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Structural elucidation and Hirshfeld surface analysis of a fused thiophene ester: methyl 3-[(naphtho[2,1-*b*]thiophen-5-yl)methyl]-1-benzothiophene-2-carboxylate

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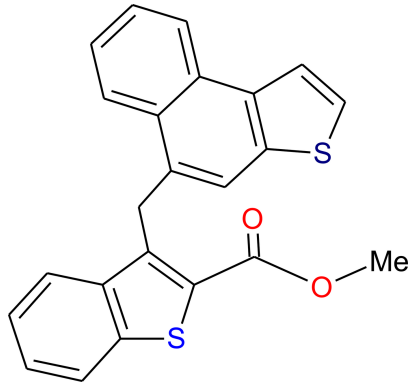
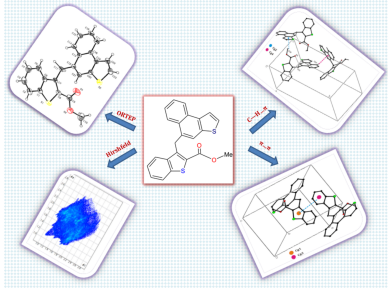
The title compound, $C_{23}H_{16}O_2S_2$, is a benzo[*b*]thiophene-2-carboxylate derivative and consists of naphthothiophene and benzothiophene moieties bridged by a methylene group. The dihedral angle between the two aromatic ring systems is 88.5 (2)°. Intramolecular C—H···O interactions generate an *S*(6) ring motif. The acetate group assumes an extended conformation. Weak C—H···π and π–π stacking interactions are present in the crystal structure, together with a short S···S interaction of 3.77 (8) Å. A Hirshfeld surface analysis indicates that H···H interactions contribute the most to the crystal packing (34.9%).Please give email addresses for all authors

1. Chemical context

Benzothiophenes are important components of organic semiconductors (OSCs) due to their potential for elongated and highly delocalized electronic structures (Huang *et al.*, 2012). OSCs have consistently attracted attention for their distinctive properties, such as mechanical flexibility and chemical versatility (Katz *et al.*, 2001). In this regard, benzothieno[3,2-*b*]benzothiophene derivatives are also highly promising materials for organic light-emitting diodes (OLEDs) (Izawa *et al.*, 2009) and organic field-effect transistors (OFET). In this context, we present here the synthesis, crystal structure and Hirshfeld surface analysis of the benzothiophene derivative $C_{23}H_{16}O_2S_2$.





2. Structural commentary

The molecular structure of the title compound is displayed in Fig. 1. The naphthothiophene group makes a dihedral angle of

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

*Cg*2 and *Cg*4 are the centroids of the S2/C19/C20/C22/C23 and C12/C13/C18-C21 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*B*···O1	0.97	2.44	3.007 (3)	117
C10—H10*A*···*Cg*2^{i}	0.96	2.86	3.397 (3)	116
C17—H17···*Cg*4^{ii}	0.93	2.98	3.689 (2)	134

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

88.5 (2)° with the benzothiophene group. Atom S2 deviates by 0.064 (1) Å from the least-squares plane of the naphthothiophene group; atom C8 deviates by −0.018 (2) Å from the least-squares plane of the benzothiophene group, most probably due to the bulky substitution by an acetate moiety. The latter assumes an extended conformation as can be seen from the C10—O2—C9—C8 torsion angle of −175.2 (2)°. The benzothiophene-2-carboxylate moiety is nearly planar, with the largest deviation from the least-squares plane of 0.011 (2) Å for atom C7. The molecular conformation is stabilized by a weak intramolecular C11—H11*B*···O1hydrogen bond involving the methylene group (C11) and the keto group (C9═O1) (Table 1, Fig. 2), which generates an *S*(6) ring motif (Bernstein *et al.*, 1995).

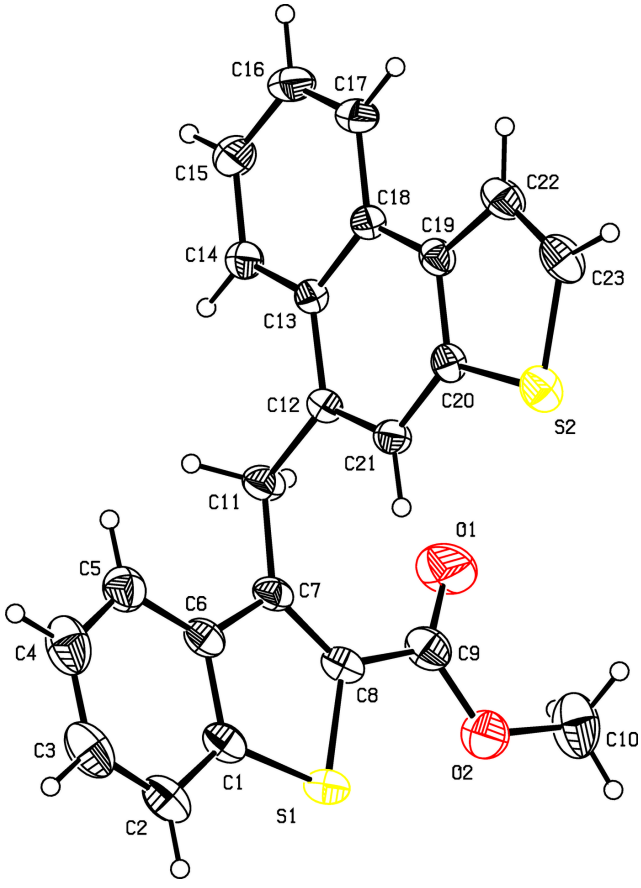


Figure 1
The molecular structure of the title compound showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

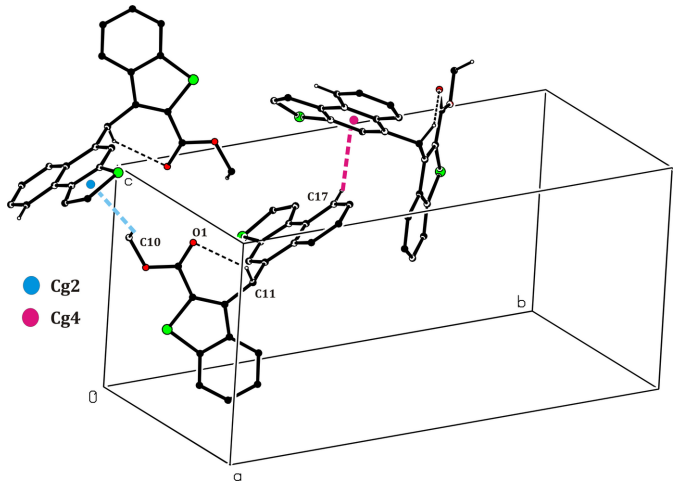


Figure 2
C—H···π and intramolecular C—H···O interaction (dashed line) in the title structure.

3. Supramolecular features

There are no hydrogen-bonding interactions in the crystal. Instead, C—H···*Cg* interactions (*Cg* is the centre of gravity of an aromatic ring) are present, *viz*. C10—H10*A*···*Cg*2^{i} between the methyl group and the thiophene ring (S2/C19/C20/C22/C23) attached to the naptho group, and C17—H17···*Cg*4^{ii} between a carbon atom of the naptho group and the central phenyl ring (C12/C13/C18-C21) of an adjacent naphthothiophene group (Table 1, Fig. 2). In addition, π–π stacking is realized (Fig. 3) between the thiophene ring of the benzothiophene group (*Cg*1; S1,C1,C6–C8) and the phenyl ring (*Cg*3; C1–C6) of the benzothiophene group of an

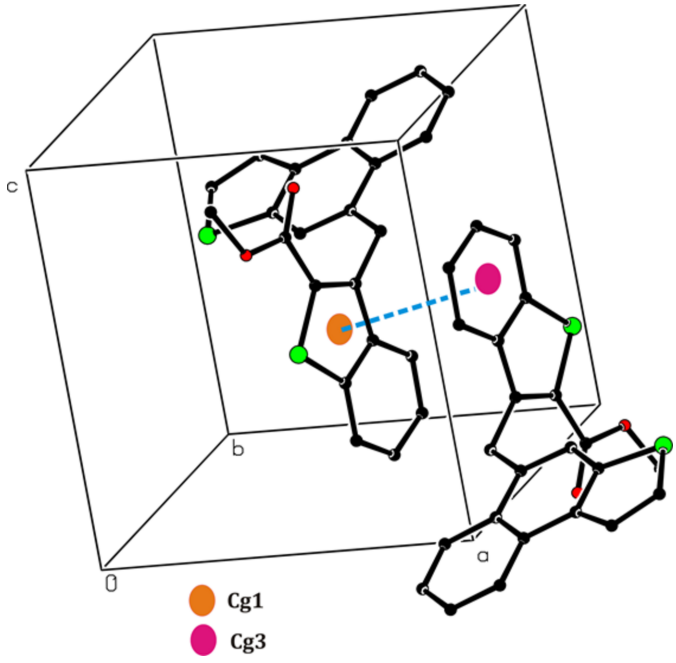


Figure 3
Relevant π–π interactions in the crystal of the title compound.

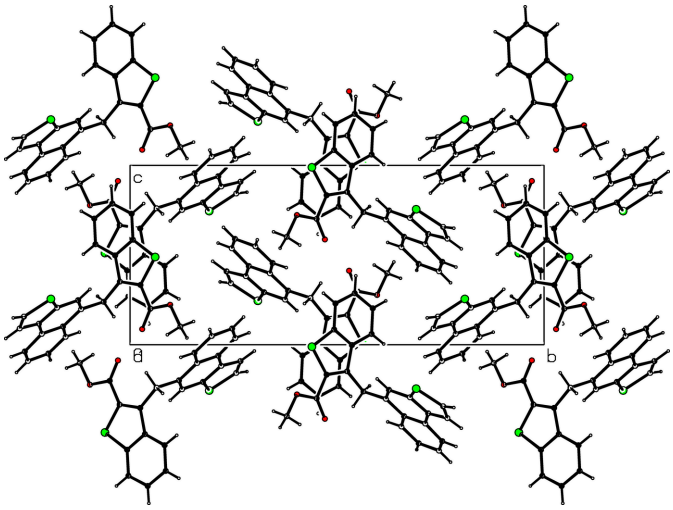


Figure 4
The molecular packing viewed down the *a* axis.

adjacent molecule (symmetry code: $2 - x, -y, 1 - z$) at a $Cg1\cdots Cg3$ distance of 3.9275 (2) Å with a slippage of 1.705 (3) Å. The molecular packing is shown in Fig. 4.

4. Hirshfeld surface analysis

Hirshfeld surface (HS) analysis (Hirshfeld, 1977) was carried out using *CrystalExplorer* (Spackman *et al.*, 2021). In the HS plotted over d_{norm}, the white surface indicates contacts with distances equal to the sum of the van der Waals radii, and the red and blue colours indicate distances shorter (in close contact) or longer (distinct contacts) than the van der Waals radii, respectively (Venkatesan *et al.*, 2016). The Hirshfeld surfaces plotted over different quantities are depicted in Fig. 5. Two-dimensional fingerprint plots showing the occurrence of all intermolecular contacts (McKinnon *et al.*, 2007) are presented in Fig. 6. The most important interaction originates from H···H contacts, contributing 34.9% to the overall crystal packing, which is reflected as widely scattered points of high density due to the large hydrogen content of the molecule. Almost as significant is the contribution from the C···H/H···C interactions (33.0%), indicating that the C—H···π interactions contribute significantly, likely hydrogen atoms interact with the π-electron-rich region to favour layered or offset stacking. Through electrostatic stabilization assisted by dispersion, three-dimensional packing efficiency is enhanced with a slight directionality. More contributions due to S···H/H···S interactions (15.6%) stem from the polarizability of the sulfur atom in weak hydrogen bond-like contacts. Sulfur atoms have soft donor properties, which allow them to participate in stabilizing intermolecular interactions. In the same way, O···H/H···O interactions (9.3%) define classical weak hydrogen-bonding pathways mediated by electronegative oxygen atoms. Electrostatic stabilization occurs as a consequence of these contacts and arrangement of molecules in the lattice in a suitable manner. This lessens the rotational and translational degrees of freedom. The S···S contacts (1.5%) represent only a small percentage, but they are structurally

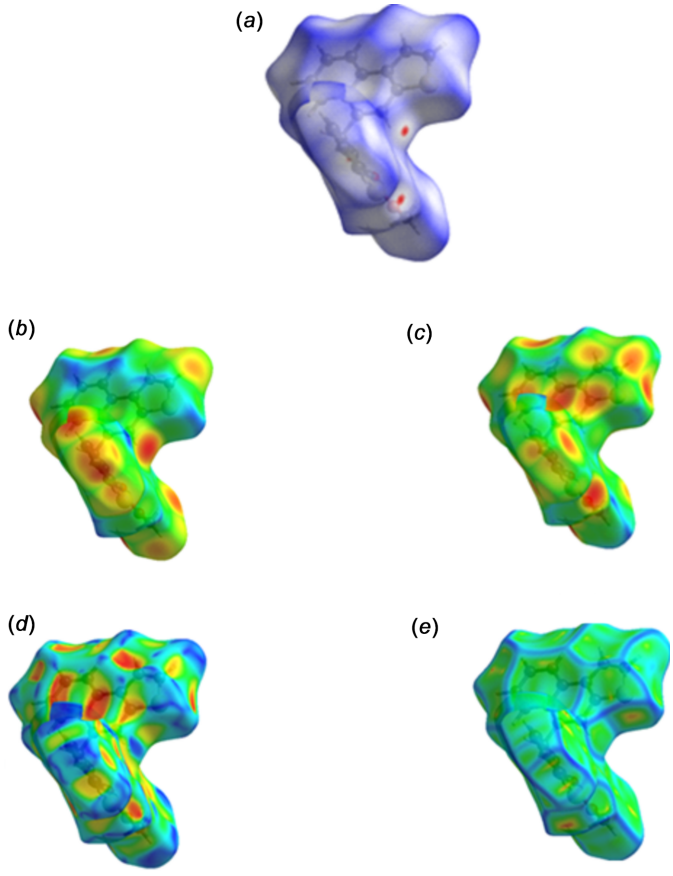


Figure 5
View of the three-dimensional Hirshfeld surface of the title compound mapped over (*a*) d_{norm}, (*b*) d_i, (*c*) d_e, (*d*) shape index and (*e*) curvedness.

important. The presence of short chalcogen–chalcogen contacts is known to enhance the lattice compactness via favourable overlap of their orbitals and associated dispersion interactions that lead to local densification. Such changes also

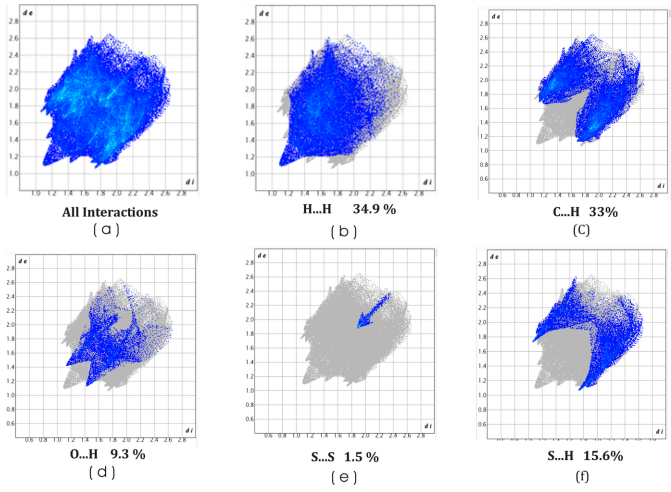


Figure 6
Two-dimensional fingerprint plots for the compound, showing (*a*) all interactions, and delineated into (*b*) H···H (*c*) C···H (*d*) H···O / O···H, (*e*) S···S and (*f*) S···H interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

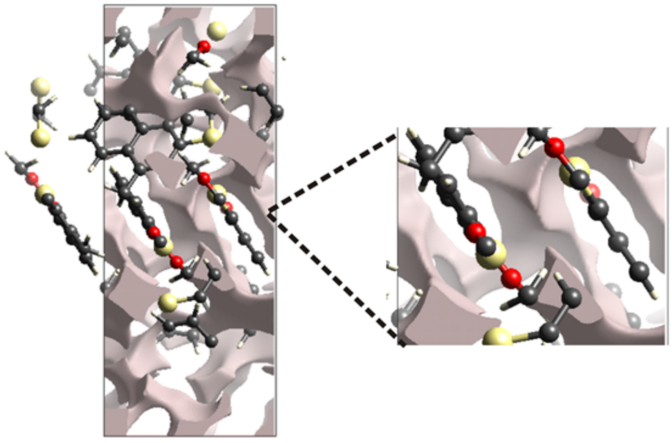


Figure 7
Plot showing the crystal voids in the crystal structure.

promote packing rigidity. These interactions can often serve as reinforcing elements of the packing within a crystal. When combined, these interactions give rise to a hierarchy of stabilization. The global stabilization is induced by the H···H dispersion forces, while the molecular stacking is being controlled by C—H···π interactions. Also, the directional locking and local reinforcement is conferred by the heteroatom-mediated contacts (S···H, O···H, S···S).

To analyse the crystal mechanical stability of the title crystal, a void evaluation was performed by summing the electron densities of the spherically symmetric atoms included in the asymmetric unit (Fig. 7). The void surface is recognized as an isosurface. The crystal voids within the unit cell are characterized by their volume and surface, which are 213.21 Å^3 and 654.88 Å^2, respectively. Considering the crystal volume of 1861.12 Å^3, the proportion of void space within the unit cell is 11.45%.

5. Database survey

A search of the Cambridge Structural Database (Version 5.37; Groom *et al.*, 2016). for benzothiophene-2-carboxylate moieties resulted in 18 hits. Entries CUDLEV (Ivachtchenko *et al.*, 2019) and QAVXOD (Shen *et al.*, 2017) are the closest analogues of the title compound. CUDLEV crystallizes in the monoclinic space group $P2_1/c$. QAVXOD crystallizes in the monoclinic space group $P2_1/n$. In CUDLEV, all atoms of the benzothiophene fragment lie in the plane within 0.02 Å. In CUDLEV, the ester substituent is turned significantly to the bicyclic system and the molecules are bound by very weak C—H···O intermolecular hydrogen bonds. Both related structures are distinguished by the nature of their substituents (morpholine-4-sulfonyl and biphenyl-4-yl groups, respectively), thus reflecting the structural flexibility of these compounds.

6. Synthesis and crystallization

The domino reaction of methyl 3-(bromomethyl)-1-benzothiophene-2-carboxylate (0.3 g, 1.05 mmol) with naphtho[2,1-*b*]thiophene (0.19 g, 1.05 mmol) using $ZnBr_2$ (0.47 g, 2.10 mmol) was carried out in dry 1,2-dichloroethane (10 ml) at room temperature under N_2 atmosphere for 6 h. The reaction mixture was then poured into crushed ice (50 g) and acidified with conc. HCl (2 ml). The crude product was then extracted with dichloromethane (3 × 10 ml) and dried with Na_2SO_4. The subsequent removal of the solvent *in vacuo* was followed by column chromatographic purification on silica gel (eluent: 2% ethyl acetate in hexane) afforded the title compound (0.23 g, 69%) as a colorless solid. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a solution in ethyl acetate at room temperature.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{16}O_2S_2$
M_r	388.48
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	8.8381 (4), 22.0387 (9), 9.5910 (3)
β (°)	94.968 (1)
V (Å^3)	1861.12 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.30
Crystal size (mm)	0.27 × 0.12 × 0.08
Data collection	
Diffractometer	Bruker APEXII CCD area detector diffractometer
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.922, 0.976
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	38099, 4271, 3717
R_{int}	0.068
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.651
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.122, 1.06
No. of reflections	4271
No. of parameters	246
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.30

Computer programs: *APEX4* and *SAINT* (Bruker, 2018), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All hydrogen atoms were positioned geometrically and refined as riding with C—H = 0.93 Å (aromatic CH) with U_{iso}(H) = 1.5U_{eq}(C) for methyl groups and 1.2U_{eq}(C) for other H atoms.

Acknowledgements

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References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.

Bruker (2018). *APEX4* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA

Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

Hirshfeld, H. L. (1977). *Theor. Chim. Acta* **44**, 129–138.

Huang, J., Luo, H., Wang, L., Guo, Y., Zhang, W., Chen, H., Zhu, M., Liu, Y. & Yu, G. (2012). *Org. Lett.* **14**, 3300–3303.

Ivachtchenko, A. V., Mitkin, O. D., Kravchenko, D. V., Kovalenko, S. M., Shishkina, S. V., Bunyatyan, N. D., Konovalova, I. S., Dmitrieva, I. G., Ivanov, V. V. & Langer, T. (2019). *Heliyon* **5**, e02738.

Izawa, T., Mori, H., Shinmura, Y., Iwatani, M., Miyazaki, E., Takimiya, K., Hung, H.-W., Yahiro, M. & Adachi, C. (2009). *Chem. Lett.* **38**, 420–421.

Katz, H. E., Bao, Z. & Gilat, S. L. (2001). *Acc. Chem. Res.* **34**, 359–369.

Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.

McKinnon, J. J., Jayatilaka, D. & Spackman, M. A. (2007). *Chem. Commun.* pp. 3814–3816.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sheldrick, G. M. (2015). *Acta Cryst.* A**71**, 3–8.

Shen, C., Spannenberg, A., Auer, M. & Wu, X.-F. (2017). *Adv. Synth. Catal.* **359**, 941–946.

Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.

Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.

Venkatesan, P., Thamotharan, S., Ilangovan, A., Liang, H. & Sundius, T. (2016). *Spectrochim. Acta A Mol. Biomol. Spectrosc.* **153**, 625–636.

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Structural elucidation and Hirshfeld surface analysis of a fused thiophene ester: methyl 3-[(naphtho[2,1-*b*]thiophen-5-yl)methyl]-1-benzothiophene-2-carboxylate

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Computing details

Methyl 3-[(naphtho[2,1-*b*]thiophen-5-yl)methyl]-1-benzothiophene-2-carboxylate

Crystal data

$C_{23}H_{16}O_2S_2$
M_r = 388.48
Monoclinic, $P2_1/c$
a = 8.8381 (4) Å
b = 22.0387 (9) Å
c = 9.5910 (3) Å
β = 94.968 (1)°
V = 1861.12 (13) Å^3
Z = 4
$F(000)$ = 808
D_x = 1.386 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3717 reflections
θ = 2.5–27.6°
μ = 0.30 mm^{-1}
T = 293 K
Block, colourless
0.27 × 0.12 × 0.08 mm

Data collection

Bruker APEXII CCD area detector diffractometer
ω and φ scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.922, T_{max} = 0.976
38099 measured reflections
4271 independent reflections
3717 reflections with $I > 2\sigma(I)$
R_{int} = 0.068
θ_{max} = 27.6°, θ_{min} = 2.5°
h = −11→11
k = −28→28
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.122
S = 1.06
4271 reflections
246 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 0.840P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 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	0.34542 (6)	0.43934 (2)	0.98904 (5)	0.05024 (18)
S2	0.62927 (6)	0.69125 (3)	0.75510 (5)	0.05271 (18)
C12	0.20885 (19)	0.61820 (7)	0.69839 (17)	0.0356 (4)
C18	0.2214 (2)	0.71310 (8)	0.56103 (18)	0.0388 (4)
C21	0.35626 (19)	0.62550 (8)	0.74821 (18)	0.0390 (4)
H21	0.402611	0.597043	0.809487	0.047*
C13	0.13745 (19)	0.66204 (7)	0.60185 (17)	0.0357 (4)
C20	0.43935 (19)	0.67627 (8)	0.70710 (17)	0.0377 (4)
C11	0.1169 (2)	0.56398 (9)	0.7392 (2)	0.0463 (4)
H11A	0.021974	0.578523	0.770724	0.056*
H11B	0.092280	0.539324	0.656601	0.056*
C19	0.3754 (2)	0.72038 (8)	0.61743 (18)	0.0392 (4)
C8	0.2809 (2)	0.47487 (8)	0.83337 (19)	0.0449 (4)
C7	0.1938 (2)	0.52451 (8)	0.85167 (19)	0.0407 (4)
C6	0.1804 (2)	0.53600 (8)	0.9982 (2)	0.0451 (4)
O2	0.4202 (2)	0.40316 (7)	0.72290 (17)	0.0672 (4)
C14	−0.0138 (2)	0.65562 (9)	0.5444 (2)	0.0460 (4)
H14	−0.070818	0.622626	0.570122	0.055*
C22	0.4825 (3)	0.76670 (9)	0.5912 (2)	0.0534 (5)
H22	0.459031	0.800284	0.534715	0.064*
C17	0.1512 (2)	0.75430 (10)	0.4623 (2)	0.0559 (5)
H17	0.206170	0.787242	0.433174	0.067*
C1	0.2574 (2)	0.49295 (9)	1.0853 (2)	0.0484 (5)
C15	−0.0784 (2)	0.69733 (11)	0.4510 (2)	0.0597 (6)
H15	−0.178874	0.692640	0.415114	0.072*
C9	0.3271 (3)	0.45074 (10)	0.7011 (2)	0.0550 (5)
C23	0.6207 (3)	0.75655 (10)	0.6568 (2)	0.0577 (5)
H23	0.703206	0.782216	0.649718	0.069*
C5	0.1042 (3)	0.58349 (10)	1.0601 (2)	0.0576 (5)
H5	0.052588	0.612757	1.004688	0.069*
C3	0.1833 (3)	0.54270 (13)	1.2871 (3)	0.0724 (7)
H3	0.183439	0.545460	1.383885	0.087*
C2	0.2580 (3)	0.49621 (11)	1.2304 (2)	0.0604 (6)
H2	0.308492	0.467139	1.287243	0.072*
O1	0.2888 (3)	0.47072 (10)	0.58721 (17)	0.0950 (7)
C4	0.1066 (3)	0.58634 (13)	1.2031 (3)	0.0750 (7)
H4	0.056388	0.617783	1.244485	0.090*
C16	0.0055 (3)	0.74655 (11)	0.4097 (3)	0.0663 (6)
H16	−0.038849	0.774302	0.345523	0.080*

C10	0.4826 (4)	0.37858 (14)	0.6016 (3)	0.0848 (9)
H10A	0.402080	0.362650	0.538502	0.127*
H10B	0.552652	0.346662	0.629634	0.127*
H10C	0.534757	0.410000	0.555647	0.127*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0610 (3)	0.0447 (3)	0.0441 (3)	0.0015 (2)	−0.0002 (2)	0.01029 (19)
S2	0.0415 (3)	0.0644 (3)	0.0513 (3)	−0.0154 (2)	−0.0015 (2)	0.0013 (2)
C12	0.0382 (8)	0.0342 (8)	0.0347 (8)	−0.0025 (7)	0.0046 (6)	0.0031 (6)
C18	0.0417 (9)	0.0341 (8)	0.0417 (9)	0.0039 (7)	0.0095 (7)	0.0038 (7)
C21	0.0385 (9)	0.0397 (9)	0.0385 (8)	−0.0011 (7)	0.0011 (7)	0.0060 (7)
C13	0.0373 (8)	0.0355 (8)	0.0350 (8)	0.0023 (6)	0.0071 (6)	0.0021 (6)
C20	0.0360 (8)	0.0417 (9)	0.0357 (8)	−0.0051 (7)	0.0039 (6)	−0.0027 (7)
C11	0.0429 (10)	0.0451 (10)	0.0497 (10)	−0.0087 (8)	−0.0017 (8)	0.0133 (8)
C19	0.0444 (9)	0.0346 (8)	0.0397 (9)	−0.0036 (7)	0.0098 (7)	−0.0013 (7)
C8	0.0537 (11)	0.0416 (9)	0.0389 (9)	−0.0077 (8)	0.0022 (8)	0.0064 (7)
C7	0.0428 (9)	0.0348 (9)	0.0440 (9)	−0.0096 (7)	0.0020 (7)	0.0084 (7)
C6	0.0476 (10)	0.0403 (9)	0.0479 (10)	−0.0133 (8)	0.0064 (8)	0.0041 (8)
O2	0.0871 (12)	0.0582 (9)	0.0584 (9)	0.0076 (8)	0.0173 (8)	−0.0084 (7)
C14	0.0388 (9)	0.0500 (10)	0.0494 (10)	0.0007 (8)	0.0045 (8)	0.0096 (8)
C22	0.0599 (12)	0.0437 (10)	0.0576 (12)	−0.0141 (9)	0.0114 (9)	0.0052 (9)
C17	0.0540 (12)	0.0453 (11)	0.0691 (13)	0.0046 (9)	0.0102 (10)	0.0228 (10)
C1	0.0546 (11)	0.0476 (10)	0.0431 (10)	−0.0133 (9)	0.0040 (8)	0.0044 (8)
C15	0.0395 (10)	0.0728 (14)	0.0656 (13)	0.0062 (10)	−0.0018 (9)	0.0188 (11)
C9	0.0650 (13)	0.0511 (12)	0.0492 (11)	−0.0099 (10)	0.0063 (9)	−0.0003 (9)
C23	0.0567 (12)	0.0579 (12)	0.0593 (12)	−0.0260 (10)	0.0092 (10)	−0.0006 (10)
C5	0.0621 (13)	0.0470 (11)	0.0655 (13)	−0.0057 (10)	0.0162 (10)	−0.0015 (9)
C3	0.0880 (18)	0.0823 (17)	0.0487 (12)	−0.0267 (15)	0.0168 (12)	−0.0091 (12)
C2	0.0714 (14)	0.0693 (14)	0.0408 (10)	−0.0208 (11)	0.0061 (9)	0.0033 (10)
O1	0.1355 (19)	0.1086 (16)	0.0410 (9)	0.0244 (14)	0.0078 (10)	0.0073 (9)
C4	0.0850 (18)	0.0702 (16)	0.0741 (16)	−0.0156 (14)	0.0316 (14)	−0.0211 (13)
C16	0.0545 (13)	0.0663 (14)	0.0773 (15)	0.0120 (11)	0.0016 (11)	0.0347 (12)
C10	0.092 (2)	0.0868 (19)	0.0798 (18)	−0.0116 (16)	0.0312 (15)	−0.0345 (15)

Geometric parameters (Å, º)

S1—C1	1.726 (2)	O2—C10	1.436 (3)
S1—C8	1.7377 (18)	C14—C15	1.373 (3)
S2—C23	1.719 (2)	C14—H14	0.9300
S2—C20	1.7334 (17)	C22—C23	1.343 (3)
C12—C21	1.358 (2)	C22—H22	0.9300
C12—C13	1.445 (2)	C17—C16	1.353 (3)
C12—C11	1.516 (2)	C17—H17	0.9300
C18—C17	1.416 (3)	C1—C2	1.393 (3)
C18—C13	1.421 (2)	C15—C16	1.391 (3)
C18—C19	1.430 (3)	C15—H15	0.9300

C21—C20	1.413 (2)	C9—O1	1.199 (3)
C21—H21	0.9300	C23—H23	0.9300
C13—C14	1.408 (2)	C5—C4	1.371 (4)
C20—C19	1.385 (2)	C5—H5	0.9300
C11—C7	1.502 (2)	C3—C2	1.358 (4)
C11—H11A	0.9700	C3—C4	1.393 (4)
C11—H11B	0.9700	C3—H3	0.9300
C19—C22	1.429 (2)	C2—H2	0.9300
C8—C7	1.358 (3)	C4—H4	0.9300
C8—C9	1.466 (3)	C16—H16	0.9300
C7—C6	1.443 (3)	C10—H10A	0.9600
C6—C1	1.401 (3)	C10—H10B	0.9600
C6—C5	1.404 (3)	C10—H10C	0.9600
O2—C9	1.338 (3)		

C1—S1—C8	91.25 (9)	C23—C22—C19	112.82 (19)
C23—S2—C20	91.03 (10)	C23—C22—H22	123.6
C21—C12—C13	119.91 (15)	C19—C22—H22	123.6
C21—C12—C11	121.49 (15)	C16—C17—C18	121.10 (19)
C13—C12—C11	118.58 (15)	C16—C17—H17	119.4
C17—C18—C13	118.88 (17)	C18—C17—H17	119.4
C17—C18—C19	121.93 (17)	C2—C1—C6	121.4 (2)
C13—C18—C19	119.16 (15)	C2—C1—S1	127.37 (18)
C12—C21—C20	120.11 (16)	C6—C1—S1	111.26 (14)
C12—C21—H21	119.9	C14—C15—C16	120.4 (2)
C20—C21—H21	119.9	C14—C15—H15	119.8
C14—C13—C18	118.18 (16)	C16—C15—H15	119.8
C14—C13—C12	122.05 (16)	O1—C9—O2	123.5 (2)
C18—C13—C12	119.76 (15)	O1—C9—C8	125.3 (2)
C19—C20—C21	122.34 (16)	O2—C9—C8	111.24 (18)
C19—C20—S2	111.39 (13)	C22—C23—S2	113.05 (15)
C21—C20—S2	126.25 (14)	C22—C23—H23	123.5
C7—C11—C12	115.01 (15)	S2—C23—H23	123.5
C7—C11—H11A	108.5	C4—C5—C6	119.4 (2)
C12—C11—H11A	108.5	C4—C5—H5	120.3
C7—C11—H11B	108.5	C6—C5—H5	120.3
C12—C11—H11B	108.5	C2—C3—C4	121.2 (2)
H11A—C11—H11B	107.5	C2—C3—H3	119.4
C20—C19—C22	111.70 (17)	C4—C3—H3	119.4
C20—C19—C18	118.67 (15)	C3—C2—C1	118.6 (2)
C22—C19—C18	129.57 (17)	C3—C2—H2	120.7
C7—C8—C9	127.41 (18)	C1—C2—H2	120.7
C7—C8—S1	113.54 (14)	C5—C4—C3	120.8 (2)
C9—C8—S1	119.02 (15)	C5—C4—H4	119.6
C8—C7—C6	111.25 (16)	C3—C4—H4	119.6
C8—C7—C11	126.90 (17)	C17—C16—C15	120.40 (19)
C6—C7—C11	121.84 (17)	C17—C16—H16	119.8
C1—C6—C5	118.58 (19)	C15—C16—H16	119.8

C1—C6—C7	112.68 (17)	O2—C10—H10A	109.5
C5—C6—C7	128.74 (19)	O2—C10—H10B	109.5
C9—O2—C10	116.3 (2)	H10A—C10—H10B	109.5
C15—C14—C13	120.99 (18)	O2—C10—H10C	109.5
C15—C14—H14	119.5	H10A—C10—H10C	109.5
C13—C14—H14	119.5	H10B—C10—H10C	109.5
C13—C12—C21—C20	0.8 (3)	C11—C7—C6—C1	178.39 (16)
C11—C12—C21—C20	179.42 (16)	C8—C7—C6—C5	178.07 (19)
C17—C18—C13—C14	−1.5 (3)	C11—C7—C6—C5	−2.4 (3)
C19—C18—C13—C14	−179.66 (16)	C18—C13—C14—C15	0.3 (3)
C17—C18—C13—C12	177.65 (17)	C12—C13—C14—C15	−178.87 (19)
C19—C18—C13—C12	−0.5 (2)	C20—C19—C22—C23	1.1 (3)
C21—C12—C13—C14	178.28 (17)	C18—C19—C22—C23	−176.02 (19)
C11—C12—C13—C14	−0.4 (3)	C13—C18—C17—C16	1.7 (3)
C21—C12—C13—C18	−0.9 (2)	C19—C18—C17—C16	179.7 (2)
C11—C12—C13—C18	−179.58 (16)	C5—C6—C1—C2	0.7 (3)
C12—C21—C20—C19	0.8 (3)	C7—C6—C1—C2	179.98 (17)
C12—C21—C20—S2	−177.49 (14)	C5—C6—C1—S1	−179.07 (15)
C23—S2—C20—C19	0.66 (14)	C7—C6—C1—S1	0.2 (2)
C23—S2—C20—C21	179.08 (17)	C8—S1—C1—C2	−179.21 (19)
C21—C12—C11—C7	7.8 (3)	C8—S1—C1—C6	0.54 (15)
C13—C12—C11—C7	−173.54 (16)	C13—C14—C15—C16	0.9 (4)
C21—C20—C19—C22	−179.62 (16)	C10—O2—C9—O1	4.1 (4)
S2—C20—C19—C22	−1.1 (2)	C10—O2—C9—C8	−175.28 (19)
C21—C20—C19—C18	−2.1 (3)	C7—C8—C9—O1	−2.9 (4)
S2—C20—C19—C18	176.38 (13)	S1—C8—C9—O1	179.0 (2)
C17—C18—C19—C20	−176.14 (18)	C7—C8—C9—O2	176.42 (19)
C13—C18—C19—C20	1.9 (2)	S1—C8—C9—O2	−1.6 (2)
C17—C18—C19—C22	0.9 (3)	C19—C22—C23—S2	−0.6 (2)
C13—C18—C19—C22	178.91 (18)	C20—S2—C23—C22	0.00 (18)
C1—S1—C8—C7	−1.23 (15)	C1—C6—C5—C4	−0.3 (3)
C1—S1—C8—C9	177.06 (16)	C7—C6—C5—C4	−179.4 (2)
C9—C8—C7—C6	−176.57 (18)	C4—C3—C2—C1	0.3 (4)
S1—C8—C7—C6	1.5 (2)	C6—C1—C2—C3	−0.7 (3)
C9—C8—C7—C11	3.9 (3)	S1—C1—C2—C3	179.00 (18)
S1—C8—C7—C11	−177.94 (14)	C6—C5—C4—C3	−0.1 (4)
C12—C11—C7—C8	−92.0 (2)	C2—C3—C4—C5	0.1 (4)
C12—C11—C7—C6	88.6 (2)	C18—C17—C16—C15	−0.5 (4)
C8—C7—C6—C1	−1.1 (2)	C14—C15—C16—C17	−0.8 (4)

Hydrogen-bond geometry (Å, º)

*Cg*2 and *Cg*4 are the centroids of the S2/C19/C20/C22/C23 and C12/C13/C18-C21 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*B*···O1	0.97	2.44	3.007 (3)	117

C10—H10*A*···*Cg*2^{i}	0.96	2.86	3.397 (3)	116
C17—H17···*Cg*4^{ii}	0.93	2.98	3.689 (2)	134

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