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Crystal structures of three 1-oxo-1,2-dihydronaphthalene derivatives: dimethyl 4-(4-methoxyphenyl)-2-(4-methylphenyl)-1-oxo-1,2-dihydronaphthalene-2,3-dicarboxylate, dimethyl 1-oxo-2-(pyren-4-yl)-4-(thiophen-2-yl)-1,2-dihydronaphthalene-2,3-dicarboxylate and ethyl 1-oxo-2-phenyl-2,4-bis(thiophen-2-yl)-1,2-dihydronaphthalene-3-carboxylate

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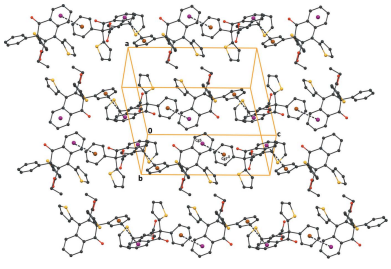
In the title 1-oxo-1,2-dihydronaphthalene derivatives, $C_{28}H_{24}O_6$, (I), $C_{34}H_{22}O_5S$, (II), and $C_{27}H_{20}O_3S_2$, (III), the cyclohexa-1,3-diene rings of the 1,2-dihydronaphthalene ring systems adopt half-chair, boat and half-chair conformations, respectively. The carbonyl O atoms attached to the dihydronaphthalene ring systems are each significantly deviated from the mean plane of the 1,2-dihydronaphthalene ring system, by 0.6162 (12) Å in (I), 0.6016 (16) Å in (II) and 0.515 (3) Å in (III). The mean planes of the 1,2-dihydronaphthalene ring systems make dihedral angles of 85.83 (3), 88.19 (3) and 81.67 (8)°, respectively, with the methylphenyl ring in (I), the pyrene ring in (II) and the phenyl ring in (III). In (I), the molecular structure is stabilized by an intramolecular C—H···O hydrogen bond, generating an $S(6)$ ring motif. In the crystal of (I), molecules are linked by an intermolecular C—H···O hydrogen bond, which generates a $C(8)$ zigzag chain running along [100]. Adjacent chains are further connected by C—H···π and offset π–π interactions [centroid–centroid distance = 3.6572 (9) Å], forming a double-chain structure. In the crystals of (II) and (III), molecules are linked into chain structures by offset π–π interactions with centroid–centroid distances of 3.5349 (12) and 3.8845 (13) Å for (II) and 3.588 (2) Å for (III). In (II) and (III), the thiophene rings are orientationally disordered over two sites, with occupancy ratios of 0.69:0.31 for (II), and 0.528 (4):0.472 (4) and 0.632 (5):0.368 (5) for (III).



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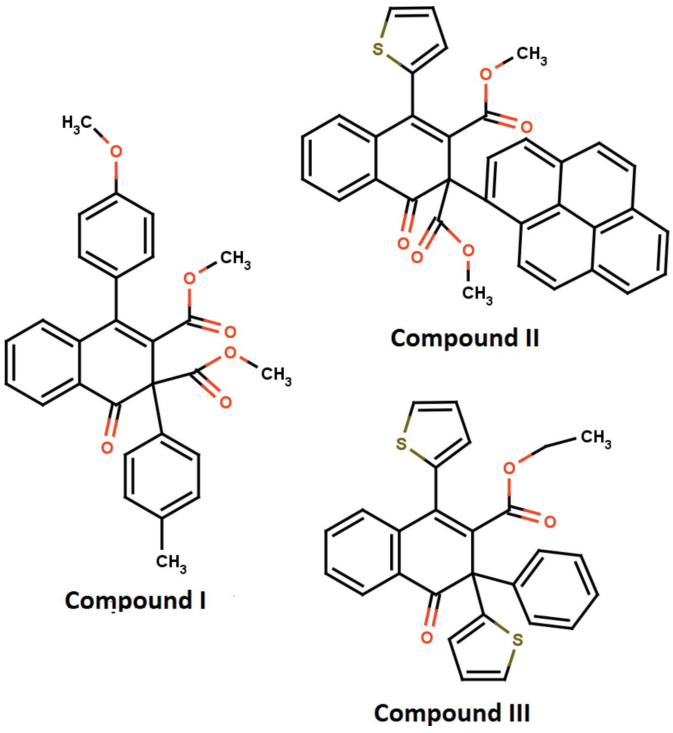
1. Chemical context

Naphthalene derivatives have been employed extensively in many fields, and some of them possess important biological and commercial applications, including use as disinfectants, insecticides and auxin plant hormones, and rooting agents (Morikawa & Takahashi, 2004). The bicyclic naphthalene skeleton constitutes a large number of clinical drugs, such as propranolol (Crowther & Smith, 1968), naproxen (Harrison *et al.*, 1970), an anti-inflammatory agent (Goudie *et al.*, 1978) and methallenestril (a non-steroid oestrogen). Dihydroxynaphthalene derivatives are a class of intermediates important for applications in dye synthesis (Bianchi *et al.*, 1997) or as

monomers in the preparation of polymers, such as polyesters (Blundell & Buckingham, 1985; Aitken *et al.*, 1992) and polynapthooxazines (Shen & Ishida, 1996). 1,2,3,4-Tetrahydronaphthalene derivatives are used for the treatment of central nervous system disorders (Jerussi *et al.*, 2004; Taber *et al.*, 2004). Tetrahydronaphthalene derivatives are also used in liquid crystal display elements (Ray *et al.*, 2003). 1-Naphthaleneacetic acid is well known as a growth regulator/stimulator in a variety of fruits and vegetables (Garriz *et al.*, 2004; Li *et al.*, 2004). Against this background, we synthesized the title compounds (I), (II) and (III) and report herein on their crystal structures and molecular conformations.



2. Structural commentary

The molecular structures of the title compounds (I), (II) and (III) are shown in Figs. 1, 2 and 3, respectively. The cyclohexa-1,3-diene rings (C1/C6–C10) of the 1,2-dihydro naphthalene ring systems of compounds (I), (II) and (III) adopt half-chair, boat and half-chair conformations, respectively, with puckering and smallest displacement parameters of q = 0.3370 (16) Å, θ = 115.7 (3)°, φ = 337.2 (3)° and ΔC_s = 5.4 (2) for (I), q = 0.257 (2) Å, θ = 66.6 (4)°, φ = 136.9 (5)° and ΔC_s = 6.9 (2) for (II), and q = 0.287 (3) Å, θ = 114.7 (6)°, φ = 337.2 (7)° and ΔC_s = 4.4 (4) for (III). In each compound, the carbonyl oxygen atom O1 deviates significantly from the mean plane of the 1,2-dihydronapthalene ring system [by 0.6453 (13) Å for (I), 0.6016 (16) Å for (II) and 0.548 (3) Å for (III)]. The mean planes of the 1,2-dihydronaphthalene ring systems make dihedral angles of 85.83 (3), 88.19 (3) and 81.67 (8)° with the methylphenyl ring in (I), the pyrene ring in (II) and the phenyl ring in (III).

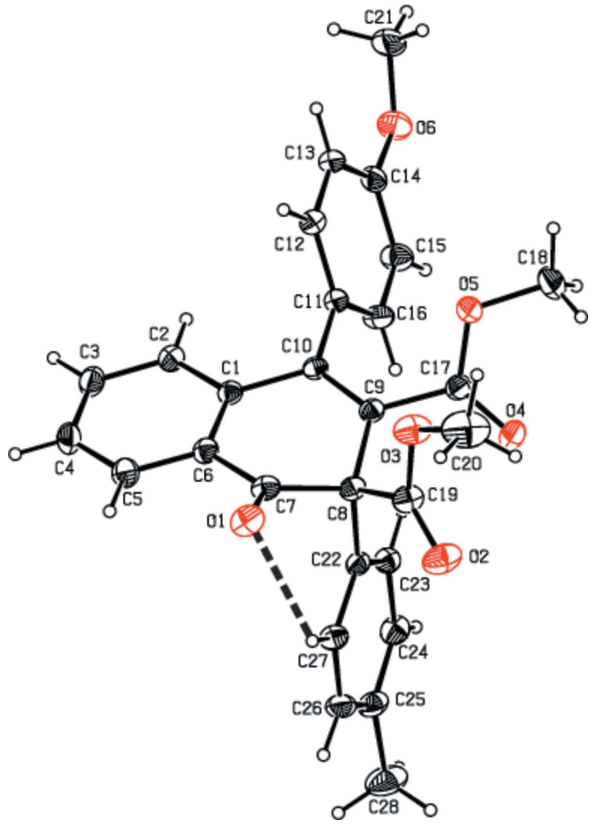


Figure 1
The molecular structure of compound (I), with the atom-numbering scheme. The intramolecular C—H···O interaction with an $S(6)$ ring motif is shown as a dashed line. Displacement ellipsoids are drawn at the 30% probability level. H atoms are shown as spheres of arbitrary radius.

In (I), the methoxyphenyl ring is inclined by 19.41 (5) and 67.84 (4)°, respectively, to the methylphenyl ring and the mean plane of 1,2-dihydronaphthalene ring system. The methyl group carbon atom C28 deviates slightly [by 0.115 (2) Å] from

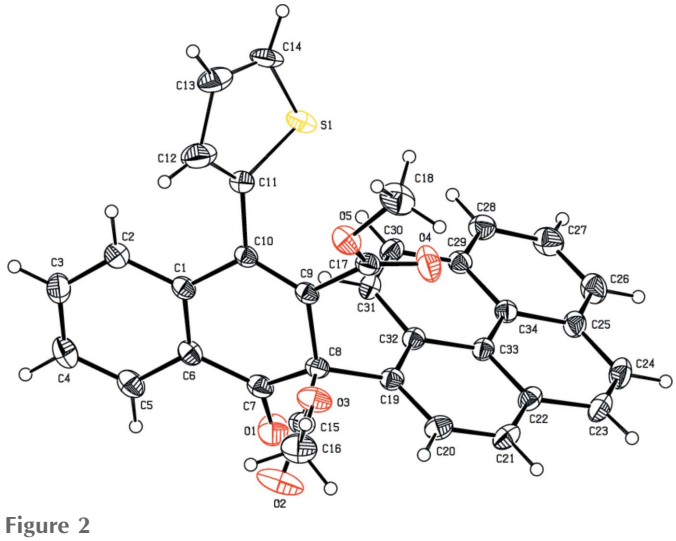


Figure 2
The molecular structure of compound (II), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are shown as spheres of arbitrary radius. For the sake of clarity, the minor component of the disordered thiophene ring has been omitted.

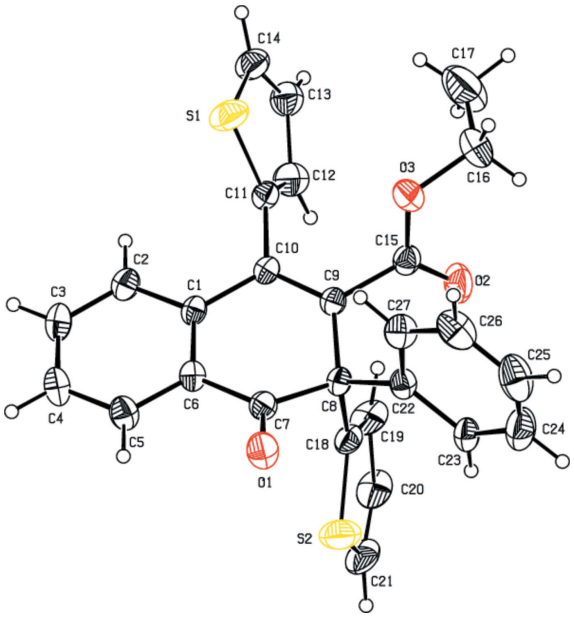


Figure 3
The molecular structure of compound (III), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are shown as spheres of arbitrary radius. For the sake of clarity, the minor components of the disordered thiophene rings have been omitted.

the C22–C27 ring. The molecular structure is stabilized by an intramolecular C—H···O hydrogen bond with an $S(6)$ ring motif (Table 1). In (II), the pyrene moiety is essentially planar with a maximum deviation of 0.085 (2) Å for atom C27. The thiophene ring is orientationally disordered over two sites with an occupancy ratio of 0.69:0.31. In (III), the two thiophene rings are also disordered with occupancy ratios of 0.528 (4):0.472 (4) and 0.632 (5):0.368 (5).

3. Supramolecular features

In the crystal of compound (I), the molecules are linked *via* C—H···O hydrogen bonds (C16—H16···O1^{i}; Table 1), generating a $C(8)$ zigzag chain along to [100]. Adjacent chains are further linked into a double-chain structure (Fig. 4) through C—H···π and π–π interactions [C3—H3···*Cg*4^{ii}; Table 1; *Cg*1···*Cg*1^{ii} = 3.6572 (9) Å, interplanar distance = 3.443 (1) Å, slippage = 1.232 Å; *Cg*1 and *Cg*4 are the centroids of the C1–C6 and C22–C27 benzene rings, respectively].

In the crystal of (II), the molecules are linked by offset π–π interactions, forming a chain along [101] [*Cg*3···*Cg*6^{iii} = 3.5349 (12) Å, interplanar distance = 3.466 (1) Å; *Cg*3···*Cg*7^{iii} = 3.8845 (13) Å, interplanar distance = 3.468 (1) Å; *Cg*3, *Cg*6 and *Cg*7 are the centroids of the C1–C6, C22–C25/C33/C34 and C25–C29/C34 benzene rings, respectively; symmetry code: (iii) $-\frac{1}{2}+x$, 1/2-*y*, $-\frac{1}{2}+z$; Fig. 5]. In the crystal of (III), the molecules are linked into a chain along [001] by an offset π–π interaction [*Cg*5···*Cg*7^{iv} = 3.888 (2) Å, interplanar distance = 3.632 (1) Å; *Cg*5 and *Cg*7 are the centroids of the benzene C1–C6 and C22–C27 rings, respectively; symmetry code: (iv) *x*, 3/2-*y*, $\frac{1}{2}+z$; Fig. 6].

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

*Cg*4 is the centroid of the C22–C27 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C27—H27···O1	0.93	2.52	3.109 (2)	121
C16—H16···O1^{i}	0.93	2.52	3.344 (3)	148
C3—H3···*Cg*4^{ii}	0.93	2.78	3.656 (2)	157

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

4. Synthesis and crystallization

Compound (I): To a stirred solution of 1-(4-methoxyphenyl)-3-*p*-tolylisobenzofuran (1 g, 3.31 mmol) in dry dichloromethane (DCM), dimethyl acetylenedicarboxylate (DMAD) (0.52 g, 3.64 mmol) was added and the reaction mixture was stirred at room temperature for 1 h. Removal of the solvent was followed by column chromatographic purification (silica gel; 15% ethyl acetate in hexane) gave the isobenzofuran–DMAD adduct as a colorless solid (1.31 g, 87%). To a stirred solution of isobenzofuran–DMAD adduct (0.30 g, 0.678 mmol) in dry DCM, $BF_3{\cdot}OEt_2$ (0.04 g, 0.28 mmol) was added and the reaction mixture was stirred at room temperature for 5 min. Removal of the solvent followed by column chromatographic purification (silica gel; 15% ethyl acetate in hexane) gave compound (I) (0.28 g, 94%) as a colorless solid. Single crystals suitable for X-ray diffraction were prepared by slow evaporation from an ethyl acetate solution of (I) at room temperature, m.p. 480–481 K.

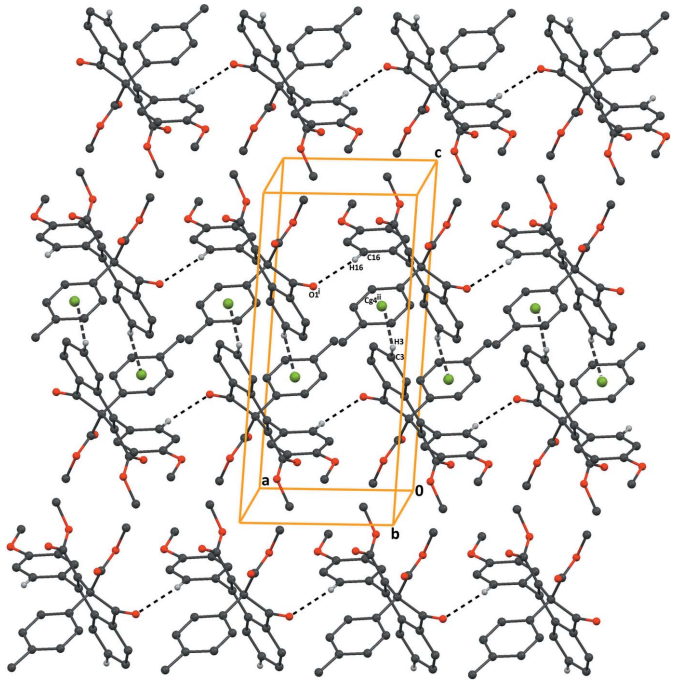


Figure 4
A packing diagram of compound (I), viewed along the *b* axis, showing the C16—H16···O1^{i} and C3—H3···*Cg*4^{ii} interactions (dashed lines). *Cg*4 is the centroid of the C22–C27 benzene ring. [Symmetry codes: (i) $-1+x, y, z$; (ii) $2-x, 1-y, 1-z$.]

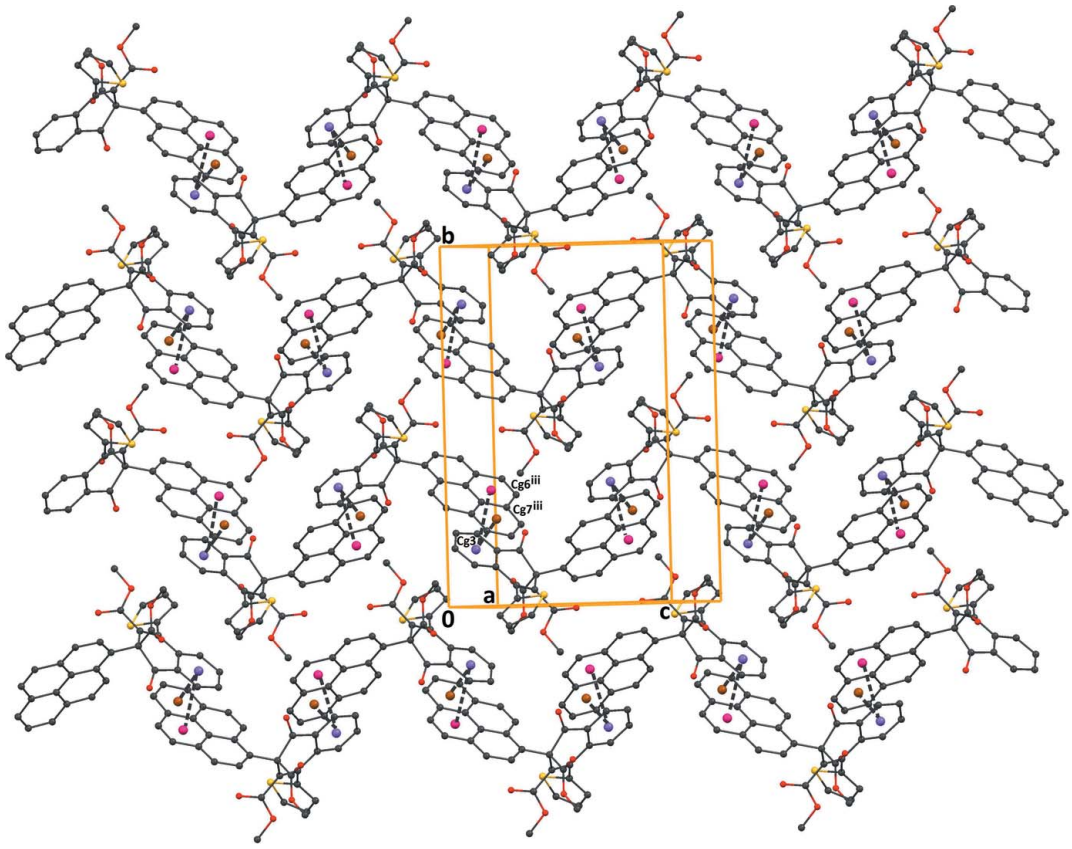


Figure 5
A packing diagram of compound (II), viewed approximately along the *a* axis, showing the π–π interactions (dashed lines). H atoms have been omitted for clarity. *Cg*3, *Cg*6 and *Cg*7 are the centroids of the C1–C6, C22–C25/C33/C34 and C25–C29/C34 benzene rings, respectively. [Symmetry code: (iii) $-\frac{1}{2}+x, \frac{1}{2}-y, -\frac{1}{2}+z$.]

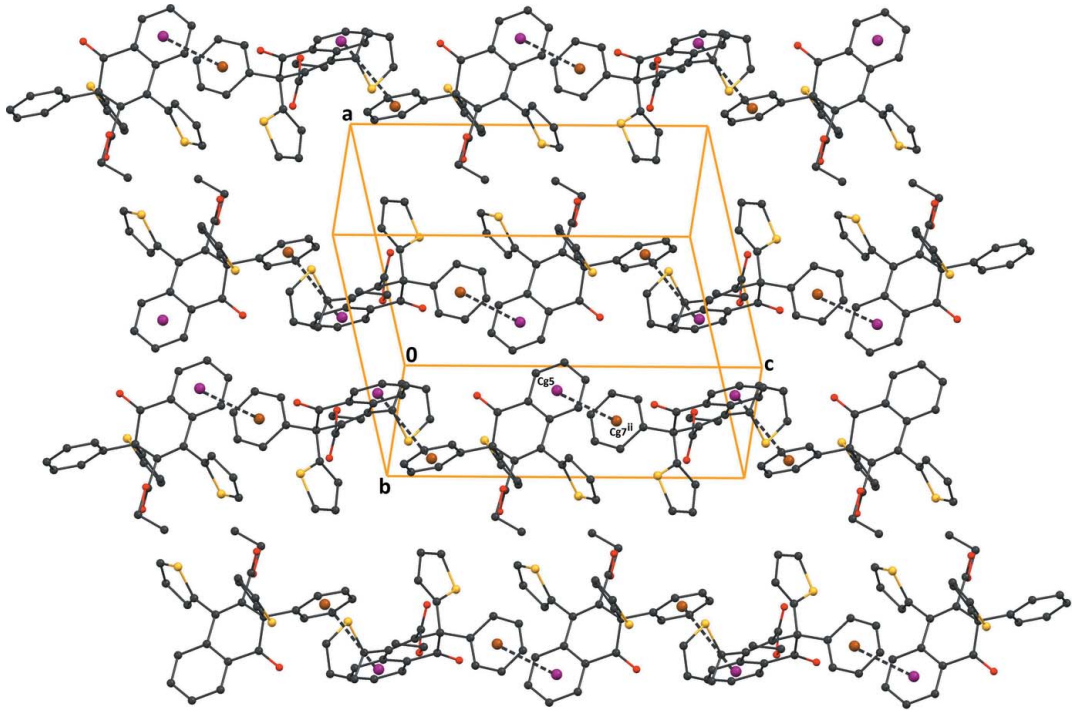


Figure 6
A packing diagram of compound (III), showing the π–π interactions (dashed lines). H atoms have been excluded for clarity. *Cg*5 and *Cg*7 are the centroids of the C1–C6 and C22–C27 benzene rings, respectively. [Symmetry code: (iv) $x, \frac{3}{2}-y, -\frac{1}{2}+z$.]

Table 2
Experimental details.

	(I)	(II)	(III)
Crystal data			
Chemical formula	$C_{28}H_{24}O_6$	$C_{34}H_{22}O_5S$	$C_{27}H_{20}O_3S_2$
M_r	456.47	542.58	456.55
Crystal system, space group	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/c$
Temperature (K)	296	296	296
a, b, c (Å)	7.5256 (2), 10.2095 (3), 15.6299 (4)	10.9268 (10), 18.9670 (14), 12.2628 (9)	12.1263 (11), 11.8009 (11), 16.0657 (13)
α, β, γ (°)	93.990 (1), 94.679 (1), 101.089 (2)	90, 93.030 (2), 90	90, 100.181 (2), 90
V (Å^3)	1170.06 (6)	2537.9 (4)	2262.8 (3)
Z	2	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.09	0.17	0.26
Crystal size (mm)	0.35 × 0.30 × 0.25	0.25 × 0.25 × 0.20	0.25 × 0.25 × 0.15
Data collection			
Diffractometer	Bruker Kappa APEXII CCD	Bruker Kappa APEXII CCD	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)	Multi-scan (*SADABS*; Bruker, 2008)	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.969, 0.978	0.958, 0.966	0.937, 0.962
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22413, 4119, 3346	21576, 4457, 3341	29901, 4110, 2685
R_{int}	0.027	0.031	0.044
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595	0.595	0.603
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.111, 1.03	0.039, 0.105, 1.04	0.061, 0.147, 1.09
No. of reflections	4119	4457	4110
No. of parameters	311	400	364
No. of restraints	0	56	100
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.21	0.22, −0.22	0.24, −0.24

Computer programs: *APEX2*and *SAINT* (Bruker, 2008), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2015).

Compound (II): To a stirred solution of 1-(pyren-1-yl)-3-(thiophen-2-yl)isobenzofuran (0.50 g, 1.25 mmol) in dry DCM (10 ml), DMAD (0.19 g, 1.32 mmol) was added and the reaction mixture was stirred at room temperature for 1 h. To this, $BF_3{\cdot}OEt_2$ (0.075 g, 0.53 mmol) was added and stirred at room temperature for 5 min. Removal of the solvent followed by column chromatographic purification (silia gel; 15% ethyl acetate in hexane) afforded compound (II) as a yellow solid. Single crystals suitable for X-ray diffraction were prepared by slow evaporation from an ethyl acetate solution of (II) at room temperature, m.p. 469–471 K.

Compound (III): To a solution of 1,3-di(thiophen-2-yl)isobenzo furan (0.50 g, 1.77 mmol) in dry toluene (15 ml), ethyl-3-phenylpropiolate (0.34 g, 1.95 mmol) was added and refluxed till the consumption of 1,3-di(thiophen-2-yl)isobenzofuran (disappearance of fluorescent colour in 8 h). After removal of toluene *in vacuo*, the crude adduct was dissolved in dry DCM (15 ml), $BF_3{\cdot}OEt_2$ (0.075 g, 0.52 mmol) was added and the reaction mixture was stirred for 10 min at room temperature. Removal of the solvent was followed by column chromatographic purification (silica gel; 15% ethyl accetate in hexane) which afforded compound (III) as a green solid (0.53 g, 65%). Single crystals suitable for X-ray diffraction were prepared by slow evaporation from an ethyl acetate solution of (III) at room temperature, m.p. 383–385 K.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. For all compounds, H atoms were localized in difference Fourier maps and were then constrained geometrically with C—H = 0.93, 0.96 and 0.97 Å for aryl, methyl and methylene H atoms, respectively, allowing for rotation of the methyl groups. The U_{iso}(H) values were set to 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for other H atoms. In compound (II), the thiophene ring is disordered and the occupancy ratio was refined to 0.691 (3):0.309 (3), which was then fixed at 0.69:0.31 in the final refinement. In compound (III), the two thiophene rings are disordered with refined occupancy ratios of 0.528 (4):0.472 (4) and 0.632 (5):0.368 (5). For (II) and (III), ellipsoid displacement restraints (*SIMU* and *DELU*) and bond length restraints (*DFIX*) with C—S = 1.70 (1) Å, C—C = 1.50 (1) Å and C═C = 1.40 (1) Å were applied to the disordered rings.

Acknowledgements

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supporting information

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Crystal structures of three 1-oxo-1,2-dihydronaphthalene derivatives: dimethyl 4-(4-methoxyphenyl)-2-(4-methylphenyl)-1-oxo-1,2-dihydronaphthalene-2,3-dicarboxylate, dimethyl 1-oxo-2-(pyren-4-yl)-4-(thiophen-2-yl)-1,2-dihydronaphthalene-2,3-dicarboxylate and ethyl 1-oxo-2-phenyl-2,4-bis(thiophen-2-yl)-1,2-dihydronaphthalene-3-carboxylate

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Computing details

For all compounds, data collection: *APEX2* (Bruker, 2008); cell refinement: *APEX2* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2015).

(I) Dimethyl 4-(4-methoxyphenyl)-2-(4-methylphenyl)-1-oxo-1,2-dihydronaphthalene-2,3-dicarboxylate

Crystal data

$C_{28}H_{24}O_6$
M_r = 456.47
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.5256 (2) Å
b = 10.2095 (3) Å
c = 15.6299 (4) Å
α = 93.990 (1)°
β = 94.679 (1)°
γ = 101.089 (2)°
V = 1170.06 (6) Å^3
Z = 2
$F(000)$ = 480
D_x = 1.296 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4119 reflections
θ = 2.3–25.0°
μ = 0.09 mm^{-1}
T = 296 K
Block, colourless
0.35 × 0.30 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω &φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.969, T_{max} = 0.978
22413 measured reflections
4119 independent reflections
3346 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −8→8
k = −12→12
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.111$
$S = 1.03$
4119 reflections
311 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
$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 0.2906P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.19$ 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 $F^2 > 2$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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.04016 (19)	0.52685 (14)	0.34053 (9)	0.0385 (3)
C2	1.0229 (2)	0.63513 (15)	0.39596 (10)	0.0478 (4)
H2	0.9373	0.6863	0.3807	0.057*
C3	1.1303 (2)	0.66814 (17)	0.47312 (11)	0.0550 (4)
H3	1.1160	0.7407	0.5095	0.066*
C4	1.2578 (2)	0.59471 (18)	0.49645 (11)	0.0587 (5)
H4	1.3297	0.6170	0.5486	0.070*
C5	1.2791 (2)	0.48799 (18)	0.44251 (11)	0.0550 (4)
H5	1.3667	0.4387	0.4581	0.066*
C6	1.17134 (19)	0.45323 (14)	0.36521 (10)	0.0417 (3)
C7	1.1958 (2)	0.33854 (15)	0.30791 (10)	0.0446 (4)
C8	1.0303 (2)	0.27105 (14)	0.24589 (9)	0.0397 (3)
C9	0.92937 (19)	0.37508 (14)	0.21154 (9)	0.0385 (3)
C10	0.92853 (19)	0.49101 (14)	0.25739 (9)	0.0371 (3)
C11	0.8042 (2)	0.58099 (14)	0.23090 (9)	0.0401 (3)
C12	0.8649 (2)	0.70937 (15)	0.20884 (10)	0.0479 (4)
H12	0.9892	0.7416	0.2088	0.058*
C13	0.7446 (3)	0.79111 (15)	0.18672 (10)	0.0521 (4)
H13	0.7878	0.8768	0.1710	0.063*
C14	0.5606 (2)	0.74492 (16)	0.18809 (10)	0.0509 (4)
C15	0.4985 (2)	0.61764 (18)	0.21056 (12)	0.0594 (5)
H15	0.3743	0.5861	0.2118	0.071*
C16	0.6190 (2)	0.53671 (16)	0.23124 (11)	0.0522 (4)
H16	0.5749	0.4504	0.2458	0.063*
C17	0.8254 (2)	0.33536 (15)	0.12560 (10)	0.0457 (4)

C18	0.7520 (3)	0.4012 (2)	−0.01137 (12)	0.0833 (7)
H18A	0.7824	0.3208	−0.0363	0.125*
H18B	0.7902	0.4735	−0.0461	0.125*
H18C	0.6228	0.3879	−0.0088	0.125*
C19	1.0997 (2)	0.19417 (17)	0.17186 (11)	0.0523 (4)
C20	1.2394 (4)	0.2216 (3)	0.04350 (16)	0.1075 (10)
H20A	1.3518	0.1943	0.0597	0.161*
H20B	1.2588	0.2863	0.0018	0.161*
H20C	1.1505	0.1449	0.0190	0.161*
C21	0.4758 (4)	0.9350 (2)	0.12847 (14)	0.0822 (7)
H21A	0.5676	0.9976	0.1647	0.123*
H21B	0.3702	0.9736	0.1181	0.123*
H21C	0.5219	0.9148	0.0746	0.123*
C22	0.9152 (2)	0.17131 (13)	0.29922 (9)	0.0383 (3)
C23	0.7324 (2)	0.16747 (15)	0.30518 (9)	0.0435 (4)
H23	0.6760	0.2297	0.2789	0.052*
C24	0.6325 (2)	0.07153 (17)	0.35007 (11)	0.0536 (4)
H24	0.5091	0.0698	0.3528	0.064*
C25	0.7110 (3)	−0.02137 (16)	0.39079 (11)	0.0569 (5)
C26	0.8952 (3)	−0.01318 (16)	0.38729 (11)	0.0575 (5)
H26	0.9528	−0.0724	0.4162	0.069*
C27	0.9956 (2)	0.08046 (15)	0.34213 (10)	0.0494 (4)
H27	1.1194	0.0828	0.3404	0.059*
C28	0.6003 (4)	−0.1312 (2)	0.43490 (16)	0.0927 (8)
H28A	0.4822	−0.1116	0.4415	0.139*
H28B	0.6608	−0.1372	0.4906	0.139*
H28C	0.5874	−0.2150	0.4007	0.139*
O1	1.33429 (15)	0.29405 (12)	0.31246 (9)	0.0629 (3)
O2	1.0894 (2)	0.07656 (13)	0.16239 (9)	0.0765 (4)
O3	1.17487 (19)	0.28042 (13)	0.11870 (8)	0.0680 (4)
O4	0.7426 (2)	0.22389 (12)	0.10391 (8)	0.0720 (4)
O5	0.84266 (17)	0.43348 (11)	0.07425 (7)	0.0588 (3)
O6	0.42858 (19)	0.81619 (13)	0.16963 (9)	0.0736 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0357 (8)	0.0370 (7)	0.0416 (8)	0.0024 (6)	0.0060 (6)	0.0053 (6)
C2	0.0525 (9)	0.0418 (8)	0.0484 (9)	0.0102 (7)	0.0033 (7)	0.0000 (7)
C3	0.0607 (11)	0.0499 (9)	0.0493 (9)	0.0035 (8)	0.0019 (8)	−0.0061 (7)
C4	0.0537 (10)	0.0613 (11)	0.0525 (10)	−0.0007 (8)	−0.0102 (8)	−0.0034 (8)
C5	0.0391 (9)	0.0574 (10)	0.0646 (11)	0.0051 (7)	−0.0072 (8)	0.0061 (8)
C6	0.0318 (8)	0.0415 (8)	0.0495 (8)	0.0014 (6)	0.0035 (6)	0.0044 (6)
C7	0.0355 (8)	0.0419 (8)	0.0577 (9)	0.0070 (7)	0.0095 (7)	0.0103 (7)
C8	0.0398 (8)	0.0357 (7)	0.0450 (8)	0.0086 (6)	0.0099 (6)	0.0031 (6)
C9	0.0377 (8)	0.0368 (7)	0.0407 (7)	0.0038 (6)	0.0075 (6)	0.0057 (6)
C10	0.0359 (8)	0.0346 (7)	0.0404 (7)	0.0035 (6)	0.0073 (6)	0.0064 (6)
C11	0.0462 (9)	0.0358 (7)	0.0380 (7)	0.0076 (6)	0.0027 (6)	0.0035 (6)

C12	0.0503 (9)	0.0400 (8)	0.0504 (9)	0.0023 (7)	0.0011 (7)	0.0060 (7)
C13	0.0724 (12)	0.0339 (8)	0.0481 (9)	0.0083 (8)	−0.0030 (8)	0.0071 (7)
C14	0.0622 (11)	0.0471 (9)	0.0459 (8)	0.0219 (8)	−0.0059 (7)	0.0024 (7)
C15	0.0471 (10)	0.0586 (11)	0.0754 (12)	0.0143 (8)	0.0035 (8)	0.0188 (9)
C16	0.0472 (10)	0.0434 (9)	0.0674 (10)	0.0084 (7)	0.0058 (8)	0.0178 (8)
C17	0.0515 (9)	0.0404 (8)	0.0432 (8)	0.0041 (7)	0.0068 (7)	0.0026 (7)
C18	0.1029 (17)	0.0871 (15)	0.0472 (10)	−0.0074 (13)	−0.0152 (10)	0.0165 (10)
C19	0.0560 (10)	0.0487 (10)	0.0569 (10)	0.0157 (8)	0.0199 (8)	0.0045 (8)
C20	0.153 (3)	0.1032 (18)	0.0904 (17)	0.0530 (18)	0.0810 (18)	0.0205 (14)
C21	0.1208 (19)	0.0549 (11)	0.0772 (14)	0.0400 (12)	−0.0099 (13)	0.0101 (10)
C22	0.0435 (8)	0.0317 (7)	0.0391 (7)	0.0057 (6)	0.0063 (6)	0.0000 (6)
C23	0.0445 (9)	0.0430 (8)	0.0434 (8)	0.0083 (7)	0.0073 (6)	0.0042 (6)
C24	0.0519 (10)	0.0529 (10)	0.0541 (9)	0.0010 (8)	0.0181 (8)	0.0030 (8)
C25	0.0831 (13)	0.0392 (9)	0.0477 (9)	0.0033 (8)	0.0232 (9)	0.0035 (7)
C26	0.0863 (14)	0.0385 (8)	0.0514 (9)	0.0189 (9)	0.0104 (9)	0.0084 (7)
C27	0.0538 (10)	0.0401 (8)	0.0563 (9)	0.0140 (7)	0.0066 (7)	0.0046 (7)
C28	0.129 (2)	0.0605 (12)	0.0908 (16)	0.0013 (13)	0.0515 (15)	0.0203 (11)
O1	0.0382 (6)	0.0576 (7)	0.0956 (9)	0.0162 (5)	0.0070 (6)	0.0054 (6)
O2	0.1068 (11)	0.0500 (8)	0.0825 (9)	0.0275 (7)	0.0436 (8)	0.0008 (6)
O3	0.0830 (9)	0.0626 (8)	0.0690 (8)	0.0226 (7)	0.0432 (7)	0.0144 (6)
O4	0.0977 (10)	0.0488 (7)	0.0551 (7)	−0.0138 (7)	−0.0069 (7)	0.0012 (6)
O5	0.0773 (8)	0.0510 (7)	0.0415 (6)	−0.0017 (6)	−0.0036 (5)	0.0095 (5)
O6	0.0803 (10)	0.0613 (8)	0.0852 (9)	0.0335 (7)	−0.0090 (7)	0.0141 (7)

Geometric parameters (Å, º)

C1—C2	1.389 (2)	C17—O4	1.1990 (19)
C1—C6	1.397 (2)	C17—O5	1.3204 (19)
C1—C10	1.472 (2)	C18—O5	1.438 (2)
C2—C3	1.379 (2)	C18—H18A	0.9600
C2—H2	0.9300	C18—H18B	0.9600
C3—C4	1.369 (2)	C18—H18C	0.9600
C3—H3	0.9300	C19—O2	1.186 (2)
C4—C5	1.373 (2)	C19—O3	1.331 (2)
C4—H4	0.9300	C20—O3	1.444 (2)
C5—C6	1.383 (2)	C20—H20A	0.9600
C5—H5	0.9300	C20—H20B	0.9600
C6—C7	1.473 (2)	C20—H20C	0.9600
C7—O1	1.2134 (18)	C21—O6	1.412 (3)
C7—C8	1.531 (2)	C21—H21A	0.9600
C8—C9	1.522 (2)	C21—H21B	0.9600
C8—C19	1.535 (2)	C21—H21C	0.9600
C8—C22	1.542 (2)	C22—C23	1.380 (2)
C9—C10	1.342 (2)	C22—C27	1.383 (2)
C9—C17	1.487 (2)	C23—C24	1.384 (2)
C10—C11	1.487 (2)	C23—H23	0.9300
C11—C12	1.380 (2)	C24—C25	1.375 (3)
C11—C16	1.381 (2)	C24—H24	0.9300

C12—C13	1.384 (2)	C25—C26	1.379 (3)
C12—H12	0.9300	C25—C28	1.506 (3)
C13—C14	1.377 (3)	C26—C27	1.373 (2)
C13—H13	0.9300	C26—H26	0.9300
C14—O6	1.364 (2)	C27—H27	0.9300
C14—C15	1.374 (2)	C28—H28A	0.9600
C15—C16	1.374 (2)	C28—H28B	0.9600
C15—H15	0.9300	C28—H28C	0.9600
C16—H16	0.9300		

C2—C1—C6	117.75 (13)	O4—C17—O5	123.66 (15)
C2—C1—C10	122.02 (13)	O4—C17—C9	123.29 (14)
C6—C1—C10	120.21 (13)	O5—C17—C9	112.94 (13)
C3—C2—C1	121.18 (15)	O5—C18—H18A	109.5
C3—C2—H2	119.4	O5—C18—H18B	109.5
C1—C2—H2	119.4	H18A—C18—H18B	109.5
C4—C3—C2	120.32 (15)	O5—C18—H18C	109.5
C4—C3—H3	119.8	H18A—C18—H18C	109.5
C2—C3—H3	119.8	H18B—C18—H18C	109.5
C3—C4—C5	119.76 (15)	O2—C19—O3	124.44 (15)
C3—C4—H4	120.1	O2—C19—C8	126.23 (15)
C5—C4—H4	120.1	O3—C19—C8	109.33 (13)
C4—C5—C6	120.48 (16)	O3—C20—H20A	109.5
C4—C5—H5	119.8	O3—C20—H20B	109.5
C6—C5—H5	119.8	H20A—C20—H20B	109.5
C5—C6—C1	120.50 (14)	O3—C20—H20C	109.5
C5—C6—C7	119.92 (14)	H20A—C20—H20C	109.5
C1—C6—C7	119.58 (13)	H20B—C20—H20C	109.5
O1—C7—C6	122.60 (15)	O6—C21—H21A	109.5
O1—C7—C8	121.18 (14)	O6—C21—H21B	109.5
C6—C7—C8	116.07 (12)	H21A—C21—H21B	109.5
C9—C8—C7	110.59 (11)	O6—C21—H21C	109.5
C9—C8—C19	110.62 (12)	H21A—C21—H21C	109.5
C7—C8—C19	107.56 (12)	H21B—C21—H21C	109.5
C9—C8—C22	113.30 (12)	C23—C22—C27	118.00 (14)
C7—C8—C22	104.74 (11)	C23—C22—C8	122.47 (13)
C19—C8—C22	109.74 (12)	C27—C22—C8	119.53 (13)
C10—C9—C17	122.91 (13)	C22—C23—C24	120.40 (15)
C10—C9—C8	122.15 (13)	C22—C23—H23	119.8
C17—C9—C8	114.88 (12)	C24—C23—H23	119.8
C9—C10—C1	120.24 (13)	C25—C24—C23	121.70 (16)
C9—C10—C11	121.87 (13)	C25—C24—H24	119.2
C1—C10—C11	117.65 (12)	C23—C24—H24	119.2
C12—C11—C16	117.89 (14)	C24—C25—C26	117.36 (15)
C12—C11—C10	123.18 (14)	C24—C25—C28	121.8 (2)
C16—C11—C10	118.88 (13)	C26—C25—C28	120.81 (19)
C11—C12—C13	121.32 (15)	C27—C26—C25	121.52 (16)
C11—C12—H12	119.3	C27—C26—H26	119.2

C13—C12—H12	119.3	C25—C26—H26	119.2
C14—C13—C12	119.67 (15)	C26—C27—C22	120.94 (16)
C14—C13—H13	120.2	C26—C27—H27	119.5
C12—C13—H13	120.2	C22—C27—H27	119.5
O6—C14—C15	115.00 (16)	C25—C28—H28A	109.5
O6—C14—C13	125.43 (16)	C25—C28—H28B	109.5
C15—C14—C13	119.57 (15)	H28A—C28—H28B	109.5
C16—C15—C14	120.27 (17)	C25—C28—H28C	109.5
C16—C15—H15	119.9	H28A—C28—H28C	109.5
C14—C15—H15	119.9	H28B—C28—H28C	109.5
C15—C16—C11	121.27 (15)	C19—O3—C20	115.56 (15)
C15—C16—H16	119.4	C17—O5—C18	116.25 (13)
C11—C16—H16	119.4	C14—O6—C21	118.23 (17)

C6—C1—C2—C3	−0.6 (2)	C11—C12—C13—C14	1.2 (2)
C10—C1—C2—C3	−179.19 (14)	C12—C13—C14—O6	178.48 (15)
C1—C2—C3—C4	0.4 (3)	C12—C13—C14—C15	−0.7 (2)
C2—C3—C4—C5	0.3 (3)	O6—C14—C15—C16	−179.47 (16)
C3—C4—C5—C6	−0.7 (3)	C13—C14—C15—C16	−0.2 (3)
C4—C5—C6—C1	0.5 (2)	C14—C15—C16—C11	0.7 (3)
C4—C5—C6—C7	179.96 (15)	C12—C11—C16—C15	−0.2 (2)
C2—C1—C6—C5	0.1 (2)	C10—C11—C16—C15	177.47 (15)
C10—C1—C6—C5	178.74 (14)	C10—C9—C17—O4	−138.46 (18)
C2—C1—C6—C7	−179.29 (13)	C8—C9—C17—O4	38.7 (2)
C10—C1—C6—C7	−0.7 (2)	C10—C9—C17—O5	45.2 (2)
C5—C6—C7—O1	−20.2 (2)	C8—C9—C17—O5	−137.56 (14)
C1—C6—C7—O1	159.22 (15)	C9—C8—C19—O2	−135.20 (19)
C5—C6—C7—C8	155.47 (14)	C7—C8—C19—O2	103.9 (2)
C1—C6—C7—C8	−25.1 (2)	C22—C8—C19—O2	−9.5 (2)
O1—C7—C8—C9	−146.10 (15)	C9—C8—C19—O3	44.87 (18)
C6—C7—C8—C9	38.16 (17)	C7—C8—C19—O3	−76.01 (17)
O1—C7—C8—C19	−25.2 (2)	C22—C8—C19—O3	170.60 (13)
C6—C7—C8—C19	159.05 (13)	C9—C8—C22—C23	7.84 (19)
O1—C7—C8—C22	91.51 (17)	C7—C8—C22—C23	128.45 (14)
C6—C7—C8—C22	−84.24 (15)	C19—C8—C22—C23	−116.35 (15)
C7—C8—C9—C10	−29.46 (18)	C9—C8—C22—C27	−173.06 (12)
C19—C8—C9—C10	−148.52 (14)	C7—C8—C22—C27	−52.45 (16)
C22—C8—C9—C10	87.78 (16)	C19—C8—C22—C27	62.75 (17)
C7—C8—C9—C17	153.32 (12)	C27—C22—C23—C24	−2.6 (2)
C19—C8—C9—C17	34.26 (17)	C8—C22—C23—C24	176.56 (13)
C22—C8—C9—C17	−89.44 (14)	C22—C23—C24—C25	0.8 (2)
C17—C9—C10—C1	−177.56 (13)	C23—C24—C25—C26	1.7 (2)
C8—C9—C10—C1	5.4 (2)	C23—C24—C25—C28	−176.07 (17)
C17—C9—C10—C11	8.2 (2)	C24—C25—C26—C27	−2.5 (2)
C8—C9—C10—C11	−168.83 (13)	C28—C25—C26—C27	175.31 (17)
C2—C1—C10—C9	−170.09 (14)	C25—C26—C27—C22	0.8 (2)
C6—C1—C10—C9	11.4 (2)	C23—C22—C27—C26	1.8 (2)
C2—C1—C10—C11	4.4 (2)	C8—C22—C27—C26	−177.35 (14)

C6—C1—C10—C11	−174.13 (12)	O2—C19—O3—C20	2.7 (3)
C9—C10—C11—C12	−117.13 (17)	C8—C19—O3—C20	−177.38 (18)
C1—C10—C11—C12	68.45 (18)	O4—C17—O5—C18	1.3 (3)
C9—C10—C11—C16	65.36 (19)	C9—C17—O5—C18	177.56 (16)
C1—C10—C11—C16	−109.06 (16)	C15—C14—O6—C21	−166.54 (17)
C16—C11—C12—C13	−0.7 (2)	C13—C14—O6—C21	14.3 (2)
C10—C11—C12—C13	−178.28 (14)		

Hydrogen-bond geometry (Å, º)

*Cg*4 is the centroid of the C22–C27 benzene ring .

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C27—H27···O1	0.93	2.52	3.109 (2)	121
C16—H16···O1^{i}	0.93	2.52	3.344 (3)	148
C3—H3···*Cg*4^{ii}	0.93	2.78	3.656 (2)	157

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

(II) Dimethyl 1-oxo-2-(pyren-4-yl)-4-(thiophen-2-yl)-1,2-dihydronaphthalene-2,3-dicarboxylate

Crystal data

$C_{34}H_{22}O_5S$
M_r = 542.58
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 10.9268 (10) Å
b = 18.9670 (14) Å
c = 12.2628 (9) Å
β = 93.030 (2)°
V = 2537.9 (4) Å^3
Z = 4
$F(000)$ = 1128
D_x = 1.420 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4457 reflections
θ = 2.0–25.0°
μ = 0.17 mm^{-1}
T = 296 K
Block, colourless
0.25 × 0.25 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω & φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.958, T_{max} = 0.966
21576 measured reflections
4457 independent reflections
3341 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.0°, θ_{min} = 2.0°
h = −12→12
k = −22→22
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.105
S = 1.04
4457 reflections
400 parameters
56 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
$w = 1/[\sigma^2(F_o^2) + (0.042P)^2 + 1.1182P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.53176 (18)	0.11069 (10)	0.09837 (15)	0.0320 (5)	
C2	0.4292 (2)	0.11714 (12)	0.02630 (16)	0.0416 (5)	
H2	0.3605	0.0895	0.0364	0.050*	
C3	0.4284 (2)	0.16390 (12)	−0.05966 (17)	0.0478 (6)	
H3	0.3601	0.1664	−0.1080	0.057*	
C4	0.5269 (2)	0.20675 (12)	−0.07487 (18)	0.0498 (6)	
H4	0.5261	0.2375	−0.1340	0.060*	
C5	0.6268 (2)	0.20404 (11)	−0.00227 (17)	0.0452 (6)	
H5	0.6923	0.2346	−0.0106	0.054*	
C6	0.63113 (19)	0.15603 (10)	0.08371 (15)	0.0351 (5)	
C7	0.73736 (19)	0.15549 (11)	0.16206 (16)	0.0376 (5)	
C8	0.76155 (18)	0.08696 (10)	0.22786 (15)	0.0321 (5)	
C9	0.64414 (18)	0.04512 (9)	0.24500 (15)	0.0297 (4)	
C10	0.53834 (18)	0.05803 (10)	0.18734 (15)	0.0299 (4)	
C11	0.42509 (18)	0.02128 (10)	0.21535 (16)	0.0336 (5)	
C15	0.84101 (19)	0.04475 (11)	0.15007 (16)	0.0392 (5)	
C16	0.8909 (2)	−0.06625 (13)	0.0818 (2)	0.0595 (7)	
H16A	0.8763	−0.0497	0.0083	0.089*	
H16B	0.8652	−0.1145	0.0865	0.089*	
H16C	0.9768	−0.0629	0.1021	0.089*	
C17	0.65383 (19)	−0.01355 (10)	0.32741 (17)	0.0355 (5)	
C18	0.5913 (3)	−0.12957 (12)	0.3641 (2)	0.0642 (7)	
H18A	0.6683	−0.1403	0.4018	0.096*	
H18B	0.5611	−0.1707	0.3258	0.096*	
H18C	0.5333	−0.1152	0.4158	0.096*	
C19	0.83524 (18)	0.10328 (10)	0.33498 (15)	0.0321 (4)	
C20	0.94999 (19)	0.07443 (11)	0.35762 (18)	0.0400 (5)	
H20	0.9840	0.0456	0.3058	0.048*	
C21	1.01527 (19)	0.08713 (11)	0.45472 (18)	0.0417 (5)	
H21	1.0915	0.0661	0.4677	0.050*	
C22	0.96935 (18)	0.13071 (10)	0.53330 (16)	0.0351 (5)	
C23	1.0356 (2)	0.14591 (12)	0.63475 (18)	0.0458 (6)	
H23	1.1102	0.1236	0.6508	0.055*	
C24	0.9928 (2)	0.19113 (12)	0.70620 (18)	0.0472 (6)	
H24	1.0394	0.2005	0.7702	0.057*	

C25	0.8774 (2)	0.22576 (11)	0.68799 (16)	0.0383 (5)	
C26	0.8312 (2)	0.27434 (12)	0.76016 (18)	0.0494 (6)	
H26	0.8772	0.2855	0.8238	0.059*	
C27	0.7194 (2)	0.30626 (13)	0.73977 (19)	0.0507 (6)	
H27	0.6915	0.3390	0.7892	0.061*	
C28	0.6483 (2)	0.29028 (11)	0.64711 (17)	0.0425 (5)	
H28	0.5721	0.3115	0.6349	0.051*	
C29	0.69065 (18)	0.24205 (10)	0.57106 (15)	0.0333 (5)	
C30	0.62192 (18)	0.22445 (10)	0.47291 (16)	0.0366 (5)	
H30	0.5443	0.2438	0.4602	0.044*	
C31	0.66595 (18)	0.18065 (10)	0.39807 (16)	0.0346 (5)	
H31	0.6182	0.1712	0.3347	0.042*	
C32	0.78410 (17)	0.14808 (10)	0.41282 (15)	0.0301 (4)	
C33	0.85277 (17)	0.16242 (10)	0.51215 (15)	0.0305 (4)	
C34	0.80620 (18)	0.20967 (10)	0.59065 (15)	0.0315 (4)	
O1	0.80805 (16)	0.20458 (8)	0.17246 (13)	0.0578 (5)	
O2	0.91056 (18)	0.07160 (9)	0.09104 (16)	0.0783 (6)	
O3	0.82234 (14)	−0.02357 (8)	0.15510 (12)	0.0491 (4)	
O4	0.69985 (18)	−0.00824 (9)	0.41768 (13)	0.0651 (5)	
O5	0.60807 (14)	−0.07340 (7)	0.28718 (12)	0.0445 (4)	
S1	0.37700 (13)	0.02866 (9)	0.34494 (12)	0.0438 (3)	0.69
C12	0.3568 (12)	−0.0254 (7)	0.1509 (9)	0.064 (3)	0.69
H12	0.3719	−0.0367	0.0790	0.076*	0.69
C13	0.2563 (11)	−0.0549 (7)	0.2127 (7)	0.0570 (16)	0.69
H13	0.1993	−0.0878	0.1856	0.068*	0.69
C14	0.2593 (8)	−0.0272 (5)	0.3137 (6)	0.0508 (18)	0.69
H14	0.2005	−0.0381	0.3633	0.061*	0.69
S1′	0.3399 (8)	−0.0324 (4)	0.1337 (6)	0.0532 (11)	0.31
C12′	0.3651 (16)	0.0294 (11)	0.3107 (10)	0.077 (5)	0.31
H12′	0.3839	0.0669	0.3574	0.092*	0.31
C13′	0.270 (2)	−0.0228 (15)	0.3377 (19)	0.064 (4)	0.31
H13′	0.2373	−0.0337	0.4040	0.077*	0.31
C14′	0.245 (3)	−0.0501 (17)	0.2351 (16)	0.055 (3)	0.31
H14′	0.1768	−0.0784	0.2214	0.066*	0.31

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0379 (12)	0.0319 (10)	0.0268 (10)	−0.0001 (9)	0.0069 (9)	−0.0045 (8)
C2	0.0402 (13)	0.0480 (13)	0.0368 (12)	−0.0005 (10)	0.0029 (10)	0.0000 (10)
C3	0.0518 (15)	0.0551 (14)	0.0360 (12)	0.0084 (12)	−0.0025 (10)	0.0018 (11)
C4	0.0671 (17)	0.0462 (13)	0.0363 (12)	0.0051 (12)	0.0041 (12)	0.0081 (10)
C5	0.0577 (15)	0.0386 (12)	0.0398 (12)	−0.0069 (11)	0.0081 (11)	0.0050 (10)
C6	0.0437 (12)	0.0311 (11)	0.0310 (11)	−0.0019 (9)	0.0056 (9)	−0.0008 (9)
C7	0.0419 (12)	0.0364 (11)	0.0352 (11)	−0.0094 (10)	0.0084 (9)	−0.0010 (9)
C8	0.0318 (11)	0.0348 (11)	0.0304 (10)	−0.0047 (9)	0.0060 (8)	−0.0018 (8)
C9	0.0353 (11)	0.0288 (10)	0.0257 (10)	−0.0042 (8)	0.0069 (8)	−0.0049 (8)
C10	0.0337 (11)	0.0302 (10)	0.0261 (10)	−0.0023 (9)	0.0062 (8)	−0.0045 (8)

C11	0.0324 (11)	0.0337 (11)	0.0351 (11)	−0.0021 (9)	0.0053 (9)	−0.0010 (9)
C15	0.0368 (12)	0.0459 (13)	0.0355 (11)	−0.0059 (10)	0.0080 (10)	−0.0035 (10)
C16	0.0592 (16)	0.0565 (15)	0.0646 (16)	0.0104 (13)	0.0199 (13)	−0.0144 (13)
C17	0.0347 (11)	0.0372 (12)	0.0349 (12)	−0.0044 (9)	0.0057 (9)	0.0014 (9)
C18	0.0783 (19)	0.0404 (13)	0.0748 (18)	−0.0105 (13)	0.0119 (15)	0.0184 (13)
C19	0.0314 (11)	0.0302 (10)	0.0346 (11)	−0.0046 (9)	0.0025 (9)	−0.0009 (8)
C20	0.0345 (12)	0.0371 (11)	0.0488 (13)	0.0013 (9)	0.0049 (10)	−0.0054 (10)
C21	0.0278 (11)	0.0399 (12)	0.0567 (14)	0.0032 (9)	−0.0037 (10)	0.0009 (10)
C22	0.0299 (11)	0.0310 (11)	0.0437 (12)	−0.0026 (9)	−0.0037 (9)	0.0029 (9)
C23	0.0347 (12)	0.0481 (13)	0.0529 (14)	−0.0006 (10)	−0.0138 (11)	0.0051 (11)
C24	0.0488 (14)	0.0503 (14)	0.0406 (12)	−0.0083 (11)	−0.0159 (11)	0.0001 (11)
C25	0.0412 (12)	0.0385 (11)	0.0345 (11)	−0.0091 (10)	−0.0050 (9)	0.0015 (9)
C26	0.0578 (16)	0.0552 (14)	0.0346 (12)	−0.0111 (12)	−0.0027 (11)	−0.0090 (11)
C27	0.0560 (16)	0.0532 (14)	0.0437 (13)	−0.0039 (12)	0.0099 (12)	−0.0147 (11)
C28	0.0395 (12)	0.0454 (12)	0.0432 (12)	0.0003 (10)	0.0065 (10)	−0.0029 (10)
C29	0.0345 (12)	0.0323 (11)	0.0332 (11)	−0.0048 (9)	0.0031 (9)	−0.0003 (9)
C30	0.0284 (11)	0.0394 (12)	0.0418 (12)	0.0037 (9)	−0.0007 (9)	0.0019 (9)
C31	0.0330 (11)	0.0367 (11)	0.0334 (11)	−0.0001 (9)	−0.0052 (9)	−0.0013 (9)
C32	0.0297 (10)	0.0270 (10)	0.0334 (10)	−0.0035 (8)	0.0002 (8)	0.0011 (8)
C33	0.0298 (11)	0.0273 (10)	0.0340 (11)	−0.0057 (8)	−0.0027 (8)	0.0036 (8)
C34	0.0335 (11)	0.0290 (10)	0.0317 (10)	−0.0065 (9)	0.0002 (9)	0.0033 (8)
O1	0.0631 (11)	0.0459 (9)	0.0633 (11)	−0.0261 (9)	−0.0084 (9)	0.0094 (8)
O2	0.0911 (15)	0.0622 (11)	0.0875 (13)	−0.0153 (11)	0.0616 (12)	−0.0073 (10)
O3	0.0542 (10)	0.0388 (8)	0.0567 (10)	−0.0007 (7)	0.0249 (8)	−0.0075 (7)
O4	0.0869 (14)	0.0657 (11)	0.0405 (10)	−0.0292 (10)	−0.0160 (9)	0.0160 (8)
O5	0.0590 (10)	0.0298 (8)	0.0451 (8)	−0.0050 (7)	0.0070 (7)	0.0016 (6)
S1	0.0458 (6)	0.0438 (6)	0.0437 (7)	0.0005 (5)	0.0210 (6)	0.0062 (5)
C12	0.041 (5)	0.068 (6)	0.083 (6)	−0.010 (3)	0.011 (4)	0.009 (4)
C13	0.037 (3)	0.052 (3)	0.083 (4)	−0.013 (2)	0.006 (3)	0.001 (3)
C14	0.038 (3)	0.055 (3)	0.062 (5)	−0.004 (2)	0.026 (3)	0.014 (3)
S1′	0.044 (2)	0.0488 (18)	0.066 (2)	−0.0163 (16)	−0.0030 (15)	−0.0054 (15)
C12′	0.100 (8)	0.062 (7)	0.068 (9)	−0.009 (6)	−0.009 (7)	0.003 (7)
C13′	0.070 (7)	0.066 (7)	0.057 (6)	0.005 (5)	−0.001 (5)	0.001 (6)
C14′	0.048 (7)	0.057 (6)	0.058 (6)	−0.012 (5)	0.004 (5)	0.001 (5)

Geometric parameters (Å, º)

C1—C2	1.395 (3)	C20—C21	1.376 (3)
C1—C6	1.404 (3)	C20—H20	0.9300
C1—C10	1.478 (3)	C21—C22	1.384 (3)
C2—C3	1.377 (3)	C21—H21	0.9300
C2—H2	0.9300	C22—C33	1.420 (3)
C3—C4	1.369 (3)	C22—C23	1.435 (3)
C3—H3	0.9300	C23—C24	1.329 (3)
C4—C5	1.373 (3)	C23—H23	0.9300
C4—H4	0.9300	C24—C25	1.429 (3)
C5—C6	1.392 (3)	C24—H24	0.9300
C5—H5	0.9300	C25—C26	1.391 (3)

C6—C7	1.467 (3)	C25—C34	1.423 (3)
C7—O1	1.212 (2)	C26—C27	1.375 (3)
C7—C8	1.545 (3)	C26—H26	0.9300
C8—C9	1.533 (3)	C27—C28	1.376 (3)
C8—C19	1.536 (3)	C27—H27	0.9300
C8—C15	1.547 (3)	C28—C29	1.402 (3)
C9—C10	1.345 (3)	C28—H28	0.9300
C9—C17	1.503 (3)	C29—C34	1.413 (3)
C10—C11	1.477 (3)	C29—C30	1.424 (3)
C11—C12′	1.379 (9)	C30—C31	1.346 (3)
C11—C12	1.380 (7)	C30—H30	0.9300
C11—S1′	1.676 (5)	C31—C32	1.434 (3)
C11—S1	1.706 (2)	C31—H31	0.9300
C15—O2	1.191 (2)	C32—C33	1.423 (3)
C15—O3	1.314 (2)	C33—C34	1.429 (3)
C16—O3	1.448 (2)	S1—C14	1.695 (6)
C16—H16A	0.9600	C12—C13	1.477 (8)
C16—H16B	0.9600	C12—H12	0.9300
C16—H16C	0.9600	C13—C14	1.345 (6)
C17—O4	1.196 (2)	C13—H13	0.9300
C17—O5	1.325 (2)	C14—H14	0.9300
C18—O5	1.441 (3)	S1′—C14′	1.691 (9)
C18—H18A	0.9600	C12′—C13′	1.483 (10)
C18—H18B	0.9600	C12′—H12′	0.9300
C18—H18C	0.9600	C13′—C14′	1.375 (10)
C19—C20	1.383 (3)	C13′—H13′	0.9300
C19—C32	1.415 (3)	C14′—H14′	0.9300

C2—C1—C6	117.75 (18)	C20—C21—C22	121.10 (19)
C2—C1—C10	122.20 (18)	C20—C21—H21	119.4
C6—C1—C10	120.04 (18)	C22—C21—H21	119.4
C3—C2—C1	120.9 (2)	C21—C22—C33	118.72 (18)
C3—C2—H2	119.5	C21—C22—C23	122.59 (19)
C1—C2—H2	119.5	C33—C22—C23	118.68 (19)
C4—C3—C2	120.9 (2)	C24—C23—C22	121.4 (2)
C4—C3—H3	119.6	C24—C23—H23	119.3
C2—C3—H3	119.6	C22—C23—H23	119.3
C3—C4—C5	119.6 (2)	C23—C24—C25	122.2 (2)
C3—C4—H4	120.2	C23—C24—H24	118.9
C5—C4—H4	120.2	C25—C24—H24	118.9
C4—C5—C6	120.6 (2)	C26—C25—C34	118.4 (2)
C4—C5—H5	119.7	C26—C25—C24	123.5 (2)
C6—C5—H5	119.7	C34—C25—C24	118.11 (19)
C5—C6—C1	120.2 (2)	C27—C26—C25	121.7 (2)
C5—C6—C7	119.62 (19)	C27—C26—H26	119.2
C1—C6—C7	120.15 (17)	C25—C26—H26	119.2
O1—C7—C6	122.77 (19)	C26—C27—C28	120.7 (2)
O1—C7—C8	120.05 (19)	C26—C27—H27	119.6

C6—C7—C8	117.08 (17)	C28—C27—H27	119.6
C9—C8—C19	113.08 (15)	C27—C28—C29	120.1 (2)
C9—C8—C7	112.70 (16)	C27—C28—H28	120.0
C19—C8—C7	110.16 (15)	C29—C28—H28	120.0
C9—C8—C15	108.53 (15)	C28—C29—C34	119.58 (18)
C19—C8—C15	110.24 (16)	C28—C29—C30	122.49 (19)
C7—C8—C15	101.51 (15)	C34—C29—C30	117.93 (17)
C10—C9—C17	121.08 (17)	C31—C30—C29	121.97 (19)
C10—C9—C8	122.41 (17)	C31—C30—H30	119.0
C17—C9—C8	116.48 (17)	C29—C30—H30	119.0
C9—C10—C11	119.94 (17)	C30—C31—C32	122.13 (19)
C9—C10—C1	121.19 (17)	C30—C31—H31	118.9
C11—C10—C1	118.83 (17)	C32—C31—H31	118.9
C12′—C11—C12	106.9 (10)	C19—C32—C33	118.90 (17)
C12′—C11—C10	125.9 (8)	C19—C32—C31	123.96 (18)
C12—C11—C10	127.2 (5)	C33—C32—C31	117.14 (17)
C12′—C11—S1′	107.5 (8)	C22—C33—C32	120.18 (18)
C10—C11—S1′	126.4 (3)	C22—C33—C34	119.39 (17)
C12—C11—S1	113.7 (5)	C32—C33—C34	120.43 (17)
C10—C11—S1	118.77 (15)	C29—C34—C25	119.55 (18)
S1′—C11—S1	114.7 (3)	C29—C34—C33	120.33 (17)
O2—C15—O3	123.8 (2)	C25—C34—C33	120.10 (18)
O2—C15—C8	123.4 (2)	C15—O3—C16	115.83 (17)
O3—C15—C8	112.83 (16)	C17—O5—C18	116.64 (17)
O3—C16—H16A	109.5	C14—S1—C11	90.3 (3)
O3—C16—H16B	109.5	C11—C12—C13	110.1 (10)
H16A—C16—H16B	109.5	C11—C12—H12	124.9
O3—C16—H16C	109.5	C13—C12—H12	124.9
H16A—C16—H16C	109.5	C14—C13—C12	110.0 (9)
H16B—C16—H16C	109.5	C14—C13—H13	125.0
O4—C17—O5	123.28 (19)	C12—C13—H13	125.0
O4—C17—C9	124.84 (19)	C13—C14—S1	115.7 (7)
O5—C17—C9	111.85 (17)	C13—C14—H14	122.2
O5—C18—H18A	109.5	S1—C14—H14	122.2
O5—C18—H18B	109.5	C11—S1′—C14′	91.3 (11)
H18A—C18—H18B	109.5	C11—C12′—C13′	119.0 (16)
O5—C18—H18C	109.5	C11—C12′—H12′	120.5
H18A—C18—H18C	109.5	C13′—C12′—H12′	120.5
H18B—C18—H18C	109.5	C14′—C13′—C12′	99 (2)
C20—C19—C32	119.24 (18)	C14′—C13′—H13′	130.6
C20—C19—C8	121.39 (17)	C12′—C13′—H13′	130.6
C32—C19—C8	119.36 (17)	C13′—C14′—S1′	120 (2)
C21—C20—C19	121.83 (19)	C13′—C14′—H14′	120.0
C21—C20—H20	119.1	S1′—C14′—H14′	120.0
C19—C20—H20	119.1		

C6—C1—C2—C3	3.3 (3)	C33—C22—C23—C24	−3.1 (3)
C10—C1—C2—C3	−176.23 (19)	C22—C23—C24—C25	1.7 (3)

C1—C2—C3—C4	−1.9 (3)	C23—C24—C25—C26	−178.7 (2)
C2—C3—C4—C5	−1.3 (3)	C23—C24—C25—C34	1.2 (3)
C3—C4—C5—C6	2.8 (3)	C34—C25—C26—C27	0.4 (3)
C4—C5—C6—C1	−1.3 (3)	C24—C25—C26—C27	−179.7 (2)
C4—C5—C6—C7	−178.3 (2)	C25—C26—C27—C28	0.8 (4)
C2—C1—C6—C5	−1.8 (3)	C26—C27—C28—C29	−1.3 (3)
C10—C1—C6—C5	177.82 (18)	C27—C28—C29—C34	0.5 (3)
C2—C1—C6—C7	175.18 (18)	C27—C28—C29—C30	−178.9 (2)
C10—C1—C6—C7	−5.2 (3)	C28—C29—C30—C31	176.80 (19)
C5—C6—C7—O1	18.2 (3)	C34—C29—C30—C31	−2.6 (3)
C1—C6—C7—O1	−158.8 (2)	C29—C30—C31—C32	0.9 (3)
C5—C6—C7—C8	−158.20 (18)	C20—C19—C32—C33	0.3 (3)
C1—C6—C7—C8	24.8 (3)	C8—C19—C32—C33	179.53 (16)
O1—C7—C8—C9	154.96 (19)	C20—C19—C32—C31	−179.83 (18)
C6—C7—C8—C9	−28.6 (2)	C8—C19—C32—C31	−0.6 (3)
O1—C7—C8—C19	27.7 (3)	C30—C31—C32—C19	−178.20 (19)
C6—C7—C8—C19	−155.88 (16)	C30—C31—C32—C33	1.7 (3)
O1—C7—C8—C15	−89.1 (2)	C21—C22—C33—C32	1.4 (3)
C6—C7—C8—C15	87.3 (2)	C23—C22—C33—C32	−179.49 (18)
C19—C8—C9—C10	140.57 (18)	C21—C22—C33—C34	−177.61 (18)
C7—C8—C9—C10	14.8 (2)	C23—C22—C33—C34	1.5 (3)
C15—C8—C9—C10	−96.8 (2)	C19—C32—C33—C22	−1.5 (3)
C19—C8—C9—C17	−41.6 (2)	C31—C32—C33—C22	178.61 (17)
C7—C8—C9—C17	−167.35 (15)	C19—C32—C33—C34	177.44 (17)
C15—C8—C9—C17	81.0 (2)	C31—C32—C33—C34	−2.4 (3)
C17—C9—C10—C11	8.8 (3)	C28—C29—C34—C25	0.8 (3)
C8—C9—C10—C11	−173.51 (16)	C30—C29—C34—C25	−179.80 (17)
C17—C9—C10—C1	−173.60 (16)	C28—C29—C34—C33	−177.67 (17)
C8—C9—C10—C1	4.1 (3)	C30—C29—C34—C33	1.7 (3)
C2—C1—C10—C9	169.55 (18)	C26—C25—C34—C29	−1.2 (3)
C6—C1—C10—C9	−10.0 (3)	C24—C25—C34—C29	178.88 (18)
C2—C1—C10—C11	−12.8 (3)	C26—C25—C34—C33	177.23 (18)
C6—C1—C10—C11	167.65 (17)	C24—C25—C34—C33	−2.6 (3)
C9—C10—C11—C12′	66.1 (11)	C22—C33—C34—C29	179.72 (17)
C1—C10—C11—C12′	−111.6 (10)	C32—C33—C34—C29	0.8 (3)
C9—C10—C11—C12	−116.3 (9)	C22—C33—C34—C25	1.3 (3)
C1—C10—C11—C12	66.0 (9)	C32—C33—C34—C25	−177.69 (17)
C9—C10—C11—S1′	−119.4 (5)	O2—C15—O3—C16	−1.0 (3)
C1—C10—C11—S1′	62.9 (5)	C8—C15—O3—C16	178.13 (18)
C9—C10—C11—S1	56.8 (2)	O4—C17—O5—C18	13.1 (3)
C1—C10—C11—S1	−120.94 (18)	C9—C17—O5—C18	−168.72 (18)
C9—C8—C15—O2	151.5 (2)	C12′—C11—S1—C14	48 (5)
C19—C8—C15—O2	−84.2 (3)	C12—C11—S1—C14	−3.0 (9)
C7—C8—C15—O2	32.5 (3)	C10—C11—S1—C14	−177.0 (4)
C9—C8—C15—O3	−27.7 (2)	S1′—C11—S1—C14	−0.4 (6)
C19—C8—C15—O3	96.7 (2)	C12′—C11—C12—C13	−6.8 (16)
C7—C8—C15—O3	−146.61 (18)	C10—C11—C12—C13	175.2 (8)
C10—C9—C17—O4	−133.5 (2)	S1′—C11—C12—C13	−111 (20)

C8—C9—C17—O4	48.6 (3)	S1—C11—C12—C13	1.8 (14)
C10—C9—C17—O5	48.3 (2)	C11—C12—C13—C14	0.7 (17)
C8—C9—C17—O5	−129.53 (18)	C12—C13—C14—S1	−3.0 (16)
C9—C8—C19—C20	114.1 (2)	C11—S1—C14—C13	3.5 (10)
C7—C8—C19—C20	−118.8 (2)	C12′—C11—S1′—C14′	−8.1 (16)
C15—C8—C19—C20	−7.6 (2)	C12—C11—S1′—C14′	68 (19)
C9—C8—C19—C32	−65.1 (2)	C10—C11—S1′—C14′	176.6 (12)
C7—C8—C19—C32	62.0 (2)	S1—C11—S1′—C14′	0.3 (14)
C15—C8—C19—C32	173.17 (17)	C12—C11—C12′—C13′	16 (2)
C32—C19—C20—C21	1.1 (3)	C10—C11—C12′—C13′	−165.9 (17)
C8—C19—C20—C21	−178.12 (18)	S1′—C11—C12′—C13′	19 (2)
C19—C20—C21—C22	−1.3 (3)	S1—C11—C12′—C13′	−115 (6)
C20—C21—C22—C33	0.0 (3)	C11—C12′—C13′—C14′	−20 (3)
C20—C21—C22—C23	−179.1 (2)	C12′—C13′—C14′—S1′	13 (3)
C21—C22—C23—C24	176.0 (2)	C11—S1′—C14′—C13′	−4 (3)

(III) Ethyl 4-oxo-3-phenyl-1,3-bis(thiophen-2-yl)-3,4-dihydronaphthalene-2-carboxylate

Crystal data

$C_{27}H_{20}O_3S_2$
M_r = 456.55
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 12.1263 (11) Å
b = 11.8009 (11) Å
c = 16.0657 (13) Å
β = 100.181 (2)°
V = 2262.8 (3) Å^3
Z = 4
$F(000)$ = 952
D_x = 1.340 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4110 reflections
θ = 2.4–25.4°
μ = 0.26 mm^{-1}
T = 296 K
Block, green
0.25 × 0.25 × 0.15 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω & φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.937, T_{max} = 0.962
29901 measured reflections
4110 independent reflections
2685 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 25.4°, θ_{min} = 2.4°
h = −14→14
k = −14→14
l = −19→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.147
S = 1.09
4110 reflections
364 parameters
100 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
$w = 1/[\sigma^2(F_o^2) + (0.0338P)^2 + 2.9594P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C7	0.6147 (3)	0.7554 (3)	0.11948 (19)	0.0431 (7)	
C6	0.5745 (2)	0.7440 (3)	0.02783 (18)	0.0395 (7)	
C5	0.4953 (3)	0.6615 (3)	−0.0013 (2)	0.0520 (8)	
H5	0.4686	0.6143	0.0371	0.062*	
C4	0.4560 (3)	0.6491 (3)	−0.0866 (2)	0.0601 (10)	
H4	0.4034	0.5934	−0.1059	0.072*	
C3	0.4950 (3)	0.7196 (3)	−0.1430 (2)	0.0576 (9)	
H3	0.4687	0.7112	−0.2006	0.069*	
C2	0.5725 (3)	0.8026 (3)	−0.11538 (19)	0.0481 (8)	
H2	0.5976	0.8499	−0.1544	0.058*	
C1	0.6138 (2)	0.8164 (3)	−0.02929 (18)	0.0370 (7)	
C10	0.6948 (2)	0.9062 (2)	0.00282 (17)	0.0353 (7)	
C9	0.7444 (2)	0.9089 (2)	0.08432 (18)	0.0369 (7)	
C8	0.7274 (2)	0.8172 (3)	0.14761 (17)	0.0386 (7)	
C22	0.7307 (3)	0.8700 (3)	0.23534 (18)	0.0425 (7)	
C23	0.8062 (3)	0.8363 (3)	0.30966 (19)	0.0466 (8)	
H23	0.8569	0.7774	0.3082	0.056*	
C24	0.8016 (4)	0.8933 (4)	0.3830 (2)	0.0775 (13)	
H24	0.8507	0.8724	0.4319	0.093*	
C25	0.7296 (4)	0.9778 (4)	0.3875 (3)	0.0819 (14)	
H25	0.7297	1.0143	0.4388	0.098*	
C26	0.6569 (4)	1.0107 (4)	0.3185 (3)	0.0730 (12)	
H26	0.6065	1.0689	0.3225	0.088*	
C27	0.6573 (3)	0.9589 (3)	0.2428 (2)	0.0556 (9)	
H27	0.6076	0.9831	0.1953	0.067*	
C15	0.8246 (3)	1.0013 (3)	0.11778 (19)	0.0451 (8)	
C16	0.8442 (4)	1.2004 (4)	0.1385 (3)	0.0863 (14)	
H16A	0.8015	1.2542	0.1657	0.104*	
H16B	0.9087	1.1771	0.1796	0.104*	
C17	0.8813 (6)	1.2539 (5)	0.0680 (4)	0.124 (2)	
H17A	0.9295	1.2031	0.0445	0.185*	
H17B	0.9215	1.3219	0.0866	0.185*	
H17C	0.8175	1.2723	0.0256	0.185*	
C11	0.7228 (2)	0.9919 (3)	−0.05704 (19)	0.0409 (7)	
S1′	0.8516 (4)	0.9932 (5)	−0.0827 (3)	0.0552 (9)	0.472 (4)

C12′	0.6539 (15)	1.0804 (16)	−0.0903 (16)	0.074 (5)	0.472 (4)
H12′	0.5821	1.0924	−0.0791	0.089*	0.472 (4)
C13′	0.7087 (15)	1.154 (2)	−0.1462 (17)	0.069 (4)	0.472 (4)
H13′	0.6783	1.2169	−0.1766	0.083*	0.472 (4)
C14′	0.8130 (17)	1.1091 (17)	−0.1435 (15)	0.055 (3)	0.472 (4)
H14′	0.8625	1.1419	−0.1746	0.066*	0.472 (4)
S1	0.6308 (4)	1.0925 (5)	−0.1018 (4)	0.0706 (11)	0.528 (4)
C12	0.8224 (10)	1.0023 (18)	−0.0856 (12)	0.073 (5)	0.528 (4)
H12	0.8809	0.9514	−0.0697	0.087*	0.528 (4)
C13	0.8323 (16)	1.0985 (17)	−0.1430 (16)	0.062 (3)	0.528 (4)
H13	0.8940	1.1204	−0.1662	0.075*	0.528 (4)
C14	0.7295 (12)	1.1467 (19)	−0.1535 (15)	0.060 (3)	0.528 (4)
H14	0.7130	1.2091	−0.1888	0.072*	0.528 (4)
C18	0.8130 (3)	0.7232 (3)	0.14620 (19)	0.0449 (8)	
S2	0.8057 (3)	0.5957 (2)	0.1928 (2)	0.0789 (10)	0.632 (5)
C19	0.9075 (11)	0.7382 (13)	0.1097 (12)	0.065 (4)	0.632 (5)
H19	0.9268	0.8032	0.0829	0.078*	0.632 (5)
C20	0.9724 (10)	0.6299 (8)	0.1219 (8)	0.068 (2)	0.632 (5)
H20	1.0376	0.6191	0.1000	0.081*	0.632 (5)
C21	0.9295 (7)	0.5467 (11)	0.1678 (7)	0.077 (2)	0.632 (5)
H21	0.9619	0.4765	0.1826	0.093*	0.632 (5)
S2′	0.9239 (6)	0.7245 (7)	0.0999 (7)	0.083 (2)	0.368 (5)
C19′	0.795 (2)	0.6210 (14)	0.1856 (19)	0.111 (7)	0.368 (5)
H19′	0.7361	0.6020	0.2132	0.133*	0.368 (5)
C20′	0.8928 (18)	0.550 (2)	0.1728 (18)	0.099 (5)	0.368 (5)
H20′	0.9004	0.4766	0.1951	0.119*	0.368 (5)
C21′	0.973 (2)	0.5912 (13)	0.1278 (19)	0.099 (6)	0.368 (5)
H21′	1.0365	0.5554	0.1159	0.119*	0.368 (5)
O1	0.5657 (2)	0.7135 (2)	0.17142 (14)	0.0628 (7)	
O2	0.9203 (2)	0.9858 (2)	0.14859 (17)	0.0693 (7)	
O3	0.7748 (2)	1.1019 (2)	0.11081 (16)	0.0624 (7)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C7	0.0479 (18)	0.0445 (18)	0.0371 (17)	−0.0016 (15)	0.0082 (14)	−0.0013 (14)
C6	0.0351 (16)	0.0466 (18)	0.0378 (17)	0.0002 (14)	0.0087 (13)	−0.0070 (14)
C5	0.0491 (19)	0.057 (2)	0.051 (2)	−0.0095 (17)	0.0123 (15)	−0.0075 (17)
C4	0.051 (2)	0.069 (2)	0.058 (2)	−0.0145 (18)	0.0020 (17)	−0.0168 (19)
C3	0.055 (2)	0.073 (3)	0.042 (2)	−0.0038 (19)	−0.0012 (16)	−0.0138 (18)
C2	0.0466 (18)	0.059 (2)	0.0382 (18)	0.0012 (16)	0.0058 (14)	−0.0005 (16)
C1	0.0297 (14)	0.0450 (18)	0.0358 (16)	0.0059 (13)	0.0042 (12)	−0.0034 (14)
C10	0.0298 (14)	0.0426 (17)	0.0340 (16)	0.0048 (13)	0.0068 (12)	−0.0004 (13)
C9	0.0313 (15)	0.0416 (17)	0.0379 (17)	0.0010 (13)	0.0064 (12)	−0.0004 (13)
C8	0.0386 (16)	0.0447 (18)	0.0315 (16)	−0.0007 (14)	0.0039 (12)	−0.0026 (13)
C22	0.0429 (17)	0.0500 (19)	0.0358 (17)	−0.0068 (15)	0.0100 (13)	−0.0039 (14)
C23	0.0436 (18)	0.060 (2)	0.0358 (18)	−0.0077 (16)	0.0056 (14)	−0.0081 (15)
C24	0.076 (3)	0.108 (4)	0.046 (2)	−0.022 (3)	0.002 (2)	−0.005 (2)

C25	0.083 (3)	0.100 (4)	0.067 (3)	−0.024 (3)	0.027 (3)	−0.033 (3)
C26	0.081 (3)	0.066 (3)	0.081 (3)	−0.008 (2)	0.037 (3)	−0.019 (2)
C27	0.058 (2)	0.062 (2)	0.049 (2)	0.0018 (18)	0.0173 (16)	−0.0053 (18)
C15	0.0445 (19)	0.053 (2)	0.0372 (17)	−0.0040 (16)	0.0067 (14)	0.0016 (15)
C16	0.103 (3)	0.060 (3)	0.089 (3)	−0.021 (2)	−0.003 (3)	−0.018 (2)
C17	0.173 (6)	0.097 (4)	0.107 (4)	−0.066 (4)	0.041 (4)	−0.014 (3)
C11	0.0370 (16)	0.0463 (18)	0.0384 (17)	0.0006 (14)	0.0041 (13)	0.0021 (14)
S1′	0.0554 (17)	0.070 (2)	0.0429 (15)	−0.0061 (15)	0.0166 (12)	0.0080 (13)
C12′	0.079 (10)	0.073 (9)	0.065 (8)	−0.008 (7)	0.003 (7)	0.024 (6)
C13′	0.080 (8)	0.066 (7)	0.057 (6)	−0.008 (6)	−0.004 (6)	0.014 (6)
C14′	0.064 (7)	0.067 (6)	0.033 (5)	−0.017 (5)	0.010 (5)	0.013 (5)
S1	0.0579 (16)	0.0710 (19)	0.080 (3)	0.0160 (13)	0.0031 (15)	0.0267 (15)
C12	0.069 (8)	0.066 (6)	0.079 (8)	−0.004 (6)	0.004 (6)	0.011 (5)
C13	0.054 (5)	0.066 (6)	0.066 (6)	−0.002 (4)	0.006 (5)	0.004 (5)
C14	0.051 (5)	0.064 (5)	0.063 (6)	0.005 (4)	0.003 (4)	0.016 (5)
C18	0.051 (2)	0.048 (2)	0.0341 (17)	0.0095 (15)	0.0014 (14)	−0.0020 (14)
S2	0.103 (2)	0.0537 (14)	0.0785 (15)	0.0134 (14)	0.0121 (13)	0.0161 (12)
C19	0.068 (6)	0.057 (5)	0.069 (6)	0.048 (4)	0.005 (5)	−0.010 (4)
C20	0.059 (4)	0.065 (5)	0.074 (5)	0.042 (4)	0.001 (3)	−0.019 (4)
C21	0.090 (6)	0.059 (5)	0.070 (5)	0.039 (5)	−0.022 (5)	−0.009 (4)
S2′	0.064 (3)	0.083 (4)	0.108 (4)	0.010 (3)	0.029 (3)	−0.027 (3)
C19′	0.114 (11)	0.091 (11)	0.126 (13)	0.074 (9)	0.018 (9)	−0.014 (9)
C20′	0.106 (10)	0.074 (7)	0.113 (10)	0.073 (8)	0.006 (8)	−0.008 (7)
C21′	0.102 (10)	0.084 (10)	0.107 (11)	0.061 (9)	0.005 (8)	−0.020 (9)
O1	0.0707 (16)	0.0789 (18)	0.0417 (14)	−0.0247 (14)	0.0178 (12)	0.0002 (12)
O2	0.0445 (14)	0.0748 (18)	0.0813 (18)	−0.0079 (13)	−0.0092 (13)	−0.0116 (14)
O3	0.0657 (16)	0.0459 (14)	0.0711 (17)	−0.0045 (12)	0.0003 (12)	−0.0055 (12)

Geometric parameters (Å, º)

C7—O1	1.212 (4)	C16—H16B	0.9700
C7—C6	1.473 (4)	C17—H17A	0.9600
C7—C8	1.544 (4)	C17—H17B	0.9600
C6—C5	1.390 (4)	C17—H17C	0.9600
C6—C1	1.397 (4)	C11—C12	1.371 (9)
C5—C4	1.377 (5)	C11—C12′	1.384 (9)
C5—H5	0.9300	C11—S1′	1.686 (4)
C4—C3	1.375 (5)	C11—S1	1.699 (4)
C4—H4	0.9300	S1′—C14′	1.698 (9)
C3—C2	1.375 (5)	C12′—C13′	1.487 (10)
C3—H3	0.9300	C12′—H12′	0.9300
C2—C1	1.395 (4)	C13′—C14′	1.365 (9)
C2—H2	0.9300	C13′—H13′	0.9300
C1—C10	1.476 (4)	C14′—H14′	0.9300
C10—C9	1.341 (4)	S1—C14	1.697 (8)
C10—C11	1.475 (4)	C12—C13	1.481 (9)
C9—C15	1.497 (4)	C12—H12	0.9300
C9—C8	1.524 (4)	C13—C14	1.353 (8)

C8—C18	1.523 (4)	C13—H13	0.9300
C8—C22	1.535 (4)	C14—H14	0.9300
C22—C27	1.395 (4)	C18—C19	1.387 (9)
C22—C23	1.427 (4)	C18—C19′	1.397 (10)
C23—C24	1.367 (5)	C18—S2′	1.648 (6)
C23—H23	0.9300	C18—S2	1.690 (4)
C24—C25	1.336 (6)	S2—C21	1.720 (7)
C24—H24	0.9300	C19—C20	1.496 (9)
C25—C26	1.346 (6)	C19—H19	0.9300
C25—H25	0.9300	C20—C21	1.383 (8)
C26—C27	1.361 (5)	C20—H20	0.9300
C26—H26	0.9300	C21—H21	0.9300
C27—H27	0.9300	S2′—C21′	1.713 (9)
C15—O2	1.192 (4)	C19′—C20′	1.500 (10)
C15—O3	1.328 (4)	C19′—H19′	0.9300
C16—C17	1.437 (6)	C20′—C21′	1.397 (10)
C16—O3	1.458 (4)	C20′—H20′	0.9300
C16—H16A	0.9700	C21′—H21′	0.9300

O1—C7—C6	122.3 (3)	H17A—C17—H17B	109.5
O1—C7—C8	120.5 (3)	C16—C17—H17C	109.5
C6—C7—C8	117.1 (3)	H17A—C17—H17C	109.5
C5—C6—C1	120.2 (3)	H17B—C17—H17C	109.5
C5—C6—C7	119.2 (3)	C12—C11—C12′	108.1 (12)
C1—C6—C7	120.6 (3)	C12—C11—C10	126.6 (8)
C4—C5—C6	120.4 (3)	C12′—C11—C10	125.2 (9)
C4—C5—H5	119.8	C12′—C11—S1′	114.9 (8)
C6—C5—H5	119.8	C10—C11—S1′	119.7 (3)
C3—C4—C5	119.5 (3)	C12—C11—S1	110.3 (7)
C3—C4—H4	120.2	C10—C11—S1	123.1 (3)
C5—C4—H4	120.2	S1′—C11—S1	117.2 (3)
C2—C3—C4	120.9 (3)	C11—S1′—C14′	88.6 (8)
C2—C3—H3	119.5	C11—C12′—C13′	111.7 (17)
C4—C3—H3	119.5	C11—C12′—H12′	124.1
C3—C2—C1	120.5 (3)	C13′—C12′—H12′	124.1
C3—C2—H2	119.7	C14′—C13′—C12′	105 (2)
C1—C2—H2	119.7	C14′—C13′—H13′	127.3
C2—C1—C6	118.4 (3)	C12′—C13′—H13′	127.3
C2—C1—C10	122.0 (3)	C13′—C14′—S1′	119.4 (17)
C6—C1—C10	119.5 (3)	C13′—C14′—H14′	120.3
C9—C10—C11	120.4 (3)	S1′—C14′—H14′	120.3
C9—C10—C1	120.9 (3)	C14—S1—C11	90.2 (8)
C11—C10—C1	118.7 (2)	C11—C12—C13	116.8 (15)
C10—C9—C15	121.2 (3)	C11—C12—H12	121.6
C10—C9—C8	123.0 (3)	C13—C12—H12	121.6
C15—C9—C8	115.7 (2)	C14—C13—C12	103.0 (19)
C18—C8—C9	109.6 (2)	C14—C13—H13	128.5
C18—C8—C22	113.7 (2)	C12—C13—H13	128.5

C9—C8—C22	109.8 (2)	C13—C14—S1	119.7 (16)
C18—C8—C7	102.9 (2)	C13—C14—H14	120.2
C9—C8—C7	110.9 (2)	S1—C14—H14	120.2
C22—C8—C7	109.8 (2)	C19—C18—C19′	120.7 (10)
C27—C22—C23	117.6 (3)	C19—C18—C8	122.0 (6)
C27—C22—C8	118.1 (3)	C19′—C18—C8	117.3 (9)
C23—C22—C8	124.3 (3)	C19′—C18—S2′	114.8 (9)
C24—C23—C22	117.8 (3)	C8—C18—S2′	127.8 (4)
C24—C23—H23	121.1	C19—C18—S2	114.4 (6)
C22—C23—H23	121.1	C8—C18—S2	123.5 (3)
C25—C24—C23	122.7 (4)	S2′—C18—S2	108.7 (4)
C25—C24—H24	118.7	C18—S2—C21	94.5 (5)
C23—C24—H24	118.7	C18—C19—C20	106.8 (10)
C24—C25—C26	120.7 (4)	C18—C19—H19	126.6
C24—C25—H25	119.6	C20—C19—H19	126.6
C26—C25—H25	119.6	C21—C20—C19	115.9 (11)
C25—C26—C27	120.1 (4)	C21—C20—H20	122.0
C25—C26—H26	120.0	C19—C20—H20	122.0
C27—C26—H26	120.0	C20—C21—S2	108.2 (10)
C26—C27—C22	121.2 (4)	C20—C21—H21	125.9
C26—C27—H27	119.4	S2—C21—H21	125.9
C22—C27—H27	119.4	C18—S2′—C21′	98.3 (11)
O2—C15—O3	124.6 (3)	C18—C19′—C20′	103.3 (18)
O2—C15—C9	124.1 (3)	C18—C19′—H19′	128.3
O3—C15—C9	111.3 (3)	C20′—C19′—H19′	128.3
C17—C16—O3	110.7 (4)	C21′—C20′—C19′	121 (2)
C17—C16—H16A	109.5	C21′—C20′—H20′	119.6
O3—C16—H16A	109.5	C19′—C20′—H20′	119.6
C17—C16—H16B	109.5	C20′—C21′—S2′	103 (2)
O3—C16—H16B	109.5	C20′—C21′—H21′	128.7
H16A—C16—H16B	108.1	S2′—C21′—H21′	128.7
C16—C17—H17A	109.5	C15—O3—C16	117.2 (3)
C16—C17—H17B	109.5		

O1—C7—C6—C5	−16.1 (5)	C1—C10—C11—S1	69.7 (5)
C8—C7—C6—C5	160.0 (3)	C12—C11—S1′—C14′	13 (9)
O1—C7—C6—C1	162.8 (3)	C12′—C11—S1′—C14′	−3.0 (18)
C8—C7—C6—C1	−21.1 (4)	C10—C11—S1′—C14′	−177.8 (10)
C1—C6—C5—C4	0.9 (5)	S1—C11—S1′—C14′	1.5 (11)
C7—C6—C5—C4	179.8 (3)	C12—C11—C12′—C13′	1 (3)
C6—C5—C4—C3	−0.5 (5)	C10—C11—C12′—C13′	177.9 (17)
C5—C4—C3—C2	−0.2 (6)	S1′—C11—C12′—C13′	3 (3)
C4—C3—C2—C1	0.4 (5)	S1—C11—C12′—C13′	−118 (16)
C3—C2—C1—C6	0.0 (4)	C11—C12′—C13′—C14′	−2 (3)
C3—C2—C1—C10	−178.5 (3)	C12′—C13′—C14′—S1′	0 (3)
C5—C6—C1—C2	−0.7 (4)	C11—S1′—C14′—C13′	2 (2)
C7—C6—C1—C2	−179.6 (3)	C12—C11—S1—C14	−1.9 (16)
C5—C6—C1—C10	177.8 (3)	C12′—C11—S1—C14	61 (14)

C7—C6—C1—C10	−1.1 (4)	C10—C11—S1—C14	178.9 (10)
C2—C1—C10—C9	−171.3 (3)	S1′—C11—S1—C14	−0.4 (11)
C6—C1—C10—C9	10.3 (4)	C12′—C11—C12—C13	−1 (3)
C2—C1—C10—C11	7.2 (4)	C10—C11—C12—C13	−177.5 (17)
C6—C1—C10—C11	−171.2 (3)	S1′—C11—C12—C13	−166 (11)
C11—C10—C9—C15	3.0 (4)	S1—C11—C12—C13	3 (3)
C1—C10—C9—C15	−178.6 (3)	C11—C12—C13—C14	−3 (3)
C11—C10—C9—C8	−174.3 (3)	C12—C13—C14—S1	2 (3)
C1—C10—C9—C8	4.2 (4)	C11—S1—C14—C13	0 (2)
C10—C9—C8—C18	88.2 (3)	C9—C8—C18—C19	15.9 (11)
C15—C9—C8—C18	−89.2 (3)	C22—C8—C18—C19	−107.4 (11)
C10—C9—C8—C22	−146.3 (3)	C7—C8—C18—C19	133.9 (11)
C15—C9—C8—C22	36.3 (3)	C9—C8—C18—C19′	−166.1 (16)
C10—C9—C8—C7	−24.7 (4)	C22—C8—C18—C19′	70.7 (16)
C15—C9—C8—C7	157.9 (3)	C7—C8—C18—C19′	−48.0 (16)
O1—C7—C8—C18	91.3 (3)	C9—C8—C18—S2′	11.2 (6)
C6—C7—C8—C18	−84.9 (3)	C22—C8—C18—S2′	−112.1 (6)
O1—C7—C8—C9	−151.7 (3)	C7—C8—C18—S2′	129.2 (6)
C6—C7—C8—C9	32.1 (4)	C9—C8—C18—S2	−167.6 (3)
O1—C7—C8—C22	−30.1 (4)	C22—C8—C18—S2	69.1 (4)
C6—C7—C8—C22	153.7 (3)	C7—C8—C18—S2	−49.6 (3)
C18—C8—C22—C27	178.5 (3)	C19—C18—S2—C21	−0.5 (11)
C9—C8—C22—C27	55.3 (3)	C19′—C18—S2—C21	170 (14)
C7—C8—C22—C27	−66.9 (4)	C8—C18—S2—C21	−177.2 (5)
C18—C8—C22—C23	0.1 (4)	S2′—C18—S2—C21	3.8 (6)
C9—C8—C22—C23	−123.0 (3)	C19′—C18—C19—C20	1 (2)
C7—C8—C22—C23	114.8 (3)	C8—C18—C19—C20	178.8 (8)
C27—C22—C23—C24	−0.1 (5)	S2′—C18—C19—C20	−33 (8)
C8—C22—C23—C24	178.2 (3)	S2—C18—C19—C20	2.0 (16)
C22—C23—C24—C25	0.3 (6)	C18—C19—C20—C21	−3.2 (19)
C23—C24—C25—C26	0.2 (7)	C19—C20—C21—S2	2.9 (15)
C24—C25—C26—C27	−0.9 (7)	C18—S2—C21—C20	−1.4 (9)
C25—C26—C27—C22	1.1 (6)	C19—C18—S2′—C21′	145 (10)
C23—C22—C27—C26	−0.6 (5)	C19′—C18—S2′—C21′	−3 (2)
C8—C22—C27—C26	−179.0 (3)	C8—C18—S2′—C21′	−179.9 (11)
C10—C9—C15—O2	−119.3 (4)	S2—C18—S2′—C21′	−1.0 (12)
C8—C9—C15—O2	58.2 (4)	C19—C18—C19′—C20′	−2 (3)
C10—C9—C15—O3	62.5 (4)	C8—C18—C19′—C20′	−179.8 (15)
C8—C9—C15—O3	−120.1 (3)	S2′—C18—C19′—C20′	3 (3)
C9—C10—C11—C12	69.2 (13)	S2—C18—C19′—C20′	−12 (12)
C1—C10—C11—C12	−109.3 (12)	C18—C19′—C20′—C21′	−1 (4)
C9—C10—C11—C12′	−106.8 (15)	C19′—C20′—C21′—S2′	0 (4)
C1—C10—C11—C12′	74.7 (15)	C18—S2′—C21′—C20′	2 (2)
C9—C10—C11—S1′	67.6 (4)	O2—C15—O3—C16	3.7 (5)
C1—C10—C11—S1′	−111.0 (4)	C9—C15—O3—C16	−178.1 (3)
C9—C10—C11—S1	−111.7 (4)	C17—C16—O3—C15	96.6 (5)