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3,4-Dimethyl-2-(2-oxo-2-phenylethyl)-2*H*,4*H*-pyrazolo[4,3-c][1,2]benzothiazine-5,5-dione

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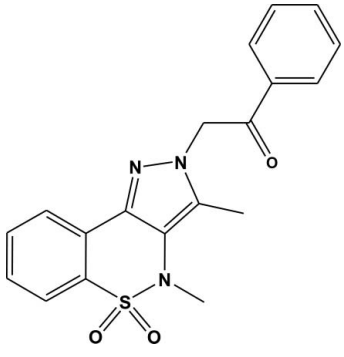
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.005 Å; R factor = 0.069; wR factor = 0.146; data-to-parameter ratio = 16.8.

In the title molecule, $C_{19}H_{17}N_3O_3S$, the heterocyclic thiazine ring adopts a half-chair conformation with the S and N atoms displaced by 0.530 (5) and 0.229 (6) Å, respectively, on opposite sides of the mean plane formed by the remaining ring atoms. The ethanone group lies at an angle of 3.8 (3)° with respect to the benzene ring, which lies almost perendicular to the pyrazole ring, with a dihedral between the two planes of 89.22 (11)°. Weak intermolecular C—H···O hydrogen-bonding interactions are present.

Related literature

For the biological activity of pyrazoles, see: Farag *et al.* (2008); Ciciani *et al.* (2008); Cunico *et al.* (2006); Ahmad *et al.* (2010). For related structures, see: Siddiqui *et al.* (2008).



Experimental

Crystal data

$C_{19}H_{17}N_3O_3S$ M_r = 367.42
Monoclinic, $C2/c$
a = 24.380 (6) Å
b = 11.141 (4) Å
c = 14.996 (5) Å
β = 120.76 (2)°
V = 3500.1 (19) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 200 K
0.12 × 0.10 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
T_{min} = 0.975, T_{max} = 0.983
12615 measured reflections
3970 independent reflections
2847 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.146
S = 1.15
3970 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O2^{i}	0.95	2.43	3.246 (5)	144
C9—H9B···O1^{ii}	0.98	2.46	3.413 (4)	163
C11—H11C···O1^{iii}	0.98	2.44	3.406 (4)	168

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

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* (Otwinowski & Minor, 1997); 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, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2383).

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supplementary materials

Acta Cryst. (2012). E**68**, o502 [**doi:10.1107/S1600536812002188**]

3,4-Dimethyl-2-(2-oxo-2-phenylethyl)-2*H*,4*H*-pyrazolo[4,3-*c*][1,2]benzothiazine-5,5-dione

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Comment

Both benzothiazines and pyrazoles are known as versatile biologically active heterocyclic nuclei. Pyrazoles are found to be cytotoxic agents (Ciciani *et al.*, 2008), anti-tumor (Farag *et al.*, 2008), anti-malarial (Cunico *et al.*, 2006), *etc*. In continuation of our research interests in biologically active molecules (Ahmad *et al.*, 2010), we have fused both of these heterocycles and herein report the synthesis and crystal structure of the title compound.

The bond distances and angles in the title molecule (Fig. 1) agree very well with the corresponding bond distances and angles reported in closely related compounds (Siddiqui *et al.*, 2008). The heterocyclic thiazine ring adopts a half chair conformation with atoms S1 and N1 displaced by 0.530 (5) and 0.229 (6) Å, respectively, on opposite sides from the mean plane formed by the remaining ring atoms. The ethanone group O3/C12/C13/C14 is oriented at 3.8 (3) °, with the benzene ring (C14–C19) which lies almost perpendicular to the pyrazolyl ring (N2/N3/C7/C8/C10) with a dihedral between the two planes of 89.22 (11)°. The structure is devoid of classical hydrogen bonds. However, intermolecular hydrogen bonding interactions of C—H···O type are present (Table 1).

Experimental

Equimolar quantities of 3,4-dimethyl-2,4-dihydropyrazolo[4,3-*c*][1,2] benzothiazine 5,5-dioxide (1.0 g, 4.01 mmol) and corresponding phenacyl bromide (0.80 g, 4.01 mmol) were dissolved in acetonitrile (20 ml) followed by the addition of equimolar K_2CO_3 (0.55 g, 4.01 mmol). The mixture was subjected to reflux for 7 h. The completion of reaction was monitored with the help of TLC. The precipitates of the title compound were collected and washed with methanol. The crystals suitable for X-ray crystallographic analysis were grown from a solution of $CHCl_3$:MeOH in 1:1 ratio.

Refinement

Though all the H atoms could be distinguished in the difference Fourier map, the H-atoms were included at geometrically idealized positions and refined in riding-model approximation with the following constraints: C—H = 0.95, 0.98 and 0.99 Å, for aryl, methyl and methylene H-atoms, respectively. The U_{iso}(H) were included at 1.5U_{eq}(C methyl) or 1.2U_{eq}(C non-methyl). The final difference map was essentially featureless.

Figures

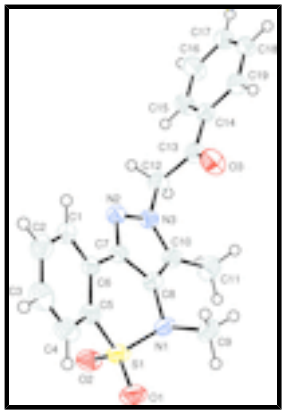

Fig. 1. The title molecule with displacement ellipsoids plotted at the 30% probability level.

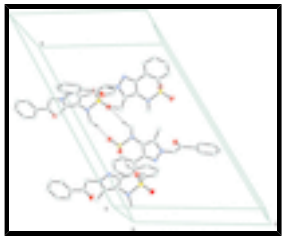

Fig. 2. A part of the unit cell showing intermolecular hydrogen bonding interactions as dashed lines. H-atoms not involved in hydrogen bonding have been excluded for clarity.

3,4-Dimethyl-2-(2-oxo-2-phenylethyl)-2*H*,4*H*- pyrazolo[4,3-*c*][1,2]benzothiazine-5,5-dione

Crystal data

$C_{19}H_{17}N_3O_3S$	$F(000) = 1536$
$M_r = 367.42$	$D_x = 1.394$ Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 6235 reflections
a = 24.380 (6) Å	θ = 1.0–27.5°
b = 11.141 (4) Å	μ = 0.21 mm^{-1}
c = 14.996 (5) Å	*T* = 200 K
β = 120.76 (2)°	Block, colorless
V = 3500.1 (19) Å^3	0.12 × 0.10 × 0.08 mm
Z = 8	

Data collection

Nonius KappaCCD diffractometer	3970 independent reflections
Radiation source: fine-focus sealed tube	2847 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.073$
ω and φ scans	$\theta_{max} = 27.5°$, $\theta_{min} = 2.1°$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)	$h = -31 \rightarrow 30$
$T_{min} = 0.975$, $T_{max} = 0.983$	$k = -14 \rightarrow 14$
12615 measured reflections	$l = -18 \rightarrow 19$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.069$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.146$	H-atom parameters constrained
$S = 1.15$	$w = 1/[\sigma^2(F_o^2) + (0.025P)^2 + 10.0879P]$ where $P = (F_o^2 + 2F_c^2)/3$
3970 reflections	$(\Delta/\sigma)_{max} < 0.001$
237 parameters	$\Delta\rho_{max} = 0.27$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.44$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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}
S1	0.37478 (4)	0.35736 (7)	0.23368 (6)	0.0377 (2)
O1	0.41198 (11)	0.3575 (2)	0.18465 (19)	0.0511 (6)
O2	0.33464 (11)	0.4586 (2)	0.21844 (19)	0.0470 (6)
O3	0.42366 (12)	0.1146 (2)	0.65556 (19)	0.0555 (7)
N1	0.42423 (11)	0.3433 (2)	0.3603 (2)	0.0348 (6)
N2	0.31406 (11)	0.2240 (2)	0.43305 (19)	0.0333 (6)
N3	0.35687 (12)	0.2864 (2)	0.51876 (19)	0.0337 (6)
C1	0.26868 (14)	0.0818 (3)	0.2346 (2)	0.0356 (7)
H1	0.2551	0.0498	0.2788	0.043*
C2	0.24943 (16)	0.0283 (3)	0.1398 (3)	0.0445 (8)
H2	0.2219	−0.0394	0.1190	0.053*
C3	0.26953 (17)	0.0715 (3)	0.0750 (3)	0.0496 (9)
H3	0.2563	0.0329	0.0106	0.059*
C4	0.30886 (17)	0.1711 (3)	0.1036 (3)	0.0447 (8)
H4	0.3230	0.2010	0.0595	0.054*
C5	0.32727 (14)	0.2264 (3)	0.1974 (2)	0.0347 (7)
C6	0.30809 (13)	0.1828 (3)	0.2652 (2)	0.0311 (6)
C7	0.33508 (13)	0.2388 (3)	0.3667 (2)	0.0304 (6)

C8	0.39001 (14)	0.3110 (3)	0.4110 (2)	0.0320 (6)
C9	0.48457 (15)	0.2765 (3)	0.3945 (3)	0.0445 (8)
H9A	0.5120	0.2825	0.4701	0.067*
H9B	0.5067	0.3109	0.3614	0.067*
H9C	0.4748	0.1919	0.3747	0.067*
C10	0.40399 (14)	0.3389 (3)	0.5091 (2)	0.0354 (7)
C11	0.45835 (17)	0.4063 (3)	0.5944 (3)	0.0501 (9)
H11A	0.4820	0.4479	0.5668	0.075*
H11B	0.4869	0.3501	0.6487	0.075*
H11C	0.4420	0.4651	0.6236	0.075*
C12	0.35231 (15)	0.2791 (3)	0.6109 (2)	0.0365 (7)
H12A	0.3071	0.2675	0.5907	0.044*
H12B	0.3673	0.3555	0.6499	0.044*
C13	0.39244 (14)	0.1753 (3)	0.6804 (2)	0.0351 (7)
C14	0.39025 (14)	0.1515 (3)	0.7764 (2)	0.0345 (7)
C15	0.35436 (16)	0.2220 (3)	0.8039 (2)	0.0432 (8)
H15	0.3320	0.2899	0.7632	0.052*
C16	0.35119 (18)	0.1929 (4)	0.8912 (3)	0.0551 (10)
H16	0.3268	0.2414	0.9102	0.066*
C17	0.38329 (16)	0.0941 (3)	0.9503 (3)	0.0442 (8)
H17	0.3802	0.0735	1.0091	0.053*
C18	0.41977 (15)	0.0256 (3)	0.9241 (2)	0.0389 (7)
H18	0.4425	−0.0417	0.9656	0.047*
C19	0.42368 (15)	0.0537 (3)	0.8375 (2)	0.0378 (7)
H19	0.4492	0.0063	0.8200	0.045*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0417 (4)	0.0377 (4)	0.0452 (5)	0.0021 (4)	0.0305 (4)	0.0067 (4)
O1	0.0548 (15)	0.0607 (16)	0.0576 (15)	0.0012 (13)	0.0430 (13)	0.0104 (13)
O2	0.0550 (15)	0.0386 (13)	0.0570 (15)	0.0097 (11)	0.0356 (13)	0.0128 (12)
O3	0.0629 (16)	0.0654 (18)	0.0503 (15)	0.0271 (14)	0.0377 (13)	0.0125 (13)
N1	0.0318 (13)	0.0371 (15)	0.0427 (15)	−0.0028 (11)	0.0243 (12)	0.0012 (12)
N2	0.0305 (13)	0.0380 (14)	0.0324 (13)	0.0011 (11)	0.0169 (11)	0.0020 (11)
N3	0.0353 (13)	0.0373 (14)	0.0313 (13)	0.0017 (12)	0.0190 (11)	0.0019 (11)
C1	0.0288 (15)	0.0397 (18)	0.0354 (17)	0.0004 (14)	0.0144 (14)	0.0027 (14)
C2	0.0388 (18)	0.0427 (19)	0.0447 (19)	−0.0034 (15)	0.0160 (16)	−0.0040 (16)
C3	0.054 (2)	0.053 (2)	0.0355 (18)	0.0026 (18)	0.0183 (17)	−0.0076 (17)
C4	0.053 (2)	0.050 (2)	0.0370 (18)	0.0111 (17)	0.0275 (17)	0.0050 (16)
C5	0.0332 (16)	0.0378 (17)	0.0358 (16)	0.0070 (14)	0.0196 (14)	0.0080 (14)
C6	0.0265 (14)	0.0351 (16)	0.0311 (16)	0.0044 (12)	0.0143 (12)	0.0051 (13)
C7	0.0276 (14)	0.0348 (16)	0.0315 (15)	0.0022 (13)	0.0171 (13)	0.0034 (13)
C8	0.0322 (15)	0.0333 (16)	0.0350 (16)	−0.0010 (13)	0.0204 (13)	0.0001 (13)
C9	0.0341 (17)	0.047 (2)	0.059 (2)	0.0022 (16)	0.0292 (17)	0.0043 (18)
C10	0.0341 (16)	0.0352 (17)	0.0391 (17)	0.0011 (14)	0.0203 (14)	0.0011 (14)
C11	0.046 (2)	0.054 (2)	0.050 (2)	−0.0121 (18)	0.0240 (18)	−0.0155 (18)
C12	0.0428 (17)	0.0383 (17)	0.0343 (16)	0.0014 (15)	0.0241 (15)	−0.0009 (14)

C13	0.0324 (15)	0.0393 (17)	0.0348 (16)	0.0031 (14)	0.0179 (14)	−0.0005 (14)
C14	0.0312 (15)	0.0403 (17)	0.0320 (16)	−0.0004 (14)	0.0162 (13)	0.0009 (14)
C15	0.0458 (19)	0.050 (2)	0.0403 (18)	0.0174 (17)	0.0265 (16)	0.0124 (16)
C16	0.058 (2)	0.070 (3)	0.049 (2)	0.025 (2)	0.036 (2)	0.015 (2)
C17	0.0404 (18)	0.057 (2)	0.0380 (18)	0.0040 (17)	0.0223 (16)	0.0093 (17)
C18	0.0358 (16)	0.0367 (17)	0.0371 (17)	0.0002 (14)	0.0136 (14)	0.0045 (14)
C19	0.0362 (17)	0.0367 (18)	0.0411 (18)	0.0059 (14)	0.0202 (15)	0.0002 (14)

Geometric parameters (Å, °)

S1—O1	1.430 (2)	C8—C10	1.365 (4)
S1—O2	1.433 (2)	C9—H9A	0.9800
S1—N1	1.656 (3)	C9—H9B	0.9800
S1—C5	1.766 (3)	C9—H9C	0.9800
O3—C13	1.211 (4)	C10—C11	1.490 (4)
N1—C8	1.432 (3)	C11—H11A	0.9800
N1—C9	1.486 (4)	C11—H11B	0.9800
N2—C7	1.342 (3)	C11—H11C	0.9800
N2—N3	1.361 (3)	C12—C13	1.530 (4)
N3—C10	1.362 (4)	C12—H12A	0.9900
N3—C12	1.444 (4)	C12—H12B	0.9900
C1—C2	1.383 (4)	C13—C14	1.491 (4)
C1—C6	1.396 (4)	C14—C15	1.386 (4)
C1—H1	0.9500	C14—C19	1.387 (4)
C2—C3	1.381 (5)	C15—C16	1.388 (4)
C2—H2	0.9500	C15—H15	0.9500
C3—C4	1.383 (5)	C16—C17	1.378 (5)
C3—H3	0.9500	C16—H16	0.9500
C4—C5	1.383 (4)	C17—C18	1.374 (4)
C4—H4	0.9500	C17—H17	0.9500
C5—C6	1.406 (4)	C18—C19	1.386 (4)
C6—C7	1.454 (4)	C18—H18	0.9500
C7—C8	1.404 (4)	C19—H19	0.9500
O1—S1—O2	118.56 (15)	N1—C9—H9C	109.5
O1—S1—N1	107.98 (14)	H9A—C9—H9C	109.5
O2—S1—N1	107.12 (14)	H9B—C9—H9C	109.5
O1—S1—C5	109.31 (15)	N3—C10—C8	104.9 (3)
O2—S1—C5	108.32 (14)	N3—C10—C11	123.6 (3)
N1—S1—C5	104.67 (14)	C8—C10—C11	131.4 (3)
C8—N1—C9	115.7 (3)	C10—C11—H11A	109.5
C8—N1—S1	110.62 (19)	C10—C11—H11B	109.5
C9—N1—S1	117.0 (2)	H11A—C11—H11B	109.5
C7—N2—N3	103.8 (2)	C10—C11—H11C	109.5
N2—N3—C10	113.6 (2)	H11A—C11—H11C	109.5
N2—N3—C12	118.5 (2)	H11B—C11—H11C	109.5
C10—N3—C12	127.5 (3)	N3—C12—C13	111.0 (2)
C2—C1—C6	120.0 (3)	N3—C12—H12A	109.4
C2—C1—H1	120.0	C13—C12—H12A	109.4
C6—C1—H1	120.0	N3—C12—H12B	109.4

C3—C2—C1	121.1 (3)	C13—C12—H12B	109.4
C3—C2—H2	119.4	H12A—C12—H12B	108.0
C1—C2—H2	119.4	O3—C13—C14	122.5 (3)
C2—C3—C4	120.0 (3)	O3—C13—C12	119.7 (3)
C2—C3—H3	120.0	C14—C13—C12	117.8 (3)
C4—C3—H3	120.0	C15—C14—C19	119.7 (3)
C3—C4—C5	119.1 (3)	C15—C14—C13	121.7 (3)
C3—C4—H4	120.4	C19—C14—C13	118.6 (3)
C5—C4—H4	120.4	C14—C15—C16	119.8 (3)
C4—C5—C6	121.7 (3)	C14—C15—H15	120.1
C4—C5—S1	120.1 (2)	C16—C15—H15	120.1
C6—C5—S1	118.1 (2)	C17—C16—C15	120.4 (3)
C1—C6—C5	117.9 (3)	C17—C16—H16	119.8
C1—C6—C7	123.9 (3)	C15—C16—H16	119.8
C5—C6—C7	118.0 (3)	C18—C17—C16	119.8 (3)
N2—C7—C8	110.7 (3)	C18—C17—H17	120.1
N2—C7—C6	125.7 (3)	C16—C17—H17	120.1
C8—C7—C6	123.5 (3)	C17—C18—C19	120.5 (3)
C10—C8—C7	107.0 (3)	C17—C18—H18	119.8
C10—C8—N1	128.5 (3)	C19—C18—H18	119.8
C7—C8—N1	124.5 (3)	C18—C19—C14	119.8 (3)
N1—C9—H9A	109.5	C18—C19—H19	120.1
N1—C9—H9B	109.5	C14—C19—H19	120.1
H9A—C9—H9B	109.5		
O1—S1—N1—C8	−164.8 (2)	C6—C7—C8—C10	−174.9 (3)
O2—S1—N1—C8	66.5 (2)	N2—C7—C8—N1	179.7 (3)
C5—S1—N1—C8	−48.4 (2)	C6—C7—C8—N1	3.3 (5)
O1—S1—N1—C9	−29.4 (3)	C9—N1—C8—C10	74.8 (4)
O2—S1—N1—C9	−158.1 (2)	S1—N1—C8—C10	−149.2 (3)
C5—S1—N1—C9	87.0 (2)	C9—N1—C8—C7	−103.0 (4)
C7—N2—N3—C10	−0.4 (3)	S1—N1—C8—C7	33.0 (4)
C7—N2—N3—C12	−173.6 (3)	N2—N3—C10—C8	1.3 (3)
C6—C1—C2—C3	1.3 (5)	C12—N3—C10—C8	173.8 (3)
C1—C2—C3—C4	−0.9 (5)	N2—N3—C10—C11	−176.5 (3)
C2—C3—C4—C5	−0.3 (5)	C12—N3—C10—C11	−4.0 (5)
C3—C4—C5—C6	1.3 (5)	C7—C8—C10—N3	−1.6 (3)
C3—C4—C5—S1	−177.4 (3)	N1—C8—C10—N3	−179.7 (3)
O1—S1—C5—C4	−27.1 (3)	C7—C8—C10—C11	176.0 (3)
O2—S1—C5—C4	103.5 (3)	N1—C8—C10—C11	−2.2 (6)
N1—S1—C5—C4	−142.5 (3)	N2—N3—C12—C13	90.0 (3)
O1—S1—C5—C6	154.2 (2)	C10—N3—C12—C13	−82.2 (4)
O2—S1—C5—C6	−75.3 (3)	N3—C12—C13—O3	1.9 (4)
N1—S1—C5—C6	38.8 (3)	N3—C12—C13—C14	−176.9 (3)
C2—C1—C6—C5	−0.3 (4)	O3—C13—C14—C15	179.8 (3)
C2—C1—C6—C7	−174.6 (3)	C12—C13—C14—C15	−1.4 (5)
C4—C5—C6—C1	−0.9 (4)	O3—C13—C14—C19	−2.1 (5)
S1—C5—C6—C1	177.8 (2)	C12—C13—C14—C19	176.6 (3)
C4—C5—C6—C7	173.6 (3)	C19—C14—C15—C16	−1.2 (5)
S1—C5—C6—C7	−7.7 (4)	C13—C14—C15—C16	176.8 (3)

N3—N2—C7—C8	−0.7 (3)	C14—C15—C16—C17	−0.3 (6)
N3—N2—C7—C6	175.7 (3)	C15—C16—C17—C18	1.4 (6)
C1—C6—C7—N2	−18.5 (5)	C16—C17—C18—C19	−1.1 (5)
C5—C6—C7—N2	167.3 (3)	C17—C18—C19—C14	−0.4 (5)
C1—C6—C7—C8	157.4 (3)	C15—C14—C19—C18	1.5 (5)
C5—C6—C7—C8	−16.8 (4)	C13—C14—C19—C18	−176.6 (3)
N2—C7—C8—C10	1.5 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O2^{i}	0.95	2.43	3.246 (5)	144
C9—H9B···O1^{ii}	0.98	2.46	3.413 (4)	163.
C11—H11C···O1^{iii}	0.98	2.44	3.406 (4)	168.

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

Fig. 1

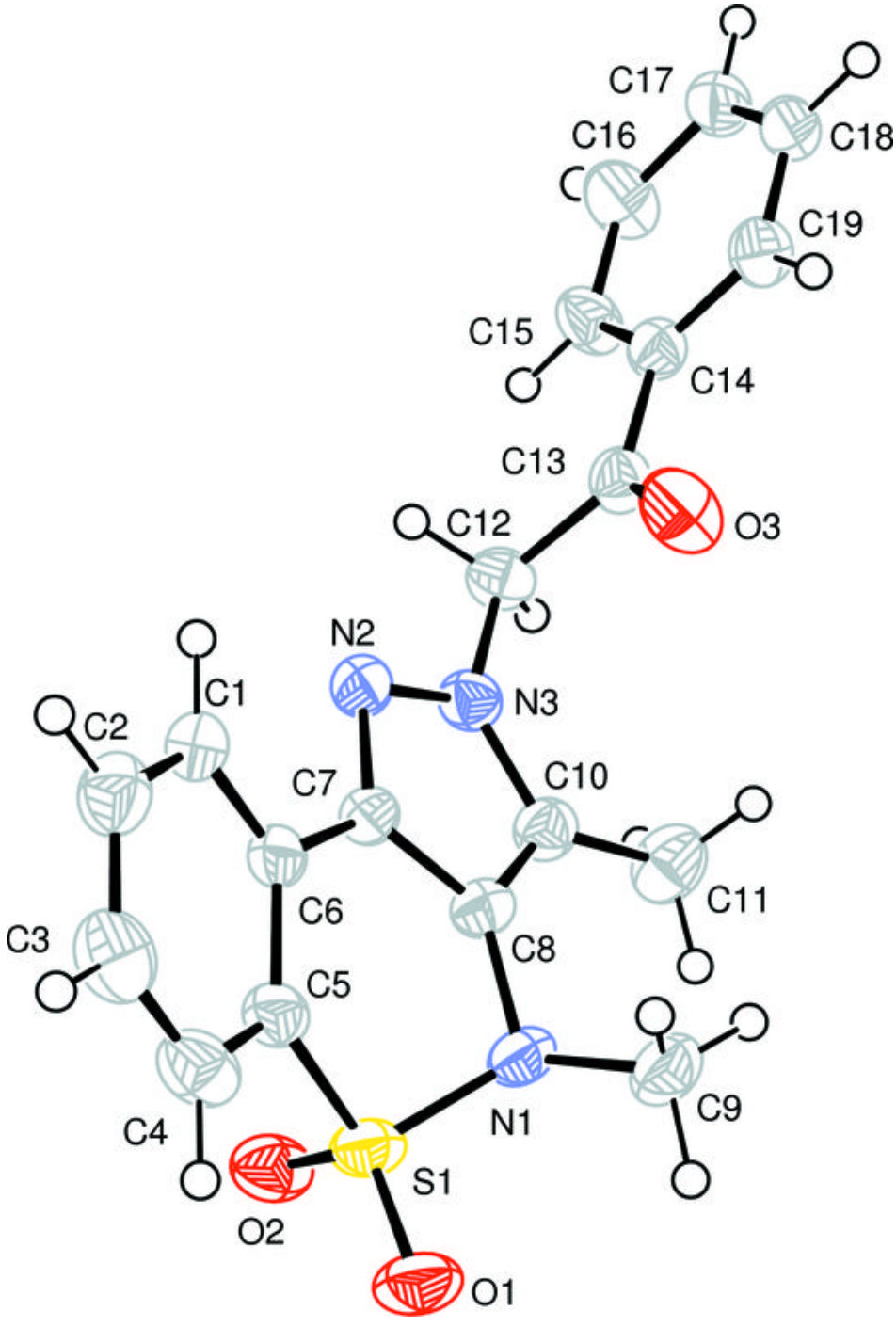
C17
C16
C18
C19
C15
C14
C13
O3
C12
N2
N3
C1
C2
C7
C10
C11
C6
C8
C3
C5
C4
N1
C9
S1
O2
O1

Fig. 2