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1,1,3-Trioxo-2,3-dihydro-1,2-benzisothiazol-2-ylmethyl 4-phenylpiperazine-1-carbodithioate

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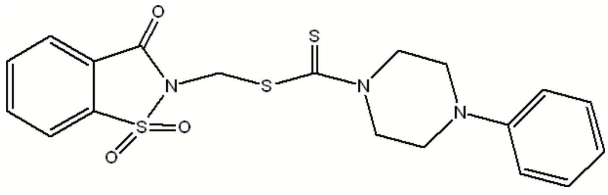
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.076; data-to-parameter ratio = 15.2.

In the title molecule, $C_{19}H_{19}N_3O_3S_3$, the mean planes of the benzisothiazole system and the phenyl ring make a dihedral angle of 8.87 (8)°. The piperazine ring has a chair conformation. The crystal structure is stabilized by weak intermolecular C—H···O interactions and weak intramolecular C—H···S interactions.

Related literature

For related literature, see: Ateş *et al.* (1995); Cao *et al.* (2005); Çapan *et al.* (1993); Cremer & Pople (1975); Farghaly & Moharram (1999); Günay *et al.* (1999); Güzel & Salman (2006); Imamura *et al.* (2001); Scozzafava *et al.* (2000); Xu *et al.* (2002).



Experimental

Crystal data

$C_{19}H_{19}N_3O_3S_3$
M_r = 433.58
Triclinic, $P\overline{1}$
a = 8.0390 (5) Å
b = 11.7619 (7) Å
c = 11.8796 (8) Å
α = 109.029 (5)°
β = 103.791 (5)°
γ = 102.326 (5)°
V = 978.02 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.41 mm^{-1}
T = 296 K
0.72 × 0.68 × 0.57 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.759, T_{max} = 0.802
18676 measured reflections
3838 independent reflections
3472 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.076
S = 1.04
3838 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O2^{i}	0.93	2.43	3.226 (2)	143
C8—H8B···S3	0.97	2.54	3.1134 (18)	117
C10—H10A···S3	0.97	2.56	3.075 (2)	113
C13—H13B···S2	0.97	2.38	2.9324 (18)	116

Symmetry code: (i) $-x+1, -y, -z+1$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2418).

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supplementary materials

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1,1,3-Trioxo-2,3-dihydro-1,2-benzisothiazol-2-ylmethyl 4-phenylpiperazine-1-carbodithioate

M. Akkurt, S.P. Yalçin, Ö. Güzel, A. Salman and O. Büyükgüngör

Comment

Considerable interest has been focused on dithiocarbamates which have shown to possess a broad spectrum of biological activities such as fungicidal (Ateş *et al.*, 1995; Günay *et al.*, 1999; Farghaly & Moharram, 1999; Xu *et al.*, 2002) and antibacterial (Günay *et al.*, 1999; Çapan *et al.*, 1993; Imamura *et al.*, 2001) effects. Dithiocarbamates are known also to be active as anticancer agents (Scozzafava *et al.*, 2000; Cao *et al.*, 2005). In our previous report (Güzel & Salman, 2006), (1,1-dioxido-3-oxo-1,2-benzisothiazol-2(3*H*)-yl)methyl N,*N*-disubstituted dithiocarbamate and (1,1-dioxido-3-oxo-1,2-benzisothiazol-2(3*H*)-yl)methyl *O*-alkyldithiocarbonate derivatives have been demonstrated to be potent antimycobacterial and antitumor activities. We now report the crystal structure of (1,1-dioxido-3-oxo-1,2-benzisothiazol-2(3*H*)-yl)methyl 4-phenylpiperazin-1-carbodithioate which has potent antimycobacterial activity.

In the title compound (Fig. 1), all bond lengths and angles are within the normal range. The C1—C7/N1/S1 ring system are almost planar, with the mean deviations of 0.039 (2) Å for C6 and −0.052 (1) Å for N1. The dihedral angle between the C1—C7/N1/S1 ring and the phenyl ring is 8.87 (8)°. The N2/N3/C10—C13 ring system has a chair conformation [puckering parameters (Cremer & Pople, 1975): Q = 0.5601 (18) Å, θ = 1.28 (17) ° and φ = 17 (6)°].

The crystal structure is stabilized by weak intermolecular C—H···O interactions (Fig. 1) and weak intramolecular C—H···S interactions (Table 1).

Experimental

The ethanolic solution of 2-(chloromethyl)-1,2-benzisothiazol-3(2*H*)-on 1,1-dioxide (5 mmol) and potassium 4-phenylpiperazin-1-carbodithioate (5 mmol) were refluxed for 1 h. After evaporation of the solvent *in vacuo*, products were washed with water and purified by recrystallization from ethanol (Güzel & Salman, 2006).

Yellow powder (62%); mp 445–450 K; IR (KBr): ν 1733 (C═O), 1243 (C═S). ^{1}H-NMR ($CDCl_3$ / 200 MHz): δ 3.15 (t, 4H, J=5.15 Hz, pip. $C_{3,5}$—H), 4.13 (br s, 4H, pip. $C_{2,6}$—H), 5.70 (s, 2H, N—CH_2—S), 6.69–6.77 (m, 3H, phenyl $C_{3,4,5}$—H), 7.06–7.14 (m, 2H, phenyl $C_{2,6}$—H), 7.71–7.81 (m, 3H, bzi. $C_{5,6,7}$—H), 7.91–7.95 (m, 1H, bzi. C_4—H); EIMS: m/*z* 433 (M^+). Analysis calculated for $C_{19}H_{19}N_3O_3S_3$: C 52.63, H 4.42, N 9.69, S 22.19%. Found: C 53.01, H 4.32, N 9.57, S 22.15%.

Refinement

All H atoms were positioned geometrically, with C—H = 0.93–0.97Å and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

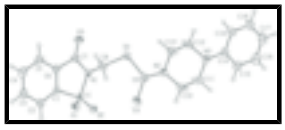

Fig. 1. An *ORTEP* view of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

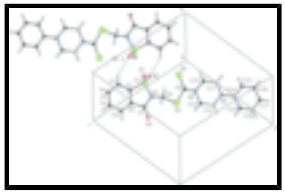

Fig. 2. View of the weak intermolecular C—H···O hydrogen bonding interactions in the unit cell.

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Crystal data

$C_{19}H_{19}N_3O_3S_3$	$Z = 2$
$M_r = 433.58$	$F_{000} = 452$
Triclinic, $P\overline{1}$	$D_x = 1.472$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.0390$ (5) Å	Cell parameters from 41005 reflections
$b = 11.7619$ (7) Å	$\theta = 2.8$–27.9°
$c = 11.8796$ (8) Å	$\mu = 0.41$ mm^{-1}
$\alpha = 109.029$ (5)°	$T = 296$ K
$\beta = 103.791$ (5)°	Prism, colourless
$\gamma = 102.326$ (5)°	0.72 × 0.68 × 0.57 mm
$V = 978.02$ (12) Å^3	

Data collection

Stoe IPDS2 diffractometer	3838 independent reflections
Monochromator: plane graphite	3472 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{int} = 0.042$
$T = 296$ K	$\theta_{max} = 26.0^\circ$
ω scans	$\theta_{min} = 2.8^\circ$
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$h = -9 \rightarrow 9$
$T_{min} = 0.759$, $T_{max} = 0.802$	$k = -14 \rightarrow 14$
18676 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.029$	H-atom parameters constrained
$wR(F^2) = 0.076$	$w = 1/[\sigma^2(F_o^2) + (0.0359P)^2 + 0.2749P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
3838 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
253 parameters	$\Delta\rho_{min} = -0.34$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating –*R*-factor-obs *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	0.29371 (4)	0.07783 (3)	0.52191 (3)	0.0315 (1)
S2	0.16223 (6)	0.36814 (4)	0.44690 (4)	0.0465 (1)
S3	0.29352 (7)	0.19904 (4)	0.26112 (4)	0.0552 (2)
O1	0.16370 (15)	−0.03381 (10)	0.42204 (10)	0.0460 (3)
O2	0.46502 (14)	0.12296 (10)	0.51054 (10)	0.0410 (3)
O3	0.13194 (18)	0.32432 (11)	0.71142 (13)	0.0584 (4)
N1	0.20056 (16)	0.19455 (11)	0.55194 (12)	0.0372 (4)
N2	0.34280 (18)	0.44371 (12)	0.31506 (13)	0.0455 (4)
N3	0.32077 (17)	0.60864 (12)	0.18385 (12)	0.0404 (4)
C1	0.31709 (18)	0.07322 (13)	0.67057 (13)	0.0335 (4)
C2	0.3811 (2)	−0.00962 (15)	0.71439 (15)	0.0428 (5)
C3	0.3814 (2)	0.00154 (19)	0.83429 (17)	0.0540 (6)
C4	0.3238 (3)	0.0924 (2)	0.90612 (16)	0.0590 (6)
C5	0.2636 (2)	0.17575 (17)	0.86153 (15)	0.0520 (5)
C6	0.26044 (19)	0.16530 (13)	0.74175 (13)	0.0380 (4)
C7	0.1914 (2)	0.23932 (14)	0.67370 (15)	0.0405 (4)
C8	0.0837 (2)	0.21508 (15)	0.45184 (16)	0.0444 (5)
C9	0.27614 (19)	0.34041 (14)	0.33358 (14)	0.0386 (4)
C10	0.4363 (2)	0.44362 (17)	0.22371 (18)	0.0514 (6)
C11	0.3388 (2)	0.48396 (16)	0.12594 (16)	0.0483 (5)
C12	0.2318 (2)	0.61100 (14)	0.27846 (15)	0.0421 (4)
C13	0.3282 (2)	0.56965 (14)	0.37590 (16)	0.0474 (5)
C14	0.25681 (19)	0.66404 (14)	0.10005 (15)	0.0407 (4)

C15	0.2437 (2)	0.61482 (18)	−0.02674 (16)	0.0531 (5)
C16	0.1895 (2)	0.6746 (2)	−0.10496 (18)	0.0631 (6)
C17	0.1431 (2)	0.7823 (2)	−0.0613 (2)	0.0634 (7)
C18	0.1535 (3)	0.83086 (18)	0.0631 (2)	0.0619 (7)
C19	0.2096 (2)	0.77347 (16)	0.14331 (18)	0.0522 (6)
H2	0.42200	−0.06990	0.66600	0.0510*
H3	0.42140	−0.05360	0.86680	0.0650*
H4	0.32560	0.09760	0.98620	0.0710*
H5	0.22590	0.23760	0.91090	0.0620*
H8A	−0.03450	0.20420	0.46140	0.0530*
H8B	0.06920	0.15030	0.37150	0.0530*
H10A	0.44220	0.35920	0.18260	0.0620*
H10B	0.55890	0.50130	0.26710	0.0620*
H11A	0.40470	0.48600	0.06770	0.0580*
H11B	0.21970	0.42230	0.07810	0.0580*
H12A	0.10800	0.55520	0.23680	0.0500*
H12B	0.22930	0.69630	0.32010	0.0500*
H13A	0.44800	0.63030	0.42370	0.0570*
H13B	0.26230	0.56760	0.43420	0.0570*
H15	0.27190	0.54080	−0.05910	0.0640*
H16	0.18450	0.64110	−0.18870	0.0760*
H17	0.10550	0.82150	−0.11460	0.0760*
H18	0.12230	0.90380	0.09400	0.0740*
H19	0.21580	0.80840	0.22720	0.0630*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0363 (2)	0.0290 (2)	0.0322 (2)	0.0115 (1)	0.0144 (1)	0.0131 (1)
S2	0.0589 (2)	0.0422 (2)	0.0546 (2)	0.0244 (2)	0.0265 (2)	0.0284 (2)
S3	0.0783 (3)	0.0425 (2)	0.0592 (3)	0.0326 (2)	0.0289 (2)	0.0251 (2)
O1	0.0512 (6)	0.0366 (5)	0.0378 (5)	0.0078 (5)	0.0094 (5)	0.0074 (4)
O2	0.0429 (5)	0.0425 (6)	0.0495 (6)	0.0176 (4)	0.0258 (5)	0.0229 (5)
O3	0.0701 (8)	0.0444 (6)	0.0756 (8)	0.0302 (6)	0.0432 (7)	0.0212 (6)
N1	0.0429 (6)	0.0368 (6)	0.0424 (7)	0.0192 (5)	0.0197 (5)	0.0206 (5)
N2	0.0558 (8)	0.0368 (7)	0.0522 (8)	0.0176 (6)	0.0254 (6)	0.0207 (6)
N3	0.0424 (6)	0.0386 (6)	0.0428 (7)	0.0144 (5)	0.0173 (5)	0.0163 (5)
C1	0.0330 (6)	0.0347 (7)	0.0327 (7)	0.0072 (5)	0.0125 (5)	0.0143 (6)
C2	0.0425 (8)	0.0489 (9)	0.0465 (8)	0.0180 (7)	0.0178 (7)	0.0262 (7)
C3	0.0528 (9)	0.0714 (12)	0.0513 (10)	0.0214 (8)	0.0178 (8)	0.0396 (9)
C4	0.0634 (11)	0.0774 (13)	0.0381 (8)	0.0157 (9)	0.0182 (8)	0.0285 (9)
C5	0.0585 (10)	0.0535 (10)	0.0390 (8)	0.0131 (8)	0.0227 (7)	0.0107 (7)
C6	0.0383 (7)	0.0352 (7)	0.0365 (7)	0.0066 (6)	0.0150 (6)	0.0106 (6)
C7	0.0416 (7)	0.0336 (7)	0.0494 (8)	0.0117 (6)	0.0233 (7)	0.0147 (6)
C8	0.0372 (7)	0.0449 (8)	0.0566 (9)	0.0135 (6)	0.0132 (7)	0.0284 (7)
C9	0.0394 (7)	0.0386 (7)	0.0392 (7)	0.0158 (6)	0.0079 (6)	0.0188 (6)
C10	0.0565 (9)	0.0497 (9)	0.0671 (11)	0.0260 (8)	0.0351 (9)	0.0305 (8)
C11	0.0589 (10)	0.0457 (9)	0.0528 (9)	0.0242 (7)	0.0318 (8)	0.0207 (7)

C12	0.0450 (8)	0.0343 (7)	0.0466 (8)	0.0125 (6)	0.0196 (7)	0.0126 (6)
C13	0.0628 (10)	0.0338 (7)	0.0460 (8)	0.0124 (7)	0.0223 (8)	0.0154 (7)
C14	0.0335 (7)	0.0389 (8)	0.0449 (8)	0.0064 (6)	0.0099 (6)	0.0163 (6)
C15	0.0526 (9)	0.0563 (10)	0.0468 (9)	0.0163 (8)	0.0135 (7)	0.0188 (8)
C16	0.0539 (10)	0.0788 (13)	0.0497 (10)	0.0104 (9)	0.0078 (8)	0.0307 (10)
C17	0.0466 (9)	0.0708 (12)	0.0734 (13)	0.0080 (9)	0.0063 (9)	0.0460 (11)
C18	0.0572 (10)	0.0500 (10)	0.0851 (14)	0.0177 (8)	0.0212 (10)	0.0364 (10)
C19	0.0573 (10)	0.0433 (9)	0.0575 (10)	0.0163 (7)	0.0193 (8)	0.0214 (8)

Geometric parameters (Å, °)

S1—O1	1.4252 (12)	C14—C15	1.395 (2)
S1—O2	1.4212 (12)	C14—C19	1.391 (3)
S1—N1	1.6792 (14)	C15—C16	1.383 (3)
S1—C1	1.7509 (15)	C16—C17	1.371 (3)
S2—C8	1.8012 (19)	C17—C18	1.374 (3)
S2—C9	1.7850 (16)	C18—C19	1.383 (3)
S3—C9	1.6579 (17)	C2—H2	0.9300
O3—C7	1.201 (2)	C3—H3	0.9300
N1—C7	1.395 (2)	C4—H4	0.9300
N1—C8	1.451 (2)	C5—H5	0.9300
N2—C9	1.328 (2)	C8—H8A	0.9700
N2—C10	1.460 (2)	C8—H8B	0.9700
N2—C13	1.465 (2)	C10—H10A	0.9700
N3—C11	1.458 (2)	C10—H10B	0.9700
N3—C12	1.465 (2)	C11—H11A	0.9700
N3—C14	1.415 (2)	C11—H11B	0.9700
C1—C2	1.379 (2)	C12—H12A	0.9700
C1—C6	1.376 (2)	C12—H12B	0.9700
C2—C3	1.387 (2)	C13—H13A	0.9700
C3—C4	1.375 (3)	C13—H13B	0.9700
C4—C5	1.377 (3)	C15—H15	0.9300
C5—C6	1.381 (2)	C16—H16	0.9300
C6—C7	1.473 (2)	C17—H17	0.9300
C10—C11	1.508 (3)	C18—H18	0.9300
C12—C13	1.509 (2)	C19—H19	0.9300
S1···O2^{i}	3.3476 (13)	C15···H12A^{v}	3.0300
S2···O3	3.4010 (15)	C15···H11B	2.9100
S3···O2	3.4335 (12)	C16···H12A^{v}	2.8600
S2···H13B	2.3800	C17···H3^{x}	3.1000
S2···H13A^{ii}	3.1400	C18···H5^{vii}	3.1000
S3···H4^{iii}	3.1900	C19···H12B	2.5300
S3···H8B	2.5400	H2···S3^{i}	3.1100
S3···H10A	2.5600	H2···O2^{i}	2.4300
S3···H18^{iv}	3.1700	H3···C17^{ix}	3.1000
S3···H2^{i}	3.1100	H4···S3^{viii}	3.1900
S3···H17^{v}	3.1800	H5···O3	2.8800

O1···C7^{vi}	3.000 (2)	H5···C11^{viii}	2.9500
O1···C6^{vi}	3.229 (2)	H5···H11B^{viii}	2.4400
O2···C12^{ii}	3.276 (2)	H5···C18^{vii}	3.1000
O2···C2^{i}	3.226 (2)	H8A···O3	2.6800
O2···S3	3.4335 (12)	H8A···C2^{vi}	2.9600
O2···S1^{i}	3.3476 (13)	H8B···S3	2.5400
O2···O2^{i}	3.0058 (17)	H8B···O1	2.6400
O2···C13^{ii}	3.292 (2)	H10A···S3	2.5600
O3···C12^{vii}	3.194 (2)	H10B···H13A	2.4700
O3···S2	3.4010 (15)	H10B···O3^{ii}	2.7600
O1···H19^{iv}	2.6400	H10B···C7^{ii}	3.0200
O1···H8B	2.6400	H11A···C15	2.5500
O2···H12B^{ii}	2.6900	H11A···H15	2.0000
O2···H13A^{ii}	2.6300	H11A···H11A^{xi}	2.5200
O2···H2^{i}	2.4300	H11B···C15	2.9100
O3···H8A	2.6800	H11B···H5^{iii}	2.4400
O3···H15^{viii}	2.8200	H11B···H12A	2.5100
O3···H5	2.8800	H11B···H15	2.5200
O3···H10B^{ii}	2.7600	H12A···H11B	2.5100
O3···H12A^{vii}	2.7000	H12A···O3^{vii}	2.7000
O3···H12B^{vii}	2.7800	H12A···C15^{v}	3.0300
N2···N3	2.866 (2)	H12A···C16^{v}	2.8600
N3···N2	2.866 (2)	H12B···C19	2.5300
C2···O2^{i}	3.226 (2)	H12B···H19	1.9800
C2···C19^{ii}	3.433 (3)	H12B···O2^{ii}	2.6900
C3···C18^{ii}	3.531 (3)	H12B···O3^{vii}	2.7800
C6···O1^{vi}	3.229 (2)	H13A···H10B	2.4700
C7···O1^{vi}	3.000 (2)	H13A···S2^{ii}	3.1400
C12···O2^{ii}	3.276 (2)	H13A···O2^{ii}	2.6300
C12···O3^{vii}	3.194 (2)	H13A···C9^{ii}	3.0500
C13···O2^{ii}	3.292 (2)	H13B···S2	2.3800
C18···C3^{ii}	3.531 (3)	H15···O3^{iii}	2.8200
C19···C2^{ii}	3.433 (3)	H15···C11	2.4700
C2···H8A^{vi}	2.9600	H15···H11A	2.0000
C3···H17^{ix}	3.0400	H15···H11B	2.5200
C7···H10B^{ii}	3.0200	H17···C3^{x}	3.0400
C9···H13A^{ii}	3.0500	H17···S3^{v}	3.1800
C11···H15	2.4700	H18···S3^{xii}	3.1700
C11···H5^{iii}	2.9500	H19···O1^{xii}	2.6400
C12···H19	2.6100	H19···C12	2.6100
C15···H11A	2.5500	H19···H12B	1.9800

O1—S1—O2	118.56 (7)	C14—C19—C18	120.80 (18)
O1—S1—N1	109.17 (7)	C1—C2—H2	122.00
O1—S1—C1	112.42 (7)	C3—C2—H2	122.00
O2—S1—N1	109.89 (7)	C2—C3—H3	119.00
O2—S1—C1	111.09 (7)	C4—C3—H3	119.00
N1—S1—C1	92.61 (7)	C3—C4—H4	119.00
C8—S2—C9	103.70 (8)	C5—C4—H4	119.00
S1—N1—C7	114.08 (11)	C4—C5—H5	121.00
S1—N1—C8	122.14 (11)	C6—C5—H5	121.00
C7—N1—C8	120.29 (14)	S2—C8—H8A	108.00
C9—N2—C10	122.90 (15)	S2—C8—H8B	109.00
C9—N2—C13	126.60 (14)	N1—C8—H8A	109.00
C10—N2—C13	110.45 (14)	N1—C8—H8B	109.00
C11—N3—C12	110.69 (14)	H8A—C8—H8B	107.00
C11—N3—C14	116.06 (13)	N2—C10—H10A	110.00
C12—N3—C14	115.49 (14)	N2—C10—H10B	110.00
S1—C1—C2	126.73 (12)	C11—C10—H10A	110.00
S1—C1—C6	110.55 (11)	C11—C10—H10B	110.00
C2—C1—C6	122.72 (14)	H10A—C10—H10B	108.00
C1—C2—C3	116.60 (16)	N3—C11—H11A	109.00
C2—C3—C4	121.33 (19)	N3—C11—H11B	109.00
C3—C4—C5	121.15 (17)	C10—C11—H11A	109.00
C4—C5—C6	118.40 (16)	C10—C11—H11B	109.00
C1—C6—C5	119.78 (15)	H11A—C11—H11B	108.00
C1—C6—C7	113.08 (13)	N3—C12—H12A	109.00
C5—C6—C7	127.04 (15)	N3—C12—H12B	109.00
O3—C7—N1	122.63 (16)	C13—C12—H12A	109.00
O3—C7—C6	127.78 (15)	C13—C12—H12B	109.00
N1—C7—C6	109.58 (14)	H12A—C12—H12B	108.00
S2—C8—N1	115.09 (12)	N2—C13—H13A	110.00
S2—C9—S3	122.16 (10)	N2—C13—H13B	110.00
S2—C9—N2	112.84 (12)	C12—C13—H13A	110.00
S3—C9—N2	125.00 (13)	C12—C13—H13B	110.00
N2—C10—C11	110.41 (14)	H13A—C13—H13B	108.00
N3—C11—C10	111.57 (14)	C14—C15—H15	120.00
N3—C12—C13	111.54 (14)	C16—C15—H15	120.00
N2—C13—C12	110.59 (14)	C15—C16—H16	119.00
N3—C14—C15	122.15 (16)	C17—C16—H16	119.00
N3—C14—C19	120.46 (15)	C16—C17—H17	121.00
C15—C14—C19	117.36 (17)	C18—C17—H17	121.00
C14—C15—C16	120.92 (18)	C17—C18—H18	119.00
C15—C16—C17	121.19 (18)	C19—C18—H18	119.00
C16—C17—C18	118.4 (2)	C14—C19—H19	120.00
C17—C18—C19	121.3 (2)	C18—C19—H19	120.00
O1—S1—N1—C7	118.00 (12)	C11—N3—C14—C15	−11.6 (2)
O2—S1—N1—C7	−110.39 (12)	C11—N3—C12—C13	54.79 (18)
C1—S1—N1—C7	3.17 (13)	C14—N3—C12—C13	−170.76 (14)
O1—S1—N1—C8	−40.93 (15)	C12—N3—C14—C19	38.5 (2)
O2—S1—N1—C8	90.68 (14)	C12—N3—C14—C15	−143.56 (16)

C1—S1—N1—C8	−155.76 (13)	C11—N3—C14—C19	170.48 (16)
O1—S1—C1—C2	64.79 (17)	C2—C1—C6—C5	−1.1 (2)
O2—S1—C1—C2	−70.73 (16)	S1—C1—C6—C5	178.41 (13)
N1—S1—C1—C2	176.78 (15)	S1—C1—C6—C7	1.70 (18)
O1—S1—C1—C6	−114.74 (12)	S1—C1—C2—C3	−177.70 (14)
O2—S1—C1—C6	109.75 (12)	C2—C1—C6—C7	−177.85 (15)
N1—S1—C1—C6	−2.75 (12)	C6—C1—C2—C3	1.8 (3)
C8—S2—C9—S3	−0.78 (13)	C1—C2—C3—C4	−1.2 (3)
C8—S2—C9—N2	179.14 (12)	C2—C3—C4—C5	0.0 (3)
C9—S2—C8—N1	95.71 (13)	C3—C4—C5—C6	0.7 (3)
S1—N1—C7—C6	−2.68 (17)	C4—C5—C6—C1	−0.1 (3)
C8—N1—C7—C6	156.68 (14)	C4—C5—C6—C7	176.08 (18)
S1—N1—C8—S2	−119.76 (12)	C5—C6—C7—O3	2.9 (3)
C7—N1—C8—S2	82.59 (17)	C1—C6—C7—N1	0.5 (2)
S1—N1—C7—O3	178.48 (14)	C1—C6—C7—O3	179.30 (18)
C8—N1—C7—O3	−22.2 (3)	C5—C6—C7—N1	−175.89 (16)
C10—N2—C9—S2	−177.89 (13)	N2—C10—C11—N3	57.1 (2)
C13—N2—C9—S2	−0.8 (2)	N3—C12—C13—N2	−55.95 (18)
C10—N2—C9—S3	2.0 (2)	N3—C14—C15—C16	−176.66 (17)
C13—N2—C9—S3	179.14 (13)	C19—C14—C15—C16	1.4 (3)
C9—N2—C10—C11	119.80 (18)	N3—C14—C19—C18	177.54 (18)
C13—N2—C10—C11	−57.72 (19)	C15—C14—C19—C18	−0.5 (3)
C10—N2—C13—C12	57.29 (18)	C14—C15—C16—C17	−1.5 (3)
C9—N2—C13—C12	−120.12 (17)	C15—C16—C17—C18	0.7 (3)
C14—N3—C11—C10	170.49 (14)	C16—C17—C18—C19	0.1 (3)
C12—N3—C11—C10	−55.34 (18)	C17—C18—C19—C14	−0.2 (3)

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, *y*, *z*−1; (iv) *x*, *y*−1, *z*; (v) −*x*, −*y*+1, −*z*; (vi) −*x*, −*y*, −*z*+1; (vii) −*x*, −*y*+1, −*z*+1; (viii) *x*, *y*, *z*+1; (ix) *x*, *y*−1, *z*+1; (x) *x*, *y*+1, *z*−1; (xi) −*x*+1, −*y*+1, −*z*; (xii) *x*, *y*+1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O2^{i}	0.93	2.43	3.226 (2)	143
C8—H8B···S3	0.97	2.54	3.1134 (18)	117
C10—H10A···S3	0.97	2.56	3.075 (2)	113
C13—H13B···S2	0.97	2.38	2.9324 (18)	116

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

Fig. 1

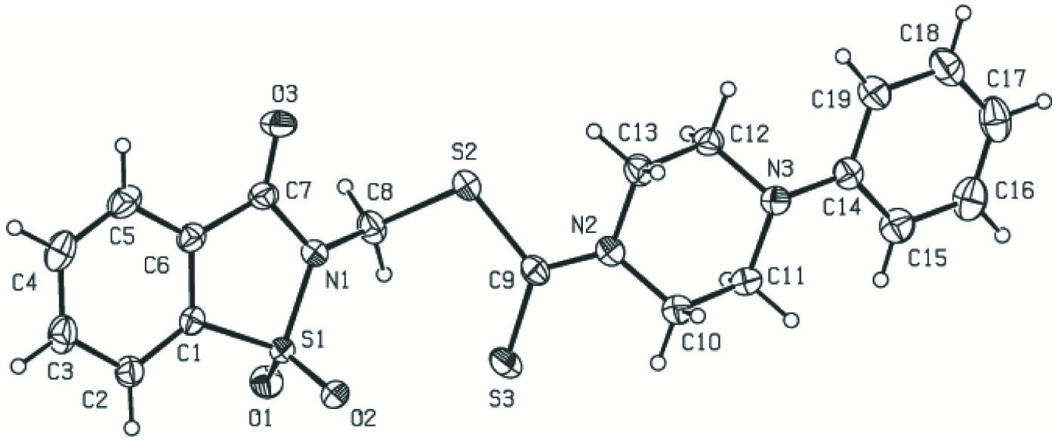
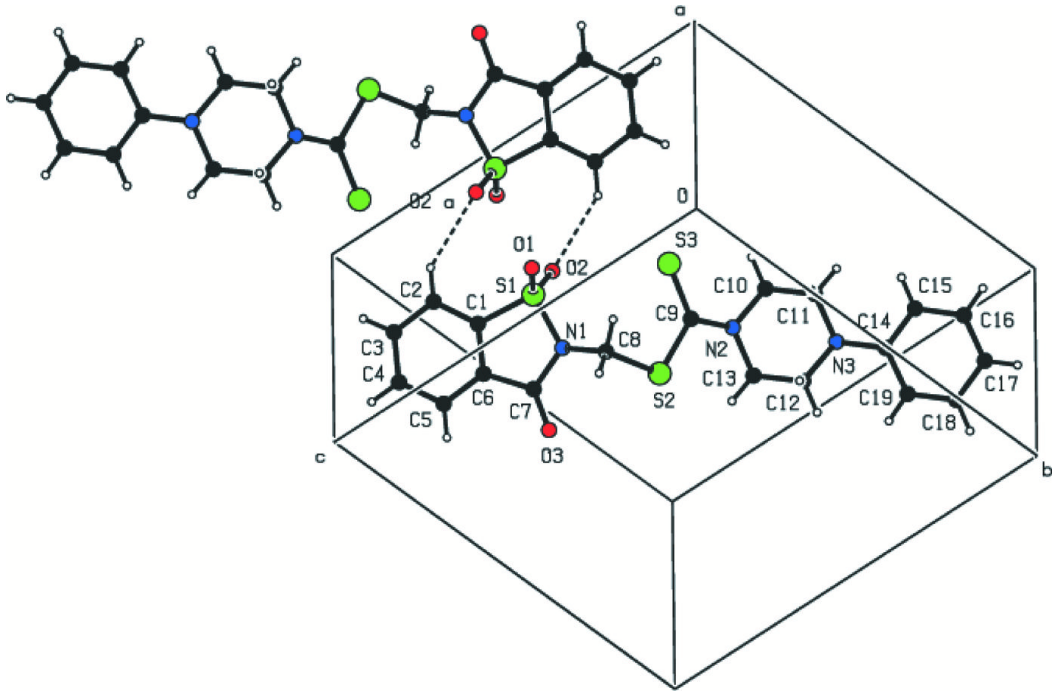

O3
C7
C8
S2
C5
C6
N1
C4
C1
S1
C3
C2
O1
O2
C9
S3
N2
C13
C12
N3
C19
C18
C17
C14
C16
C15
C11
C10

Fig. 2


a
O2
a
O
O1
S3
C2
S1
O2
C10
C15
C1
C9
C11
C14
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C8
C3
N2
N3
C4
C13
C17
C6
S2
C12
C19
C5
C7
C18
O3
c
b