—C1—C2	107.76 (18)	H10B—C10—H10C	109.5
C8—C1—S	119.19 (18)	C6—C11—H11A	109.5
C2—C1—S	133.01 (17)	C6—C11—H11B	109.5
C7—C2—C3	118.3 (2)	H11A—C11—H11B	109.5
C7—C2—C1	103.78 (19)	C6—C11—H11C	109.5
C3—C2—C1	137.9 (2)	H11A—C11—H11C	109.5
C4—C3—C2	116.1 (2)	H11B—C11—H11C	109.5
C4—C3—C9	120.8 (2)	C8—C12—H12A	109.5
C2—C3—C9	123.1 (2)	C8—C12—H12B	109.5
C3—C4—C5	124.3 (2)	H12A—C12—H12B	109.5
C3—C4—H4	117.9	C8—C12—H12C	109.5
C5—C4—H4	117.9	H12A—C12—H12C	109.5
C6—C5—C4	119.9 (2)	H12B—C12—H12C	109.5
C6—C5—C10	121.0 (2)	C14—C13—C18	120.0 (2)
C4—C5—C10	119.1 (2)	C14—C13—S	119.65 (17)
C7—C6—C5	115.1 (2)	C18—C13—S	120.10 (19)
C7—C6—C11	120.9 (2)	C15—C14—C13	120.4 (2)
C5—C6—C11	124.0 (2)	C15—C14—H14	119.8
C6—C7—O1	122.7 (2)	C13—C14—H14	119.8
C6—C7—C2	126.3 (2)	C16—C15—C14	118.8 (2)
O1—C7—C2	110.98 (19)	C16—C15—H15	120.6
C1—C8—O1	110.9 (2)	C14—C15—H15	120.6
C1—C8—C12	133.7 (2)	C15—C16—C17	121.8 (2)
O1—C8—C12	115.38 (18)	C15—C16—Cl	119.1 (2)
C3—C9—H9A	109.5	C17—C16—Cl	119.11 (17)
C3—C9—H9B	109.5	C18—C17—C16	119.2 (2)
H9A—C9—H9B	109.5	C18—C17—H17	120.4
C3—C9—H9C	109.5	C16—C17—H17	120.4
H9A—C9—H9C	109.5	C17—C18—C13	119.8 (2)
H9B—C9—H9C	109.5	C17—C18—H18	120.1
C5—C10—H10A	109.5	C13—C18—H18	120.1

O2—S—C1—C8	137.63 (18)	C8—O1—C7—C2	0.1 (2)
C13—S—C1—C8	−110.40 (19)	C3—C2—C7—C6	−0.4 (3)
O2—S—C1—C2	−44.6 (3)	C1—C2—C7—C6	−179.7 (2)
C13—S—C1—C2	67.3 (2)	C3—C2—C7—O1	−179.92 (18)
C8—C1—C2—C7	−1.4 (2)	C1—C2—C7—O1	0.7 (2)
S—C1—C2—C7	−179.29 (18)	C2—C1—C8—O1	1.5 (2)
C8—C1—C2—C3	179.5 (3)	S—C1—C8—O1	179.78 (14)
S—C1—C2—C3	1.6 (4)	C2—C1—C8—C12	−175.5 (2)
C7—C2—C3—C4	1.6 (3)	S—C1—C8—C12	2.8 (4)
C1—C2—C3—C4	−179.4 (2)	C7—O1—C8—C1	−1.1 (2)
C7—C2—C3—C9	−179.6 (2)	C7—O1—C8—C12	176.55 (19)
C1—C2—C3—C9	−0.5 (4)	O2—S—C13—C14	−13.4 (2)
C2—C3—C4—C5	−1.3 (4)	C1—S—C13—C14	−127.83 (19)
C9—C3—C4—C5	179.8 (2)	O2—S—C13—C18	172.49 (18)
C3—C4—C5—C6	−0.2 (4)	C1—S—C13—C18	58.0 (2)
C3—C4—C5—C10	178.6 (2)	C18—C13—C14—C15	−1.9 (3)
C4—C5—C6—C7	1.4 (3)	S—C13—C14—C15	−176.00 (19)
C10—C5—C6—C7	−177.4 (2)	C13—C14—C15—C16	1.4 (4)
C4—C5—C6—C11	−179.2 (2)	C14—C15—C16—C17	−0.1 (4)
C10—C5—C6—C11	2.0 (3)	C14—C15—C16—Cl	−179.48 (19)
C5—C6—C7—O1	178.34 (19)	C15—C16—C17—C18	−0.8 (4)
C11—C6—C7—O1	−1.1 (3)	Cl—C16—C17—C18	178.60 (19)
C5—C6—C7—C2	−1.1 (3)	C16—C17—C18—C13	0.3 (4)
C11—C6—C7—C2	179.4 (2)	C14—C13—C18—C17	1.0 (3)
C8—O1—C7—C6	−179.4 (2)	S—C13—C18—C17	175.08 (18)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the C13–C18 4-chlorophenyl ring and the C2–C7 benzene ring, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*A*···*Cg*1^{i}	0.96	2.76	3.613 (3)	148
C12—H12*B*···*Cg*2^{ii}	0.96	2.83	3.653 (3)	144

Symmetry codes: (i) *x*−1/2, −*y*+3/2, *z*; (ii) *x*, *y*, *z*−1.