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O-Butyl *S*-(1,1,3-trioxobenz[*d*]isothiazol-2-yl)methyl dithiocarbonate

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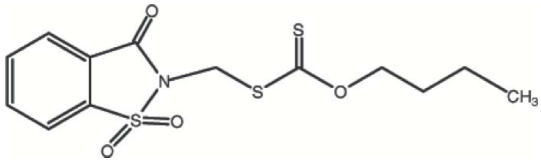
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.007 Å; R factor = 0.076; wR factor = 0.197; data-to-parameter ratio = 26.0.

The asymmetric unit in the crystal structure of the title compound, $C_{13}H_{15}NO_4S_3$, comprises two molecules. Their nine-membered fused-ring systems are planar, with maximum deviations from the mean planes for the N atoms of 0.045 (3) and −0.028 (3) Å for the two molecules. The molecules are linked by intermolecular C—H···O hydrogen bonds oriented along the [010] axis.

Related literature

For related literature, see: Güzel & Salman (2006); Pennino (1957); Tsuchima & Wakamori (1974); Uchiyama & Hashimoto (1974).



Experimental

Crystal data

$C_{13}H_{15}NO_4S_3$
M_r = 345.47
Triclinic, $P\overline{1}$
a = 8.8191 (3) Å
b = 13.4997 (2) Å
c = 14.7531 (2) Å
α = 70.270 (3)°
β = 85.255 (5)°
γ = 89.696 (5)°
V = 1647.18 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.46 mm^{-1}
T = 294 (2) K
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.913, T_{max} = 0.913
46335 measured reflections
9889 independent reflections
3931 reflections with $I > 2\sigma(I)$
R_{int} = 0.140

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.197
S = 1.01
9889 reflections
381 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2′—H2′···O3′^{i}	0.93	2.47	3.371 (5)	162
C5—H5···O2^{ii}	0.93	2.54	3.458 (6)	167
C5′—H5′···O3^{iii}	0.93	2.37	3.165 (5)	143
C8—H8*A*···O3^{iii}	0.97	2.38	3.344 (5)	170

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2107).

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supplementary materials

Acta Cryst. (2007). E**63**, o2974 [**doi:10.1107/S160053680702363X**]

O-Butyl *S*-(1,1,3-trioxobenz[*d*]isothiazol-2-yl)methyl dithiocarbonate

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Comment

Dithiocarbonate derivatives have been demonstrated to possess antifungal (Uchiyama & Hashimoto, 1974; Tsuchima & Wakamori, 1974) and antibacterial properties (Uchiyama & Hashimoto, 1974; Pennino, 1957). In our previous report (Güzel & Salman; 2006) the potent antimycobacterial and antitumor activities of the title compound were recorded. Here we report the crystal structure of the title compound which has potent antimycobacterial activity.

The asymmetric unit of the title compound (Fig. 1) reveals geometric parameters n agreement with the atom type and hybridization. The S═O and S═C distances are in the interval 1.418 (3) to 1.427 (3) and 1.612 (4) to 1.626 (5) Å, respectively. The O═S═O angles are 117.44 (17) ° for molecule A and 117.78 (17) ° for molecule B. The nine-membered fused rings of both molecules are planar; the maximum deviations from the mean planes are −0.038 (1) for S1, 0.045 (3) for N1 (ring A), and 0.016 (1) for S1', −0.028 (3) for N1' (ring B). In the asymmetric unit, the dihedral angle between the ring A and ring B of the two molecules is 3.76 (11)°. The crystal structure is stabilized by intermolecular C—H···O hydrogen bonds connecting molecules along the [010] axis (Table 2, Fig. 2).

Experimental

The ethanolic solution of 2-(chloromethyl)-1,2-benzisothiazol-3(2*H*)-on 1,1-dioxide and *O*-buthyldithiocarbonate (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. (Yield 42%, m.p. 325–327 K). IR (KBr): ν 1737 (C═O), 1246 (C═S). ^{1}H-NMR (DMSO-d_6/400 MHz): δ 0.92 (t, 3H, J=7.31 Hz, butyl CH_3), 1.39–1.48 (m, 2H, butyl C_3—H_2), 1.79–1.86 (m, 2H, butyl C_2—H_2), 4.65 (t, 2H, J=6.58 Hz, O—CH_2), 5.49 (s, 2H, N—CH_2—S), 7.99–8.14 (m, 3H, bzi, $C_{5,6,7}$—H), 8.33 (d, 1H, J=6.82 Hz, bzi, C_4—H). EIMS: m/*z* 345 (M^+), Analysis calculated for $C_{13}H_{15}NO_4S_3$: C 45.20, H 4.38, N 4.05, S 27.85%. Found: C 45.49, H 3.98, N 4.07, S 27.55%.

Refinement

H atoms were positioned geometrically, with the C—H distances in the range of 0.93 − 0.97 Å, and with U_{iso}(H) = 1.5U_{eq}(C) [U_{iso}(H) = 1.5U_{eq}(C) for methyl group].

Figures

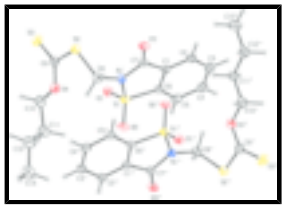

Fig. 1. Two independent molecules in the asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

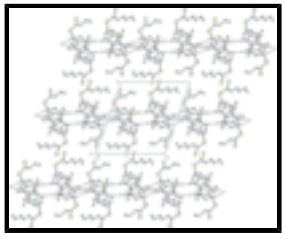

Fig. 2. Packing diagram of (I), showing hydrogen-bonding interactions (dashed lines). H atoms not involved in hydrogen contacts have been omitted.

O-Butyl *S*-(1,1,3-trioxobenz[*d*]isothiazol-2-yl)methyl dithiocarbonate

Crystal data

$C_{13}H_{15}NO_4S_3$	$Z = 4$
$M_r = 345.47$	$F_{000} = 720$
Triclinic, $P\overline{1}$	$D_x = 1.393$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.8191$ (3) Å	Cell parameters from 5653 reflections
$b = 13.4997$ (2) Å	$\theta = 2.5$–30.5º
$c = 14.7531$ (2) Å	$\mu = 0.46$ mm^{-1}
$\alpha = 70.270$ (3)º	$T = 294$ (2) K
$\beta = 85.255$ (5)º	Block, light yellow
$\gamma = 89.696$ (5)º	0.20 × 0.20 × 0.20 mm
$V = 1647.18$ (7) Å^3	

Data collection

Rigaku R-AXIS RAPID-S diffractometer	9889 independent reflections
Radiation source: fine-focus sealed tube	3931 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.140$
$T = 294$(2) K	$\theta_{max} = 30.6$º
ω scans	$\theta_{min} = 2.5$º
Absorption correction: multi-scan (Blessing, 1995)	$h = -12 \rightarrow 11$
$T_{min} = 0.913$, $T_{max} = 0.913$	$k = -19 \rightarrow 19$
46335 measured reflections	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.076$	H-atom parameters constrained
$wR(F^2) = 0.197$	$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
9889 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
381 parameters	$\Delta\rho_{min} = -0.26$ 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	1.06266 (10)	0.29619 (7)	0.05807 (7)	0.0681 (3)
S2	1.10307 (13)	0.00305 (8)	0.21582 (9)	0.0905 (4)
S3	1.21346 (16)	0.02860 (12)	0.38646 (10)	0.1256 (6)
O1	1.1357 (3)	0.30388 (19)	0.13759 (18)	0.0785 (10)
O2	0.9098 (3)	0.3310 (2)	0.0490 (2)	0.0898 (10)
O3	1.1811 (3)	0.07802 (19)	−0.03274 (19)	0.0787 (10)
O4	0.9792 (3)	0.1259 (2)	0.2981 (2)	0.0916 (11)
N1	1.0696 (3)	0.1740 (2)	0.0554 (2)	0.0649 (10)
C1	1.2230 (4)	0.2660 (3)	−0.0846 (3)	0.0625 (11)
C2	1.3151 (4)	0.2870 (3)	−0.1690 (3)	0.0769 (16)
C3	1.3590 (5)	0.3907 (4)	−0.2192 (3)	0.0915 (19)
C4	1.3136 (5)	0.4693 (4)	−0.1849 (4)	0.0953 (19)
C5	1.2219 (5)	0.4497 (3)	−0.0991 (3)	0.0839 (16)
C6	1.1782 (4)	0.3466 (3)	−0.0507 (3)	0.0636 (12)
C7	1.1599 (4)	0.1622 (3)	−0.0222 (3)	0.0645 (11)
C8	0.9852 (4)	0.0846 (3)	0.1246 (3)	0.0796 (16)
C9	1.0928 (4)	0.0605 (3)	0.3056 (3)	0.0815 (16)
C10	0.9636 (6)	0.1863 (4)	0.3638 (3)	0.114 (2)

C11	0.8268 (7)	0.2521 (4)	0.3395 (4)	0.124 (3)
C12	0.6805 (8)	0.1885 (5)	0.3673 (5)	0.158 (3)
C13	0.5369 (8)	0.2503 (5)	0.3586 (5)	0.158 (3)
S1'	0.75578 (10)	0.25022 (7)	−0.14738 (7)	0.0685 (3)
S2'	0.75963 (14)	0.51558 (9)	−0.34352 (9)	0.1022 (5)
S3'	0.7432 (2)	0.44961 (13)	−0.51090 (11)	0.1369 (7)
O1'	0.6760 (3)	0.2329 (2)	−0.22091 (18)	0.0829 (11)
O2'	0.9079 (2)	0.2140 (2)	−0.13762 (19)	0.0817 (10)
O3'	0.6476 (3)	0.48732 (19)	−0.0829 (2)	0.0874 (10)
O4'	0.9228 (3)	0.3687 (2)	−0.3707 (2)	0.0916 (11)
N1'	0.7536 (3)	0.3769 (2)	−0.1574 (2)	0.0716 (11)
C1'	0.5993 (4)	0.3005 (3)	−0.0145 (3)	0.0616 (11)
C2'	0.5069 (4)	0.2884 (3)	0.0699 (3)	0.0714 (16)
C3'	0.4636 (4)	0.1873 (3)	0.1290 (3)	0.0826 (16)
C4'	0.5106 (5)	0.1009 (3)	0.1041 (3)	0.0879 (17)
C5'	0.6011 (4)	0.1122 (3)	0.0209 (3)	0.0751 (14)
C6'	0.6423 (3)	0.2133 (3)	−0.0375 (3)	0.0637 (11)
C7'	0.6624 (4)	0.3993 (3)	−0.0845 (3)	0.0664 (14)
C8'	0.8445 (5)	0.4588 (3)	−0.2321 (3)	0.0874 (17)
C9'	0.8184 (5)	0.4344 (4)	−0.4102 (3)	0.0920 (17)
C10'	0.9840 (5)	0.2953 (4)	−0.4172 (3)	0.0928 (17)
C11'	1.1245 (5)	0.2504 (3)	−0.3682 (3)	0.0890 (17)
C12'	1.2043 (6)	0.1771 (4)	−0.4132 (3)	0.1050 (19)
C13'	1.3434 (7)	0.1294 (5)	−0.3628 (5)	0.152 (3)
H2	1.34690	0.23330	−0.19180	0.0920*
H3	1.42020	0.40700	−0.27700	0.1100*
H4	1.34510	0.53820	−0.22010	0.1150*
H5	1.19180	0.50340	−0.07580	0.1010*
H8A	0.94410	0.04200	0.09050	0.0950*
H8B	0.90040	0.10980	0.15630	0.0950*
H10C	1.05350	0.23060	0.35560	0.1360*
H10D	0.95110	0.13930	0.43030	0.1360*
H11C	0.83450	0.29040	0.27060	0.1490*
H11D	0.82490	0.30330	0.37250	0.1490*
H12C	0.68160	0.14200	0.43380	0.1900*
H12D	0.67730	0.14460	0.32720	0.1900*
H13D	0.53590	0.29190	0.40020	0.2380*
H13E	0.45040	0.20280	0.37720	0.2380*
H13F	0.53280	0.29580	0.29290	0.2380*
H8'1	0.94100	0.42950	−0.24530	0.1040*
H2'	0.47520	0.34650	0.08610	0.0860*
H8'2	0.86600	0.51460	−0.20690	0.1040*
H3'	0.40240	0.17710	0.18590	0.0990*
H4'	0.48000	0.03380	0.14480	0.1050*
H5'	0.63320	0.05410	0.00460	0.0900*
H10A	1.00950	0.33160	−0.48570	0.1110*
H10B	0.90990	0.23960	−0.40950	0.1110*
H11A	1.09620	0.21250	−0.30040	0.1070*
H11B	1.19390	0.30760	−0.37250	0.1070*

H12A	1.23470	0.21560	−0.48070	0.1260*
H12B	1.13390	0.12100	−0.41050	0.1260*
H13A	1.41410	0.18460	−0.36590	0.2270*
H13B	1.39080	0.08390	−0.39410	0.2270*
H13C	1.31350	0.08950	−0.29640	0.2270*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0650 (5)	0.0658 (5)	0.0878 (7)	0.0081 (4)	−0.0113 (5)	−0.0436 (5)
S2	0.1002 (8)	0.0636 (6)	0.1003 (8)	0.0047 (5)	0.0069 (6)	−0.0218 (6)
S3	0.1183 (11)	0.1404 (12)	0.1018 (10)	0.0155 (9)	−0.0289 (8)	−0.0153 (8)
O1	0.0813 (16)	0.0878 (17)	0.0841 (17)	−0.0013 (13)	−0.0138 (13)	−0.0508 (14)
O2	0.0624 (15)	0.0969 (19)	0.134 (2)	0.0229 (13)	−0.0190 (15)	−0.0680 (17)
O3	0.0814 (16)	0.0639 (15)	0.105 (2)	0.0118 (12)	−0.0122 (14)	−0.0465 (14)
O4	0.106 (2)	0.0890 (19)	0.088 (2)	0.0145 (16)	−0.0172 (16)	−0.0388 (16)
N1	0.0719 (18)	0.0572 (16)	0.0748 (19)	0.0004 (13)	−0.0044 (15)	−0.0347 (14)
C1	0.0578 (19)	0.064 (2)	0.074 (2)	0.0103 (16)	−0.0182 (17)	−0.0313 (18)
C2	0.069 (2)	0.092 (3)	0.076 (3)	0.013 (2)	−0.014 (2)	−0.035 (2)
C3	0.083 (3)	0.106 (4)	0.078 (3)	0.001 (3)	−0.013 (2)	−0.020 (3)
C4	0.095 (3)	0.077 (3)	0.100 (4)	0.000 (2)	−0.016 (3)	−0.010 (3)
C5	0.092 (3)	0.059 (2)	0.106 (3)	0.008 (2)	−0.022 (3)	−0.032 (2)
C6	0.063 (2)	0.059 (2)	0.073 (2)	0.0090 (16)	−0.0156 (17)	−0.0255 (17)
C7	0.0581 (19)	0.062 (2)	0.083 (2)	0.0110 (16)	−0.0159 (17)	−0.0350 (19)
C8	0.081 (2)	0.079 (3)	0.093 (3)	−0.012 (2)	−0.005 (2)	−0.048 (2)
C9	0.081 (3)	0.065 (2)	0.086 (3)	−0.001 (2)	−0.003 (2)	−0.010 (2)
C10	0.141 (4)	0.125 (4)	0.092 (3)	0.016 (3)	−0.015 (3)	−0.058 (3)
C11	0.157 (5)	0.118 (4)	0.117 (4)	0.023 (4)	−0.003 (4)	−0.068 (3)
C12	0.136 (5)	0.143 (6)	0.193 (7)	0.016 (5)	−0.003 (5)	−0.056 (5)
C13	0.154 (6)	0.152 (6)	0.172 (6)	−0.007 (5)	0.011 (5)	−0.064 (5)
S1'	0.0633 (5)	0.0718 (6)	0.0844 (7)	0.0121 (4)	−0.0105 (5)	−0.0440 (5)
S2'	0.1055 (9)	0.0873 (8)	0.0985 (9)	0.0133 (6)	0.0081 (7)	−0.0157 (6)
S3'	0.1587 (14)	0.1380 (13)	0.1141 (11)	0.0267 (10)	−0.0501 (10)	−0.0343 (9)
O1'	0.0811 (17)	0.0959 (19)	0.0939 (19)	0.0168 (14)	−0.0224 (14)	−0.0581 (16)
O2'	0.0603 (15)	0.0977 (19)	0.0991 (19)	0.0198 (13)	−0.0098 (13)	−0.0484 (15)
O3'	0.0924 (18)	0.0676 (16)	0.115 (2)	0.0044 (13)	0.0048 (15)	−0.0507 (15)
O4'	0.0881 (19)	0.104 (2)	0.0826 (19)	0.0140 (16)	−0.0060 (15)	−0.0321 (16)
N1'	0.0783 (19)	0.0649 (18)	0.079 (2)	0.0053 (15)	0.0022 (16)	−0.0362 (16)
C1'	0.0553 (18)	0.062 (2)	0.077 (2)	0.0095 (15)	−0.0122 (17)	−0.0347 (18)
C2'	0.064 (2)	0.080 (3)	0.083 (3)	0.0117 (18)	−0.0121 (19)	−0.043 (2)
C3'	0.072 (2)	0.094 (3)	0.082 (3)	0.006 (2)	−0.011 (2)	−0.029 (2)
C4'	0.075 (3)	0.074 (3)	0.107 (3)	0.008 (2)	−0.010 (2)	−0.020 (2)
C5'	0.062 (2)	0.062 (2)	0.108 (3)	0.0114 (17)	−0.015 (2)	−0.036 (2)
C6'	0.0529 (18)	0.064 (2)	0.083 (2)	0.0105 (15)	−0.0139 (17)	−0.0348 (19)
C7'	0.059 (2)	0.070 (2)	0.081 (3)	0.0091 (17)	−0.0087 (17)	−0.039 (2)
C8'	0.093 (3)	0.081 (3)	0.093 (3)	−0.012 (2)	0.016 (2)	−0.041 (2)
C9'	0.091 (3)	0.087 (3)	0.091 (3)	−0.006 (2)	0.001 (2)	−0.023 (2)
C10'	0.102 (3)	0.102 (3)	0.082 (3)	0.001 (3)	0.000 (2)	−0.043 (2)

C11'	0.094 (3)	0.084 (3)	0.090 (3)	0.000 (2)	0.002 (2)	−0.033 (2)
C12'	0.120 (4)	0.100 (3)	0.099 (3)	0.003 (3)	0.012 (3)	−0.044 (3)
C13'	0.143 (5)	0.159 (5)	0.176 (6)	0.062 (4)	−0.026 (4)	−0.085 (5)

Geometric parameters (Å, °)

S1—O1	1.418 (3)	C5—H5	0.9300
S1—O2	1.427 (3)	C8—H8B	0.9700
S1—N1	1.664 (3)	C8—H8A	0.9700
S1—C6	1.754 (4)	C10—H10C	0.9700
S2—C8	1.823 (4)	C10—H10D	0.9700
S2—C9	1.743 (5)	C11—H11C	0.9700
S3—C9	1.612 (4)	C11—H11D	0.9700
S1'—O2'	1.427 (2)	C12—H12D	0.9700
S1'—N1'	1.666 (3)	C12—H12C	0.9700
S1'—C6'	1.752 (4)	C13—H13E	0.9600
S1'—O1'	1.423 (3)	C13—H13F	0.9600
S2'—C8'	1.788 (5)	C13—H13D	0.9600
S2'—C9'	1.754 (5)	C1'—C2'	1.392 (6)
S3'—C9'	1.626 (5)	C1'—C6'	1.374 (6)
O3—C7	1.210 (5)	C1'—C7'	1.462 (6)
O4—C9	1.319 (5)	C2'—C3'	1.384 (6)
O4—C10	1.461 (6)	C3'—C4'	1.388 (6)
O3'—C7'	1.203 (5)	C4'—C5'	1.371 (6)
O4'—C9'	1.306 (6)	C5'—C6'	1.377 (6)
O4'—C10'	1.461 (6)	C10'—C11'	1.507 (6)
N1—C8	1.451 (5)	C11'—C12'	1.508 (7)
N1—C7	1.393 (5)	C12'—C13'	1.514 (8)
N1'—C8'	1.456 (5)	C2'—H2'	0.9300
N1'—C7'	1.403 (5)	C3'—H3'	0.9300
C1—C2	1.374 (6)	C4'—H4'	0.9300
C1—C6	1.386 (6)	C5'—H5'	0.9300
C1—C7	1.474 (6)	C8'—H8'1	0.9700
C2—C3	1.384 (7)	C8'—H8'2	0.9700
C3—C4	1.366 (8)	C10'—H10A	0.9700
C4—C5	1.390 (7)	C10'—H10B	0.9700
C5—C6	1.373 (6)	C11'—H11A	0.9700
C10—C11	1.489 (8)	C11'—H11B	0.9700
C11—C12	1.502 (9)	C12'—H12A	0.9700
C12—C13	1.503 (10)	C12'—H12B	0.9700
C2—H2	0.9300	C13'—H13A	0.9600
C3—H3	0.9300	C13'—H13B	0.9600
C4—H4	0.9300	C13'—H13C	0.9600
S1'···O4'	3.354 (3)	C2'···O1^{vi}	3.369 (5)
S2···O2^{i}	3.497 (4)	C2'···C6^{vi}	3.474 (6)
S2···O3	3.468 (4)	C3···C7^{ii}	3.487 (6)
S3···H10C	2.9800	C3'···O1^{vi}	3.299 (5)
S3···H13E^{ii}	3.1200	C4···C7^{ii}	3.511 (6)

S3···H10D^{iii}	3.1300	C5···O3'^{viii}	3.365 (5)
S3···H12C^{iii}	3.0700	C5'···O3^{i}	3.165 (5)
S3···H10D	2.8900	C6···C2^{ii}	3.474 (6)
S3'···H11D^{iv}	3.0700	C6'···O2	3.410 (5)
S3'···H10B	3.1500	C6'···C2^{vi}	3.560 (5)
S3'···H11B^{v}	3.1700	C7···O2'	2.852 (5)
S3'···H10A	2.8100	C7'···C3^{vi}	3.487 (6)
O1···C3'^{ii}	3.299 (5)	C7'···C4^{vi}	3.511 (6)
O1···C9	3.383 (5)	C7'···O2	2.992 (5)
O1···C10	3.402 (5)	C8···O3^{i}	3.344 (5)
O1···C2'^{ii}	3.369 (5)	C9···O1	3.383 (5)
O1···O4	2.990 (4)	C9'···O1'	3.332 (6)
O1'···C9'	3.332 (6)	C10···O1	3.402 (5)
O1'···O4'	3.081 (4)	C9···H12B^{i}	3.0600
O1'···C2^{vi}	3.347 (5)	C13···H4^{viii}	3.0300
O2···C1'	3.040 (5)	H8'1···O4'	2.2800
O2···C6'	3.410 (5)	H8'1···O2'	2.8100
O2···C7'	2.992 (5)	H2···O1'^{ii}	2.9000
O2'···C7	2.852 (5)	H2···O3	2.8600
O2'···C1	3.095 (5)	H2'···O3'	2.8900
O2'···S2^{i}	3.497 (4)	H2'···O3'^{vii}	2.4700
O2'···O3	3.197 (4)	H8'2···O3'	2.4800
O2'···N1	3.172 (4)	H3'···O1^{vi}	2.8900
O3···O2'	3.197 (4)	H4···H13F^{viii}	2.3500
O3···S2	3.468 (4)	H4···C13^{viii}	3.0300
O3···C8^{i}	3.344 (5)	H5···O2^{viii}	2.5400
O3···C5'^{i}	3.165 (5)	H5···O3'^{viii}	2.8700
O3'···C2'^{vii}	3.371 (5)	H5'···O3^{i}	2.3700
O3'···C5^{viii}	3.365 (5)	H8A···O3	2.5900
O4···O1	2.990 (4)	H8A···O3^{i}	2.3800
O4'···S1'	3.354 (3)	H8B···O4	2.3400
O4'···O1'	3.081 (4)	H8B···O2	2.8700
O1···H3'^{ii}	2.8900	H10A···S3'	2.8100
O1'···H2^{vi}	2.9000	H10A···H12A	2.5100
O2···H5^{viii}	2.5400	H10B···H12B	2.5400
O2···H8B	2.8700	H10B···S3'	3.1500
O2'···H8'1	2.8100	H10C···S3	2.9800
O2'···H11A	2.8100	H10D···S3	2.8900
O3···H2	2.8600	H10D···H12C	2.3700
O3···H5'^{i}	2.3700	H10D···S3^{iii}	3.1300
O3···H8A	2.5900	H11A···O2'	2.8100
O3···H8A^{i}	2.3800	H11A···H13C	2.5200
O3'···H8'2	2.4800	H11B···S3'^{v}	3.1700

O3'···H2'^{vii}	2.4700	H11B···H13A	2.5300
O3'···H5^{viii}	2.8700	H11D···S3^{ix}	3.0700
O3'···H2'	2.8900	H11D···H13D	2.5400
O4···H8B	2.3400	H12A···H10A	2.5100
O4···H12D	2.6900	H12B···H10B	2.5400
O4'···H8'1	2.2800	H12B···C9^{i}	3.0600
N1···O2'	3.172 (4)	H12C···H10D	2.3700
C1···O2'	3.095 (5)	H12C···S3^{iii}	3.0700
C1'···C2^{vi}	3.569 (6)	H12D···O4	2.6900
C1'···O2	3.040 (5)	H13A···H11B	2.5300
C2···C6'^{ii}	3.560 (5)	H13C···H11A	2.5200
C2···C1'^{ii}	3.569 (6)	H13D···H11D	2.5400
C2···O1'^{ii}	3.347 (5)	H13E···S3^{vi}	3.1200
C2'···O3'^{vii}	3.371 (5)	H13F···H4^{viii}	2.3500
O1—S1—O2	117.44 (17)	C11—C12—H12C	108.00
O1—S1—N1	110.72 (16)	C11—C12—H12D	108.00
O1—S1—C6	111.87 (17)	C13—C12—H12C	108.00
O2—S1—N1	108.88 (16)	C13—C12—H12D	108.00
O2—S1—C6	112.53 (18)	H12C—C12—H12D	107.00
N1—S1—C6	92.60 (18)	C12—C13—H13F	109.00
C8—S2—C9	104.7 (2)	H13E—C13—H13F	110.00
N1'—S1'—C6'	92.19 (18)	H13D—C13—H13E	109.00
O2'—S1'—C6'	113.33 (16)	H13D—C13—H13F	109.00
O1'—S1'—O2'	117.78 (17)	C12—C13—H13D	109.00
O1'—S1'—N1'	110.66 (16)	C12—C13—H13E	109.00
O1'—S1'—C6'	110.78 (16)	C2'—C1'—C6'	119.7 (4)
O2'—S1'—N1'	109.15 (15)	C2'—C1'—C7'	126.8 (4)
C8'—S2'—C9'	103.6 (2)	C6'—C1'—C7'	113.5 (4)
C9—O4—C10	118.7 (3)	C1'—C2'—C3'	118.1 (4)
C9'—O4'—C10'	120.0 (3)	C2'—C3'—C4'	120.7 (4)
S1—N1—C8	124.5 (2)	C3'—C4'—C5'	121.6 (4)
C7—N1—C8	120.5 (3)	C4'—C5'—C6'	117.0 (4)
S1—N1—C7	115.0 (3)	S1'—C6'—C1'	110.6 (3)
C7'—N1'—C8'	121.4 (3)	S1'—C6'—C5'	126.6 (3)
S1'—N1'—C7'	114.8 (2)	C1'—C6'—C5'	122.9 (4)
S1'—N1'—C8'	123.7 (2)	O3'—C7'—N1'	122.4 (4)
C2—C1—C7	126.6 (4)	O3'—C7'—C1'	128.7 (4)
C2—C1—C6	120.5 (4)	N1'—C7'—C1'	108.8 (3)
C6—C1—C7	112.9 (4)	S2'—C8'—N1'	115.4 (3)
C1—C2—C3	117.9 (4)	S2'—C9'—S3'	118.7 (3)
C2—C3—C4	120.8 (4)	S2'—C9'—O4'	113.1 (3)
C3—C4—C5	122.2 (5)	S3'—C9'—O4'	128.2 (4)
C4—C5—C6	116.2 (4)	O4'—C10'—C11'	106.5 (3)
S1—C6—C1	110.2 (3)	C10'—C11'—C12'	112.0 (4)
S1—C6—C5	127.5 (3)	C11'—C12'—C13'	112.4 (4)
C1—C6—C5	122.3 (4)	C1'—C2'—H2'	121.00
O3—C7—C1	127.7 (4)	C3'—C2'—H2'	121.00

O3—C7—N1	123.2 (4)	C2'—C3'—H3'	120.00
N1—C7—C1	109.2 (3)	C4'—C3'—H3'	120.00
S2—C8—N1	112.3 (2)	C3'—C4'—H4'	119.00
S2—C9—S3	119.5 (2)	C5'—C4'—H4'	119.00
S2—C9—O4	112.6 (3)	C4'—C5'—H5'	121.00
S3—C9—O4	128.0 (3)	C6'—C5'—H5'	122.00
O4—C10—C11	107.0 (4)	S2'—C8'—H8'1	108.00
C10—C11—C12	112.9 (5)	S2'—C8'—H8'2	108.00
C11—C12—C13	116.0 (6)	N1'—C8'—H8'1	108.00
C3—C2—H2	121.00	N1'—C8'—H8'2	108.00
C1—C2—H2	121.00	H8'1—C8'—H8'2	107.00
C2—C3—H3	120.00	O4'—C10'—H10A	110.00
C4—C3—H3	120.00	O4'—C10'—H10B	110.00
C5—C4—H4	119.00	C11'—C10'—H10A	110.00
C3—C4—H4	119.00	C11'—C10'—H10B	110.00
C4—C5—H5	122.00	H10A—C10'—H10B	109.00
C6—C5—H5	122.00	C10'—C11'—H11A	109.00
S2—C8—H8B	109.00	C10'—C11'—H11B	109.00
S2—C8—H8A	109.00	C12'—C11'—H11A	109.00
H8A—C8—H8B	108.00	C12'—C11'—H11B	109.00
N1—C8—H8A	109.00	H11A—C11'—H11B	108.00
N1—C8—H8B	109.00	C11'—C12'—H12A	109.00
C11—C10—H10C	110.00	C11'—C12'—H12B	109.00
O4—C10—H10D	110.00	C13'—C12'—H12A	109.00
C11—C10—H10D	110.00	C13'—C12'—H12B	109.00
H10C—C10—H10D	109.00	H12A—C12'—H12B	108.00
O4—C10—H10C	110.00	C12'—C13'—H13A	109.00
C10—C11—H11C	109.00	C12'—C13'—H13B	109.00
H11C—C11—H11D	108.00	C12'—C13'—H13C	109.00
C10—C11—H11D	109.00	H13A—C13'—H13B	110.00
C12—C11—H11C	109.00	H13A—C13'—H13C	109.00
C12—C11—H11D	109.00	H13B—C13'—H13C	109.00
O1—S1—N1—C7	−112.4 (3)	S1—N1—C7—C1	−1.8 (4)
O1—S1—N1—C8	70.1 (3)	S1'—N1'—C8'—S2'	86.8 (3)
O2—S1—N1—C7	117.1 (3)	S1'—N1'—C7'—O3'	−178.8 (3)
O2—S1—N1—C8	−60.5 (3)	S1'—N1'—C7'—C1'	3.3 (4)
C6—S1—N1—C7	2.2 (3)	C8'—N1'—C7'—O3'	4.4 (5)
C6—S1—N1—C8	−175.3 (3)	C8'—N1'—C7'—C1'	−173.5 (3)
O1—S1—C6—C1	111.7 (3)	C7'—N1'—C8'—S2'	−96.6 (4)
O1—S1—C6—C5	−68.4 (4)	C6—C1—C2—C3	−1.0 (6)
O2—S1—C6—C1	−113.6 (3)	C6—C1—C7—N1	0.3 (4)
O2—S1—C6—C5	66.3 (4)	C2—C1—C6—S1	−179.7 (3)
N1—S1—C6—C1	−1.9 (3)	C2—C1—C6—C5	0.4 (6)
N1—S1—C6—C5	178.0 (4)	C7—C1—C6—S1	1.2 (4)
C9—S2—C8—N1	86.9 (3)	C7—C1—C6—C5	−178.7 (4)
C8—S2—C9—S3	−165.2 (3)	C2—C1—C7—O3	2.2 (7)
C8—S2—C9—O4	16.1 (3)	C2—C1—C7—N1	−178.7 (4)
C6'—S1'—N1'—C8'	172.9 (3)	C7—C1—C2—C3	178.0 (4)
O1'—S1'—C6'—C1'	−109.8 (3)	C6—C1—C7—O3	−178.8 (4)

O1'—S1'—C6'—C5'	71.2 (3)	C1—C2—C3—C4	0.9 (6)
O2'—S1'—C6'—C1'	115.2 (3)	C2—C3—C4—C5	−0.2 (7)
O2'—S1'—C6'—C5'	−63.7 (4)	C3—C4—C5—C6	−0.5 (7)
N1'—S1'—C6'—C1'	3.3 (3)	C4—C5—C6—S1	−179.5 (3)
N1'—S1'—C6'—C5'	−175.7 (3)	C4—C5—C6—C1	0.3 (6)
O2'—S1'—N1'—C8'	57.3 (3)	O4—C10—C11—C12	70.2 (5)
C6'—S1'—N1'—C7'	−3.8 (3)	C10—C11—C12—C13	171.3 (5)
O1'—S1'—N1'—C8'	−73.9 (3)	C6'—C1'—C2'—C3'	1.1 (5)
O2'—S1'—N1'—C7'	−119.5 (3)	C7'—C1'—C2'—C3'	−177.4 (4)
O1'—S1'—N1'—C7'	109.4 (3)	C2'—C1'—C6'—S1'	179.3 (3)
C8'—S2'—C9'—O4'	−10.3 (4)	C2'—C1'—C6'—C5'	−1.7 (5)
C9'—S2'—C8'—N1'	−88.9 (3)	C7'—C1'—C6'—S1'	−2.0 (4)
C8'—S2'—C9'—S3'	170.8 (3)	C7'—C1'—C6'—C5'	177.0 (3)
C10—O4—C9—S3	6.2 (6)	C2'—C1'—C7'—O3'	0.2 (7)
C10—O4—C9—S2	−175.2 (3)	C2'—C1'—C7'—N1'	177.9 (4)
C9—O4—C10—C11	−179.7 (4)	C6'—C1'—C7'—O3'	−178.4 (4)
C10'—O4'—C9'—S2'	179.9 (3)	C6'—C1'—C7'—N1'	−0.7 (4)
C10'—O4'—C9'—S3'	−1.3 (6)	C1'—C2'—C3'—C4'	−0.4 (6)
C9'—O4'—C10'—C11'	166.8 (4)	C2'—C3'—C4'—C5'	0.1 (6)
C8—N1—C7—O3	−5.0 (5)	C3'—C4'—C5'—C6'	−0.6 (6)
C8—N1—C7—C1	175.8 (3)	C4'—C5'—C6'—S1'	−179.8 (3)
S1—N1—C8—S2	−100.8 (3)	C4'—C5'—C6'—C1'	1.4 (5)
C7—N1—C8—S2	81.8 (4)	O4'—C10'—C11'—C12'	−177.0 (3)
S1—N1—C7—O3	177.3 (3)	C10'—C11'—C12'—C13'	−178.5 (4)

Symmetry codes: (i) −*x*+2, −*y*, −*z*; (ii) *x*+1, *y*, *z*; (iii) −*x*+2, −*y*, −*z*+1; (iv) *x*, *y*, *z*−1; (v) −*x*+2, −*y*+1, −*z*−1; (vi) *x*−1, *y*, *z*; (vii) −*x*+1, −*y*+1, −*z*; (viii) −*x*+2, −*y*+1, −*z*; (ix) *x*, *y*, *z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2'—H2'···O3'^{vii}	0.93	2.47	3.371 (5)	162
C8'—H8'2···O3'	0.97	2.48	2.818 (5)	100
C5—H5···O2^{viii}	0.93	2.54	3.458 (6)	167
C5'—H5'···O3^{i}	0.93	2.37	3.165 (5)	143
C8—H8A···O3^{i}	0.97	2.38	3.344 (5)	170

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

Fig. 1

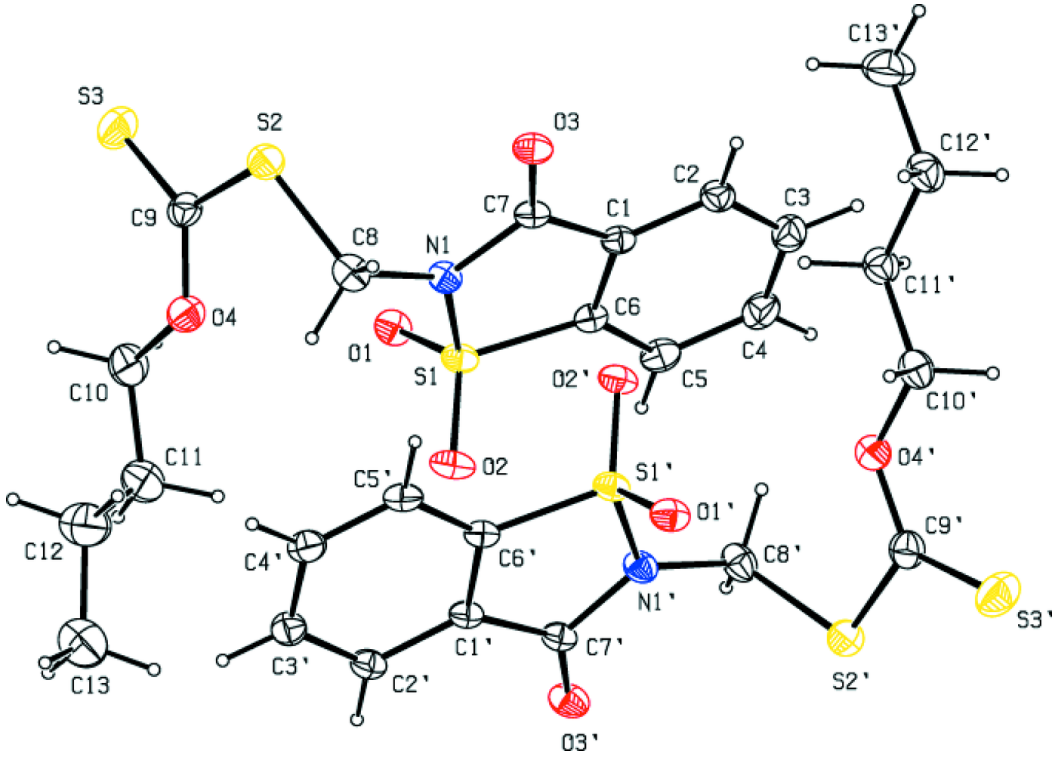
C13'
S3
S2
O3
C12'
C2
C9
C7
C1
C3
C8
N1
C11'
O4
C6
O1
S1
C4
O2'
C5
C10
C10'
C11
C5'
O2
S1'
O4'
O1'
C12
C4'
C6'
C8'
C9'
N1'
S3'
C1'
C7'
C3'
C2'
S2'
C13
O3'

Fig. 2