Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-Methyl-1-phenylbenzothieno[3,2-*d*]-imidazo[1,2-*a*]pyrimidine-2,5(1*H*,3*H*)-dione

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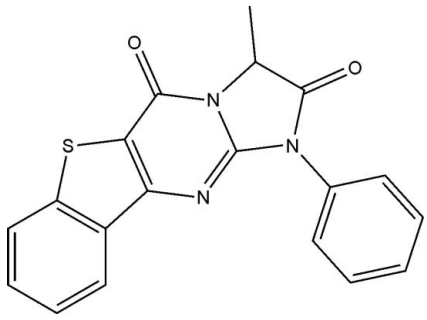
Received 6 April 2007; accepted 9 April 2007

Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.003 Å; R factor = 0.050; wR factor = 0.115; data-to-parameter ratio = 16.9.

In the molecule of the title compound, $C_{19}H_{13}N_3O_2S$, the pyrimidine ring is not planar and has a flattened-boat conformation; it also has a pseudo-mirror plane running through the bridgehead N atom and the opposite C atom. The dihedral angles between the planar fused benzene (A), thienyl (B), imidazole (D) and substituent phenyl (E) rings are A/B = 1.63 (3)°, A/D = 5.80 (2)°, B/D = 5.49 (3)° and D/E = 39.73 (3)°. In the crystal structure, intermolecular C—H···O hydrogen bonds and π–π stacking interactions may be effective in the stabilization of the structure [adjacent thiophene rings have a centroid–centroid distance of 3.79 (1) Å (symmetry code: $1-x, 2-y, 1-z$), while adjacent imidazole and benzene rings have a centroid–centroid distance of 3.48 (1) Å (symmetry codes: $\frac{1}{2}-x, \frac{1}{2}+y, z$ and $\frac{3}{2}-x, -\frac{1}{2}+y, z$)].

Related literature

For related literature, see: Allen *et al.* (1987); Cao (2007); Chambhare *et al.* (2003); Cremer & Pople (1975); Ding *et al.* (2004); Janiak (2000).



Experimental

Crystal data

$C_{19}H_{13}N_3O_2S$
M_r = 347.38
Orthorhombic, *Pbca*
a = 12.6184 (18) Å
b = 11.0787 (16) Å
c = 23.074 (3) Å
V = 3225.7 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 292 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
19405 measured reflections
3847 independent reflections
2529 reflections with $I > 2\sigma(I)$
R_{int} = 0.109

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.115
S = 0.92
3847 reflections
227 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected torsion angles (°).

N1—C7—C8—C9	2.6 (3)	C8—C7—N1—C10	−2.8 (2)
C7—C8—C9—N2	2.5 (2)	N1—C10—N2—C9	8.1 (3)
N2—C10—N1—C7	−2.4 (2)	C8—C9—N2—C10	−7.4 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C19—H19···O2^{i}	0.93	2.58	3.409 (2)	148
C16—H16···O2^{ii}	0.93	2.40	3.328 (2)	172
C5—H5···O1^{iii}	0.93	2.45	3.358 (2)	165

Symmetry codes: (i) $x-\frac{1}{2}, y, -z+\frac{3}{2}$; (ii) $-x+2, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x-\frac{1}{2}, -y+\frac{5}{2}, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; structure solution: *SHELXS97* (Sheldrick, 1997); structure refinement: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); publication material: *SHELXTL* (Bruker, 2001).

The author acknowledges the National Basic Research Program of China (No. 2004CCA00100) and the National Natural Science Foundation of China (No. 20102001).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2230).

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  doi:10.1107/S1600536807017576

supplementary materials

Acta Cryst. (2007). E**63**, o2660 [**doi:10.1107/S1600536807017576**]

3-Methyl-1-phenylbenzothieno[3,2-*d*]imidazo[1,2-*a*]pyrimidine-2,5(1*H*,3*H*)-dione

M.-H. Cao

Comment

Thienopyrimidine derivatives are of interest as possible antiviral agents, and because of their other biological properties, including antibacterial, antifungal, antiallergic and antiinflammatory activities (Chambhare *et al.*, 2003). We have recently focused on the synthesis of the fused heterocyclic systems containing thienopyrimidine via aza-Wittig reactions at room temperature (Ding *et al.*, 2004). We herein report the crystal structure of one such thienopyrimidine derivative, the title compound, (I).

In the molecule of (I), (Fig. 1) the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The ring C (N1/N2/C7—C10) is not planar having a total puckering amplitude, Q_T of 0.228 (2) Å and a flattened-boat conformation [φ = 54.10 (2)° and θ = 63.62 (3)°] (Cremer & Pople, 1975). Ring C has a pseudo mirror plane running through atoms N2 and C7, as can be deduced from the torsion angles (Table 1). Rings A (C1—C6), B (S1/C1/C6—C8), D (N2/N3/C10—C12) and E (C14—C19) are, of course, planar and the dihedral angles between them are A/B = 1.63 (3)°, A/D = 5.80 (2)°, B/D = 5.49 (3)° and D/E = 39.73 (3)°.

In the crystal structure, the weak intermolecular C—H···O hydrogen bonds (Table 2) cause to the formation of a three dimensional network (Fig. 2), in which they may be effective in the stabilization of the structure. Further stability is provided by offset π-π stacking interactions (Janiak, 2000), involving the rings; B, D and E. The adjacent B rings have a centroid-centroid distance of 3.79 (1) %A [symmetry code: 1 - x, 2 - y, 1 - z], while rings D and E have a centroid-centroid distance of 3.48 (1) %A [symmetry codes: 3/2 - x, y + 1/2, z; 3/2 - x, y - 1/2, z].

Experimental

The title compound was synthesized according to the literature method (Cao, 2007). Crystals suitable for X-ray analysis were grown from acetone at 277 K.

Refinement

H atoms were positioned geometrically, with C—H = 0.93, 0.98 and 0.96 Å for aromatic, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.5 for methyl H and x = 1.2 for all other H atoms.

Figures

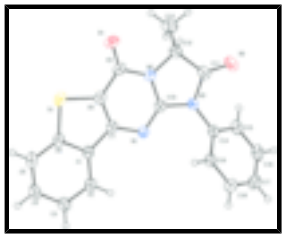

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

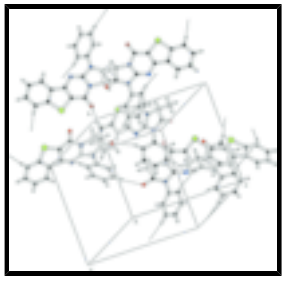

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

3-Methyl-1-phenylbenzothieno[3,2-d]imidazo[1,2-a]pyrimidine-2,5(1*H*,3H)-dione

Crystal data

$C_{19}H_{13}N_3O_2S$	F_{000} = 1440
M_r = 347.38	D_x = 1.431 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 3753 reflections
a = 12.6184 (18) Å	θ = 2.4–22.8º
b = 11.0787 (16) Å	μ = 0.22 mm^{-1}
c = 23.074 (3) Å	*T* = 292 (2) K
V = 3225.7 (8) Å^3	Block, colorless
Z = 8	0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer	2529 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.109
Monochromator: graphite	θ_{max} = 28.0º
T = 292(2) K	θ_{min} = 1.8º
φ and ω scans	*h* = −16→12
Absorption correction: none	*k* = −14→14
19405 measured reflections	*l* = −29→27
3847 independent reflections	

Refinement

Refinement on F^2	H-atom parameters constrained

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.115$

$S = 0.92$

3847 reflections

227 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$w = 1/[\sigma^2(F_o^2) + (0.0558P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 0.30$ e Å^{-3}

$\Delta\rho_{min} = -0.21$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.43864 (12)	0.97800 (15)	0.59301 (7)	0.0371 (4)
C2	0.37664 (13)	0.87999 (17)	0.60996 (8)	0.0438 (4)
H2	0.4039	0.8215	0.6347	0.053*
C3	0.27466 (14)	0.87107 (18)	0.58957 (8)	0.0518 (5)
H3	0.2330	0.8055	0.6003	0.062*
C4	0.23303 (15)	0.9589 (2)	0.55310 (8)	0.0549 (5)
H4	0.1637	0.9511	0.5400	0.066*
C5	0.29153 (15)	1.0568 (2)	0.53598 (8)	0.0535 (5)
H5	0.2628	1.1151	0.5116	0.064*
C6	0.39535 (14)	1.06644 (16)	0.55618 (7)	0.0422 (4)
C7	0.54732 (13)	1.00455 (15)	0.60685 (7)	0.0362 (4)
C8	0.58174 (14)	1.10884 (15)	0.58091 (7)	0.0409 (4)
C9	0.68825 (15)	1.15173 (16)	0.58730 (8)	0.0441 (4)
C10	0.70455 (13)	0.97290 (15)	0.64790 (7)	0.0371 (4)
C11	0.87532 (14)	0.98872 (18)	0.68008 (9)	0.0472 (5)
C12	0.85911 (13)	1.08834 (17)	0.63630 (8)	0.0470 (5)
H12	0.8682	1.1672	0.6549	0.056*
C13	0.93537 (16)	1.0761 (2)	0.58549 (10)	0.0740 (7)
H13A	0.9255	0.9990	0.5673	0.111*
H13B	1.0069	1.0827	0.5992	0.111*

H13C	0.9217	1.1390	0.5579	0.111*
C14	0.76691 (13)	0.82173 (14)	0.72199 (7)	0.0378 (4)
C15	0.84826 (14)	0.73933 (17)	0.72829 (9)	0.0472 (5)
H15	0.9104	0.7479	0.7070	0.057*
C16	0.83663 (16)	0.64405 (18)	0.76645 (10)	0.0560 (5)
H16	0.8919	0.5895	0.7715	0.067*
C17	0.74425 (18)	0.62940 (18)	0.79685 (9)	0.0576 (5)
H17	0.7363	0.5643	0.8219	0.069*
C18	0.66351 (16)	0.71136 (19)	0.79017 (9)	0.0535 (5)
H18	0.6008	0.7013	0.8108	0.064*
C19	0.67441 (13)	0.80874 (16)	0.75303 (8)	0.0432 (4)
H19	0.6199	0.8647	0.7491	0.052*
N1	0.60876 (10)	0.93359 (12)	0.64293 (6)	0.0368 (3)
N2	0.74802 (10)	1.07041 (12)	0.62043 (6)	0.0403 (4)
N3	0.78190 (10)	0.92229 (12)	0.68350 (6)	0.0393 (4)
O1	0.72739 (11)	1.24438 (12)	0.56814 (6)	0.0616 (4)
O2	0.95559 (11)	0.96797 (14)	0.70621 (7)	0.0704 (5)
S1	0.48557 (4)	1.18039 (5)	0.53977 (2)	0.05129 (17)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0397 (10)	0.0392 (10)	0.0324 (9)	0.0063 (8)	−0.0013 (7)	−0.0013 (7)
C2	0.0434 (10)	0.0456 (11)	0.0423 (10)	0.0043 (8)	−0.0025 (8)	0.0016 (8)
C3	0.0467 (11)	0.0583 (13)	0.0504 (12)	−0.0060 (10)	−0.0037 (9)	−0.0042 (10)
C4	0.0433 (11)	0.0738 (15)	0.0477 (12)	0.0029 (10)	−0.0129 (9)	−0.0055 (10)
C5	0.0558 (13)	0.0639 (14)	0.0407 (11)	0.0191 (11)	−0.0120 (9)	−0.0010 (9)
C6	0.0481 (11)	0.0449 (11)	0.0337 (10)	0.0081 (8)	−0.0039 (8)	−0.0015 (8)
C7	0.0408 (10)	0.0349 (10)	0.0329 (9)	0.0041 (7)	0.0004 (7)	0.0000 (7)
C8	0.0478 (11)	0.0387 (10)	0.0363 (10)	0.0037 (8)	0.0004 (8)	0.0038 (8)
C9	0.0546 (11)	0.0406 (11)	0.0369 (10)	−0.0025 (9)	0.0039 (9)	0.0036 (8)
C10	0.0380 (10)	0.0369 (10)	0.0365 (9)	0.0027 (8)	0.0029 (8)	−0.0006 (8)
C11	0.0369 (10)	0.0537 (12)	0.0509 (12)	−0.0030 (9)	−0.0025 (9)	−0.0032 (9)
C12	0.0411 (11)	0.0496 (12)	0.0502 (12)	−0.0097 (8)	0.0000 (8)	−0.0008 (9)
C13	0.0514 (13)	0.1027 (19)	0.0680 (15)	−0.0104 (12)	0.0124 (11)	0.0078 (14)
C14	0.0374 (10)	0.0348 (10)	0.0414 (10)	0.0019 (8)	−0.0076 (8)	−0.0007 (8)
C15	0.0403 (10)	0.0466 (12)	0.0546 (12)	0.0064 (8)	−0.0088 (9)	−0.0059 (9)
C16	0.0588 (13)	0.0429 (12)	0.0662 (14)	0.0134 (10)	−0.0237 (11)	−0.0006 (10)
C17	0.0705 (14)	0.0451 (12)	0.0572 (13)	−0.0027 (11)	−0.0145 (11)	0.0146 (10)
C18	0.0548 (12)	0.0558 (13)	0.0501 (12)	−0.0011 (10)	−0.0009 (9)	0.0097 (10)
C19	0.0417 (11)	0.0431 (11)	0.0448 (11)	0.0068 (8)	−0.0035 (8)	0.0035 (8)
N1	0.0325 (8)	0.0378 (8)	0.0402 (8)	0.0024 (6)	−0.0016 (6)	0.0051 (6)
N2	0.0391 (8)	0.0411 (9)	0.0406 (8)	−0.0046 (6)	0.0014 (6)	0.0048 (7)
N3	0.0326 (8)	0.0422 (9)	0.0432 (8)	0.0002 (6)	−0.0050 (6)	0.0043 (7)
O1	0.0727 (10)	0.0515 (9)	0.0606 (9)	−0.0163 (7)	−0.0034 (7)	0.0190 (7)
O2	0.0430 (8)	0.0753 (11)	0.0928 (12)	−0.0110 (7)	−0.0214 (8)	0.0140 (9)
S1	0.0614 (3)	0.0464 (3)	0.0461 (3)	0.0063 (2)	−0.0065 (2)	0.0134 (2)

Geometric parameters (Å, °)

C1—C2	1.394 (2)	C11—O2	1.201 (2)
C1—C6	1.407 (2)	C11—N3	1.392 (2)
C1—C7	1.439 (2)	C11—C12	1.510 (3)
C2—C3	1.374 (2)	C12—N2	1.462 (2)
C2—H2	0.9300	C12—C13	1.523 (3)
C3—C4	1.390 (3)	C12—H12	0.9800
C3—H3	0.9300	C13—H13A	0.9600
C4—C5	1.370 (3)	C13—H13B	0.9600
C4—H4	0.9300	C13—H13C	0.9600
C5—C6	1.395 (2)	C14—C19	1.377 (2)
C5—H5	0.9300	C14—C15	1.381 (2)
C6—S1	1.7416 (19)	C14—N3	1.437 (2)
C7—C8	1.372 (2)	C15—C16	1.382 (3)
C7—N1	1.383 (2)	C15—H15	0.9300
C8—C9	1.433 (3)	C16—C17	1.370 (3)
C8—S1	1.7326 (17)	C16—H16	0.9300
C9—O1	1.222 (2)	C17—C18	1.373 (3)
C9—N2	1.402 (2)	C17—H17	0.9300
C10—N1	1.2898 (19)	C18—C19	1.385 (3)
C10—N2	1.367 (2)	C18—H18	0.9300
C10—N3	1.394 (2)	C19—H19	0.9300
C2—C1—C6	119.59 (15)	N2—C12—H12	110.0
C2—C1—C7	129.19 (16)	C11—C12—H12	110.0
C6—C1—C7	111.21 (15)	C13—C12—H12	110.0
C3—C2—C1	119.05 (17)	C12—C13—H13A	109.5
C3—C2—H2	120.5	C12—C13—H13B	109.5
C1—C2—H2	120.5	H13A—C13—H13B	109.5
C2—C3—C4	120.73 (18)	C12—C13—H13C	109.5
C2—C3—H3	119.6	H13A—C13—H13C	109.5
C4—C3—H3	119.6	H13B—C13—H13C	109.5
C5—C4—C3	121.69 (18)	C19—C14—C15	120.41 (17)
C5—C4—H4	119.2	C19—C14—N3	120.93 (15)
C3—C4—H4	119.2	C15—C14—N3	118.65 (16)
C4—C5—C6	118.05 (18)	C14—C15—C16	119.52 (19)
C4—C5—H5	121.0	C14—C15—H15	120.2
C6—C5—H5	121.0	C16—C15—H15	120.2
C5—C6—C1	120.88 (18)	C17—C16—C15	120.46 (18)
C5—C6—S1	126.64 (15)	C17—C16—H16	119.8
C1—C6—S1	112.47 (13)	C15—C16—H16	119.8
C8—C7—N1	124.34 (16)	C16—C17—C18	119.70 (18)
C8—C7—C1	112.15 (15)	C16—C17—H17	120.2
N1—C7—C1	123.50 (15)	C18—C17—H17	120.2
C7—C8—C9	122.08 (16)	C17—C18—C19	120.73 (19)
C7—C8—S1	113.75 (14)	C17—C18—H18	119.6
C9—C8—S1	124.16 (13)	C19—C18—H18	119.6
O1—C9—N2	121.32 (18)	C14—C19—C18	119.18 (17)

O1—C9—C8	128.33 (17)	C14—C19—H19	120.4
N2—C9—C8	110.34 (15)	C18—C19—H19	120.4
N1—C10—N2	126.98 (15)	C10—N1—C7	112.77 (14)
N1—C10—N3	124.95 (15)	C10—N2—C9	123.00 (15)
N2—C10—N3	108.07 (14)	C10—N2—C12	112.08 (14)
O2—C11—N3	125.77 (18)	C9—N2—C12	124.40 (14)
O2—C11—C12	126.16 (17)	C11—N3—C10	110.30 (14)
N3—C11—C12	108.04 (15)	C11—N3—C14	123.81 (14)
N2—C12—C11	101.42 (14)	C10—N3—C14	125.73 (14)
N2—C12—C13	113.64 (16)	C8—S1—C6	90.41 (9)
C11—C12—C13	111.38 (17)		
C6—C1—C2—C3	0.9 (3)	C17—C18—C19—C14	1.0 (3)
C7—C1—C2—C3	−177.67 (17)	N2—C10—N1—C7	−2.4 (2)
C1—C2—C3—C4	−0.7 (3)	N3—C10—N1—C7	176.89 (15)
C2—C3—C4—C5	0.3 (3)	C8—C7—N1—C10	−2.8 (2)
C3—C4—C5—C6	0.1 (3)	C1—C7—N1—C10	178.25 (15)
C4—C5—C6—C1	0.1 (3)	N1—C10—N2—C9	8.1 (3)
C4—C5—C6—S1	178.95 (15)	N3—C10—N2—C9	−171.26 (15)
C2—C1—C6—C5	−0.6 (3)	N1—C10—N2—C12	−179.83 (16)
C7—C1—C6—C5	178.24 (15)	N3—C10—N2—C12	0.81 (19)
C2—C1—C6—S1	−179.58 (13)	O1—C9—N2—C10	172.59 (16)
C7—C1—C6—S1	−0.77 (18)	C8—C9—N2—C10	−7.4 (2)
C2—C1—C7—C8	178.66 (17)	O1—C9—N2—C12	1.5 (3)
C6—C1—C7—C8	0.0 (2)	C8—C9—N2—C12	−178.46 (15)
C2—C1—C7—N1	−2.3 (3)	C11—C12—N2—C10	−2.32 (18)
C6—C1—C7—N1	179.04 (15)	C13—C12—N2—C10	117.31 (18)
N1—C7—C8—C9	2.6 (3)	C11—C12—N2—C9	169.62 (16)
C1—C7—C8—C9	−178.41 (15)	C13—C12—N2—C9	−70.7 (2)
N1—C7—C8—S1	−178.25 (13)	O2—C11—N3—C10	179.24 (19)
C1—C7—C8—S1	0.78 (19)	C12—C11—N3—C10	−2.7 (2)
C7—C8—C9—O1	−177.43 (18)	O2—C11—N3—C14	3.6 (3)
S1—C8—C9—O1	3.5 (3)	C12—C11—N3—C14	−178.36 (15)
C7—C8—C9—N2	2.5 (2)	N1—C10—N3—C11	−178.10 (16)
S1—C8—C9—N2	−176.57 (13)	N2—C10—N3—C11	1.27 (19)
O2—C11—C12—N2	−179.01 (19)	N1—C10—N3—C14	−2.6 (3)
N3—C11—C12—N2	2.98 (18)	N2—C10—N3—C14	176.78 (14)
O2—C11—C12—C13	59.8 (3)	C19—C14—N3—C11	136.45 (18)
N3—C11—C12—C13	−118.24 (18)	C15—C14—N3—C11	−42.1 (2)
C19—C14—C15—C16	−0.6 (3)	C19—C14—N3—C10	−38.5 (2)
N3—C14—C15—C16	178.01 (16)	C15—C14—N3—C10	142.93 (17)
C14—C15—C16—C17	1.6 (3)	C7—C8—S1—C6	−1.03 (14)
C15—C16—C17—C18	−1.3 (3)	C9—C8—S1—C6	178.14 (16)
C16—C17—C18—C19	0.0 (3)	C5—C6—S1—C8	−177.92 (17)
C15—C14—C19—C18	−0.7 (3)	C1—C6—S1—C8	1.01 (14)
N3—C14—C19—C18	−179.25 (16)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

C19—H19···O2^{i}	0.93	2.58	3.409 (2)	148
C16—H16···O2^{ii}	0.93	2.40	3.328 (2)	172
C5—H5···O1^{iii}	0.93	2.45	3.358 (2)	165

Symmetry codes: (i) *x*−1/2, *y*, −*z*+3/2; (ii) −*x*+2, *y*−1/2, −*z*+3/2; (iii) *x*−1/2, −*y*+5/2, −*z*+1.

Fig. 1

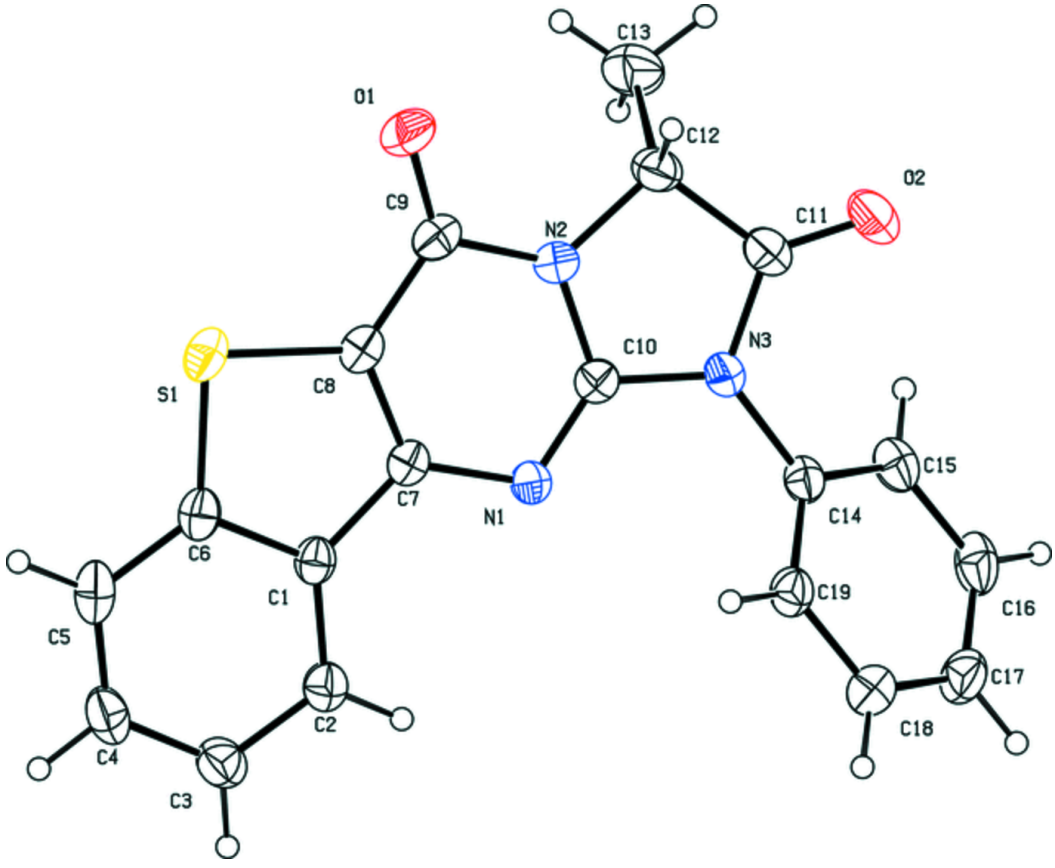
C13
O1
C12
O2
C9
N2
C11
S1
C8
C10
N3
C15
C7
N1
C14
C6
C1
C19
C16
C5
C17
C2
C18
C4
C3

Fig. 2