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N^2-[Bis(benzylsulfanyl)methylene]-2-methoxybenzohydrazide

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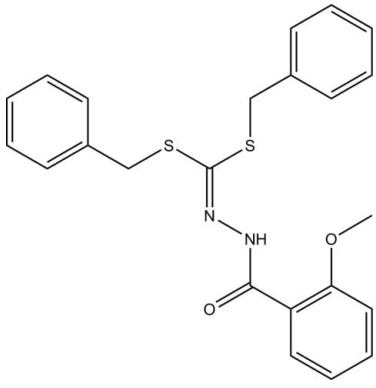
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.073; wR factor = 0.245; data-to-parameter ratio = 26.0.

The title compound, $C_{23}H_{22}N_2O_2S_2$, was obtained from the reaction of potassium N'-(2-methoxybenzoyl)hydrazinecarbodithioate and benzyl chloride. Strong intramolecular N—H···O and N—H···S hydrogen bonds are observed. Weak intermolecular C—H···O interactions link molecules into a two-dimensional framework; C—H···π interactions are also observed.

Related literature

For related literature, see: Agarwal *et al.* (2006); Jing & Yu (2007); Jing *et al.* (2006); Nematollahi & Nulu (2006); Wu *et al.* (2000).



Experimental

Crystal data

$C_{23}H_{22}N_2O_2S_2$
M_r = 422.55
Monoclinic, $P2_1/c$
a = 13.0233 (6) Å
b = 8.4361 (4) Å
c = 20.3957 (11) Å
β = 105.849 (5)°
V = 2155.61 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 296 (2) K
0.55 × 0.49 × 0.41 mm

Data collection

Oxford Diffraction Gemini R diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.890, T_{max} = 1.000 (expected range = 0.797–0.896)
16045 measured reflections
6835 independent reflections
2543 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.245
S = 1.08
6835 reflections
263 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 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
N1—H1A···O2	0.86	1.94	2.625 (3)	136
C1B—H1BB···O1^{i}	0.97	2.30	3.220 (4)	159
N1—H1A···S2	0.86	2.53	2.963 (3)	112

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2239).

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supplementary materials

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N^2-[Bis(benzylsulfanyl)methylene]-2-methoxybenzohydrazide

N. K. Singh, M. Singh and R. J. Butcher

Comment

The acidhydrazides provide an interesting series of ligands whose properties can be altered by introducing different organic substituents (Jing *et al.*; 2006, 2007). Acidhydrazides compounds were tested for pharmacological properties such as MAO inhibitory activity (Nematollahi *et al.*, 2006). Metal complexes based on acidhydrazides have attracted much attention because they show remarkable antifungal and antibacterial activites on different species of pathogenic fungi and bacteria (Agarwal *et al.*, 2006). In spite of this, there is little information on substituted acids, in particulars those containing sulfur atoms. Therefore, as a part of our ongoing research, we report here the crystal structure of a new N^2-bis(sulfanyl)derivative of 2-methoxybenzoic acid hydrazide.

The molecular structure of (I) can be divided into three different planes which contain one *o*-methoxyphenyl and two benzyl rings (Fig. 1). Atom O1 is in a *trans* configuration with respect to hydrazinic atom H1A. The dihedral angle between the *o*-methoxyphenyl ring and one benzyl ring (C6A, C5A, C4A, C3A, C2A and C7A) is 67.79 (9)°. Similarly the dihedral angle between the *o*-methoxyphenyl ring and the other benzyl ring (C3B, C4B, C5B, C6B, C7B and C2B) is 43.77(0.17)°. In addition, the C—S bond distances of 1.748 (3) Å agrees well with equivalent bonds in similar structures, being intermediate between 1.82 Å for a C—S single bond and 1.56 Å for a C=S double bond (Wu *et al.*; 2000). The corresponding C=N2 bond distance of 1.284 (4) Å is close to 1.299%A for a C=N double bond. The N1—N2 distance of 1.367 (3) Å shows partial double bond character, suggesting extensive delocalization in the (I). The three dimensional structure of I makes atoms O and N(2) potential neutral donor sites for coordination with metals. Intermolecular C—H···O hydrogen bonds link the molecules together in the solid state (Table 1, Fig 2). The crystal packing is also reinforced by a weak C—H···π interaction involving C3A–H3AA and the C2B to C7B carbons of the benzyl ring (centroid *Cg*) (Figure 2).

Experimental

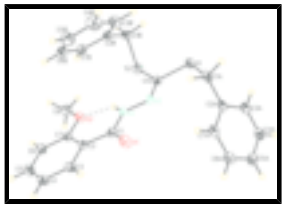
The potassium [*N*'-(2-methoxy-benzoyl)-hydrazinecarbodithioate] was synthesized by adding CS2 (4.3 ml, 45 mmol) to a methanol solution (25 ml) of 2-methoxybenzoic acid hydrazide (5.0 g, 30 mmol) in the presence of KOH (1.7 g, 30 mmol) and stirring the reaction mixture for 2 h at room temperature, yield (4.6 g, 92%), m.p. 260°C. IR (KBr, ν cm^{-1}): 3367 m, 3235 m (–NH), 1620 s (>C=O), 994 m (C=S); ^{1}H NMR (DMSO-d_6, TMS): 12.01, 9.92 (s, 2H, –NH), 3.39 (s, 3H, –OCH_3), 8.01, 7.53, 7.21, 7.12 (4*H*, aromatic); ^{13}C NMR (DMSO-d_6, TMS): 205.41 (C), 157.12 (C1), 119.07 (C2), 130.90 (C3), 120.87 (C4), 133.05 (C5), 112.22 (C6), 155.77 (C7), 56.32 (C8). Compound (I) was synthesized by dropwise addition of benzyl chloride (3 ml, 22 mmol) to a suspension of freshly prepared potassium [*N*'-(2-methoxy-benzoyl)-hydrazine]-carbodithioate (3 g, 11 mmol) in methanol (15 ml) and stirring the reaction mixture continuously for 2 h at room temperature. White single crystals of (I) (m.p. 383 K) suitable for X-ray analysis were obtained by slow evaporation of a methanol solution over a period of 1 d. (yield 1.74 g, 58%) IR (KBr, ν cm^{-1}) 3251 m (–NH), 1658 s (>C=O), 1598 s (C=N), 877 m (C—S); ^{1}H NMR (DMSO-d_6, TMS): 11.42 (s, 1H, –NH), 3.17 (s, 3H, –OCH_3), 4.29 (s, 4H, methylene); 8.03, 7.56, 7.34, 7.29 (m, 4H,

aromatic); 7.19, 7.15, 7.09(m, 10H, phenyl), ^{13}C NMR (DMSO-d_6, TMS): 157.03 (C), 164.41 (C1), 119.56 (C2), 128.28 (C3), 121.17 (C4), 133.22 (C5), 112.33 (C6), 159.44 (C7), 56.56 (C8), 35.62 (C1A, C1B), 137.27 (C2A, C2B), 129.52 (C3A, C3B, C7A, C7B), 128.56 (C4A), 127.46 (C5A, C5B).

Refinement

All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry with C—H distances of 0.96Å and U_{iso} (H) = 1.5 U_{eq} (C), but each group was allowed to rotate freely about its C—C bond. The position of the hydrazinic H atom was refined freely along with an isotropic displacement parameter. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with an N—H distance of 0.86 Å and C—H distances in the range of 0.93–0.97 Å and U_{iso}(H) = 1.2 U_{eq} (C, N).

Figures



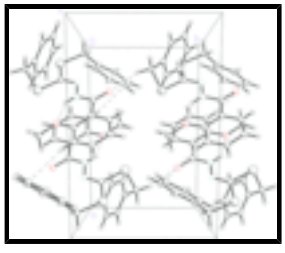


Fig. 1. The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 20% probability level. H-atoms are shown as small spheres of arbitrary radii. The dashed lines indicate intramolecular hydrogen bonds NH···O and NH···S.

N^2-[Bis(benzylsulfanyl)methylene]-2-methoxybenzohydrazide

Crystal data

$C_{23}H_{22}N_2O_2S_2$	F_{000} = 888
M_r = 422.55	D_x = 1.302 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4189 reflections
a = 13.0233 (6) Å	θ = 4.9–32.5º
b = 8.4361 (4) Å	μ = 0.27 mm^{-1}
c = 20.3957 (11) Å	T = 296 (2) K
β = 105.849 (5)º	Prism, colorless
V = 2155.61 (18) Å^3	0.55 × 0.49 × 0.41 mm
Z = 4	

Data collection

Oxford Diffraction Gemini R diffractometer	R_{int} = 0.045
Radiation source: fine-focus sealed tube	θ_{max} = 32.6º
Monochromator: graphite	θ_{min} = 4.9º
T = 296(2) K	h = −18→19
φ and ω scans	k = −11→12
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	l = −30→29
T_{min} = 0.890, T_{max} = 1.000	2 standard reflections
16045 measured reflections	every 50 reflections
6835 independent reflections	intensity decay: 2%
2543 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.073	H-atom parameters constrained
$wR(F^2)$ = 0.245	$w = 1/[\sigma^2(F_o^2) + (0.0797P)^2 + 0.9801P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.08	$(\Delta/\sigma)_{max} < 0.001$
6835 reflections	$\Delta\rho_{max}$ = 0.30 e Å^{-3}
263 parameters	$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.13312 (9)	0.80835 (13)	0.30775 (5)	0.0928 (4)
S2	0.28700 (8)	0.64554 (11)	0.41899 (5)	0.0806 (3)
O1	0.2976 (2)	1.2281 (3)	0.49188 (16)	0.1075 (10)

O2	0.46878 (18)	0.8278 (3)	0.57408 (13)	0.0796 (7)
N1	0.32261 (19)	0.9691 (3)	0.47724 (12)	0.0603 (6)
H1A	0.3562	0.8839	0.4936	0.072*
N2	0.2479 (2)	0.9653 (3)	0.41540 (13)	0.0643 (6)
C1C	0.2270 (2)	0.8288 (4)	0.38701 (17)	0.0663 (8)
C1	0.3440 (2)	1.1050 (4)	0.51253 (16)	0.0626 (7)
C2	0.4278 (2)	1.0997 (4)	0.57988 (15)	0.0594 (7)
C3	0.4481 (3)	1.2410 (4)	0.61549 (19)	0.0781 (9)
H3A	0.4109	1.3315	0.5965	0.094*
C4	0.5222 (3)	1.2513 (5)	0.6786 (2)	0.0943 (12)
H4A	0.5341	1.3474	0.7018	0.113*
C5	0.5780 (3)	1.1185 (6)	0.7067 (2)	0.0975 (12)
H5A	0.6280	1.1251	0.7490	0.117*
C6	0.5609 (3)	0.9769 (5)	0.67312 (19)	0.0812 (10)
H6A	0.5993	0.8878	0.6927	0.097*
C7	0.4866 (2)	0.9647 (4)	0.60990 (16)	0.0622 (8)
C8	0.5294 (3)	0.6904 (5)	0.6005 (2)	0.0999 (13)
H8A	0.5092	0.6050	0.5685	0.150*
H8B	0.5159	0.6608	0.6428	0.150*
H8C	0.6040	0.7127	0.6080	0.150*
C1A	0.0768 (3)	1.0064 (5)	0.2923 (2)	0.0932 (12)
H1AA	0.0045	0.9976	0.2630	0.112*
H1AB	0.0723	1.0502	0.3354	0.112*
C2A	0.1364 (2)	1.1207 (5)	0.26046 (18)	0.0723 (9)
C3A	0.1507 (3)	1.0933 (6)	0.1966 (2)	0.0888 (11)
H3AA	0.1235	1.0014	0.1730	0.107*
C4A	0.2047 (4)	1.2008 (6)	0.1677 (2)	0.1008 (13)
H4AA	0.2141	1.1802	0.1249	0.121*
C5A	0.2447 (4)	1.3368 (6)	0.2007 (3)	0.0991 (13)
H5AA	0.2815	1.4082	0.1807	0.119*
C6A	0.2308 (3)	1.3677 (5)	0.2630 (3)	0.0935 (12)
H6AA	0.2569	1.4614	0.2854	0.112*
C7A	0.1778 (3)	1.2601 (5)	0.2932 (2)	0.0857 (11)
H7AA	0.1697	1.2816	0.3363	0.103*
C1B	0.1757 (3)	0.5587 (4)	0.4454 (2)	0.0821 (10)
H1BA	0.1143	0.5501	0.4060	0.099*
H1BB	0.1952	0.4524	0.4625	0.099*
C2B	0.1451 (3)	0.6530 (4)	0.49929 (19)	0.0681 (8)
C3B	0.0472 (4)	0.7176 (5)	0.4877 (3)	0.1067 (14)
H3BA	−0.0035	0.7042	0.4460	0.128*
C4B	0.0228 (5)	0.8088 (7)	0.5419 (4)	0.141 (2)
H4BA	−0.0445	0.8530	0.5362	0.169*
C5B	0.0992 (5)	0.8280 (7)	0.6004 (3)	0.1288 (19)
H5BA	0.0842	0.8892	0.6346	0.155*
C6B	0.1938 (4)	0.7648 (7)	0.6116 (2)	0.1102 (15)
H6BA	0.2446	0.7802	0.6531	0.132*
C7B	0.2170 (3)	0.6766 (5)	0.5623 (2)	0.0893 (11)
H7BA	0.2840	0.6299	0.5711	0.107*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0911 (7)	0.0908 (7)	0.0824 (7)	−0.0100 (5)	−0.0002 (5)	−0.0070 (5)
S2	0.0829 (6)	0.0688 (6)	0.0918 (7)	0.0140 (5)	0.0268 (5)	−0.0093 (5)
O1	0.123 (2)	0.0589 (15)	0.115 (2)	0.0307 (15)	−0.0097 (17)	−0.0049 (14)
O2	0.0721 (14)	0.0592 (14)	0.0934 (17)	0.0192 (11)	−0.0015 (12)	−0.0010 (12)
N1	0.0641 (15)	0.0477 (13)	0.0659 (15)	0.0120 (11)	0.0120 (12)	0.0026 (12)
N2	0.0626 (14)	0.0667 (17)	0.0598 (15)	0.0057 (13)	0.0104 (12)	0.0051 (13)
C1C	0.0596 (17)	0.069 (2)	0.070 (2)	0.0050 (16)	0.0180 (15)	0.0000 (16)
C1	0.0639 (17)	0.0512 (17)	0.0705 (19)	0.0132 (15)	0.0143 (15)	0.0048 (15)
C2	0.0594 (16)	0.0566 (17)	0.0662 (18)	0.0019 (14)	0.0238 (14)	−0.0067 (15)
C3	0.079 (2)	0.064 (2)	0.090 (3)	−0.0039 (18)	0.021 (2)	−0.0124 (19)
C4	0.092 (3)	0.090 (3)	0.101 (3)	−0.014 (2)	0.026 (2)	−0.033 (3)
C5	0.083 (3)	0.120 (4)	0.084 (3)	−0.006 (3)	0.012 (2)	−0.015 (3)
C6	0.072 (2)	0.087 (3)	0.080 (2)	0.0040 (19)	0.0126 (18)	0.002 (2)
C7	0.0518 (16)	0.0645 (19)	0.0710 (19)	0.0038 (15)	0.0178 (15)	−0.0002 (16)
C8	0.098 (3)	0.068 (2)	0.122 (3)	0.030 (2)	0.011 (2)	0.014 (2)
C1A	0.0583 (19)	0.125 (3)	0.085 (2)	0.015 (2)	0.0006 (18)	−0.009 (2)
C2A	0.0506 (16)	0.084 (2)	0.074 (2)	0.0220 (17)	0.0020 (15)	−0.0002 (19)
C3A	0.081 (2)	0.100 (3)	0.079 (2)	0.013 (2)	0.0104 (19)	−0.018 (2)
C4A	0.101 (3)	0.125 (4)	0.076 (3)	0.005 (3)	0.025 (2)	−0.006 (3)
C5A	0.100 (3)	0.093 (3)	0.101 (3)	0.016 (2)	0.022 (3)	0.013 (3)
C6A	0.083 (3)	0.074 (3)	0.113 (3)	0.018 (2)	0.009 (2)	−0.001 (2)
C7A	0.075 (2)	0.095 (3)	0.078 (2)	0.031 (2)	0.0060 (19)	−0.013 (2)
C1B	0.094 (2)	0.0500 (18)	0.100 (3)	−0.0014 (18)	0.023 (2)	−0.0062 (18)
C2B	0.0705 (19)	0.0512 (17)	0.082 (2)	0.0035 (16)	0.0208 (17)	0.0084 (16)
C3B	0.086 (3)	0.098 (3)	0.126 (4)	0.018 (2)	0.013 (3)	−0.004 (3)
C4B	0.094 (4)	0.147 (5)	0.184 (6)	0.038 (3)	0.044 (4)	−0.021 (4)
C5B	0.116 (4)	0.145 (5)	0.135 (5)	0.005 (4)	0.050 (4)	−0.028 (4)
C6B	0.106 (4)	0.147 (4)	0.082 (3)	−0.009 (3)	0.034 (3)	0.004 (3)
C7B	0.087 (3)	0.098 (3)	0.086 (3)	0.004 (2)	0.026 (2)	0.015 (2)

Geometric parameters (Å, °)

S1—C1C	1.749 (4)	C1A—H1AB	0.9700
S1—C1A	1.817 (4)	C2A—C3A	1.385 (5)
S2—C1C	1.775 (3)	C2A—C7A	1.387 (5)
S2—C1B	1.832 (4)	C3A—C4A	1.375 (6)
O1—C1	1.217 (4)	C3A—H3AA	0.9300
O2—C7	1.352 (4)	C4A—C5A	1.360 (6)
O2—C8	1.423 (4)	C4A—H4AA	0.9300
N1—C1	1.342 (4)	C5A—C6A	1.356 (6)
N1—N2	1.367 (3)	C5A—H5AA	0.9300
N1—H1A	0.8600	C6A—C7A	1.383 (6)
N2—C1C	1.284 (4)	C6A—H6AA	0.9300
C1—C2	1.504 (4)	C7A—H7AA	0.9300
C2—C3	1.383 (5)	C1B—C2B	1.496 (5)

C2—C7	1.415 (4)	C1B—H1BA	0.9700
C3—C4	1.385 (6)	C1B—H1BB	0.9700
C3—H3A	0.9300	C2B—C3B	1.348 (5)
C4—C5	1.373 (6)	C2B—C7B	1.383 (5)
C4—H4A	0.9300	C3B—C4B	1.452 (7)
C5—C6	1.365 (6)	C3B—H3BA	0.9300
C5—H5A	0.9300	C4B—C5B	1.339 (8)
C6—C7	1.389 (5)	C4B—H4BA	0.9300
C6—H6A	0.9300	C5B—C6B	1.304 (7)
C8—H8A	0.9600	C5B—H5BA	0.9300
C8—H8B	0.9600	C6B—C7B	1.349 (6)
C8—H8C	0.9600	C6B—H6BA	0.9300
C1A—C2A	1.493 (5)	C7B—H7BA	0.9300
C1A—H1AA	0.9700		
C1C—S1—C1A	102.53 (17)	C3A—C2A—C7A	117.4 (4)
C1C—S2—C1B	98.75 (16)	C3A—C2A—C1A	121.4 (4)
C7—O2—C8	119.7 (3)	C7A—C2A—C1A	121.2 (3)
C1—N1—N2	120.4 (2)	C4A—C3A—C2A	120.6 (4)
C1—N1—H1A	119.8	C4A—C3A—H3AA	119.7
N2—N1—H1A	119.8	C2A—C3A—H3AA	119.7
C1C—N2—N1	116.6 (3)	C5A—C4A—C3A	121.0 (4)
N2—C1C—S1	120.9 (3)	C5A—C4A—H4AA	119.5
N2—C1C—S2	126.7 (3)	C3A—C4A—H4AA	119.5
S1—C1C—S2	112.4 (2)	C6A—C5A—C4A	119.7 (5)
O1—C1—N1	122.2 (3)	C6A—C5A—H5AA	120.2
O1—C1—C2	120.6 (3)	C4A—C5A—H5AA	120.2
N1—C1—C2	117.2 (3)	C5A—C6A—C7A	120.1 (4)
C3—C2—C7	117.6 (3)	C5A—C6A—H6AA	119.9
C3—C2—C1	116.1 (3)	C7A—C6A—H6AA	119.9
C7—C2—C1	126.2 (3)	C6A—C7A—C2A	121.1 (4)
C2—C3—C4	121.8 (4)	C6A—C7A—H7AA	119.4
C2—C3—H3A	119.1	C2A—C7A—H7AA	119.4
C4—C3—H3A	119.1	C2B—C1B—S2	113.2 (2)
C5—C4—C3	119.5 (4)	C2B—C1B—H1BA	108.9
C5—C4—H4A	120.3	S2—C1B—H1BA	108.9
C3—C4—H4A	120.3	C2B—C1B—H1BB	108.9
C6—C5—C4	120.6 (4)	S2—C1B—H1BB	108.9
C6—C5—H5A	119.7	H1BA—C1B—H1BB	107.7
C4—C5—H5A	119.7	C3B—C2B—C7B	118.2 (4)
C5—C6—C7	120.5 (4)	C3B—C2B—C1B	121.0 (4)
C5—C6—H6A	119.8	C7B—C2B—C1B	120.7 (3)
C7—C6—H6A	119.8	C2B—C3B—C4B	118.3 (5)
O2—C7—C6	122.5 (3)	C2B—C3B—H3BA	120.8
O2—C7—C2	117.4 (3)	C4B—C3B—H3BA	120.8
C6—C7—C2	120.0 (3)	C5B—C4B—C3B	118.6 (5)
O2—C8—H8A	109.5	C5B—C4B—H4BA	120.7
O2—C8—H8B	109.5	C3B—C4B—H4BA	120.7
H8A—C8—H8B	109.5	C6B—C5B—C4B	122.9 (5)
O2—C8—H8C	109.5	C6B—C5B—H5BA	118.5

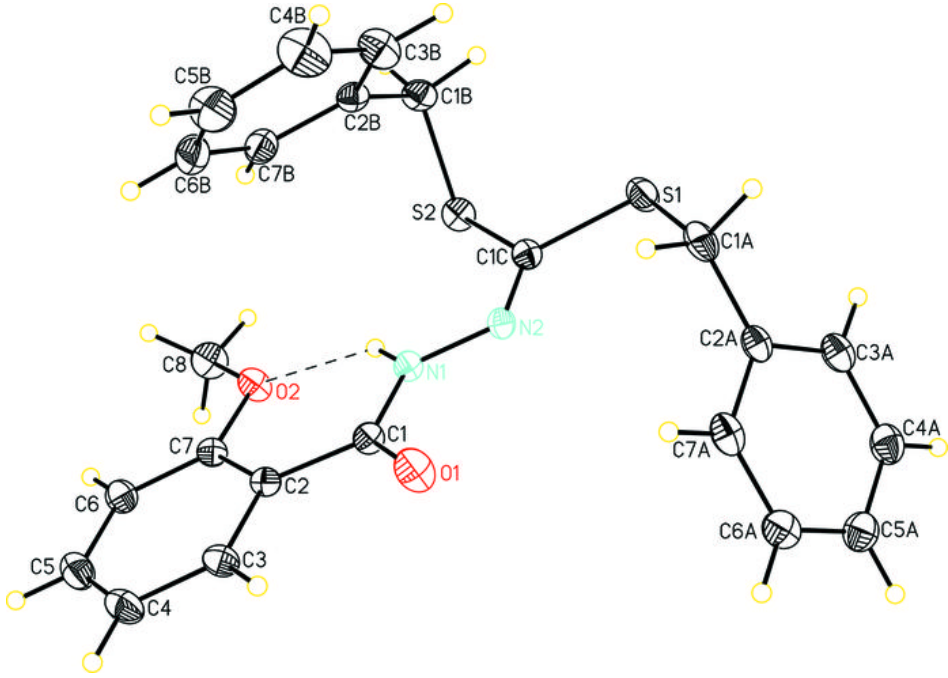
H8A—C8—H8C	109.5	C4B—C5B—H5BA	118.5
H8B—C8—H8C	109.5	C5B—C6B—C7B	119.2 (5)
C2A—C1A—S1	115.8 (2)	C5B—C6B—H6BA	120.4
C2A—C1A—H1AA	108.3	C7B—C6B—H6BA	120.4
S1—C1A—H1AA	108.3	C6B—C7B—C2B	122.7 (4)
C2A—C1A—H1AB	108.3	C6B—C7B—H7BA	118.7
S1—C1A—H1AB	108.3	C2B—C7B—H7BA	118.7
H1AA—C1A—H1AB	107.4		
C1—N1—N2—C1C	−175.5 (3)	C3—C2—C7—C6	0.4 (4)
N1—N2—C1C—S1	−179.8 (2)	C1—C2—C7—C6	−179.1 (3)
N1—N2—C1C—S2	−1.3 (4)	C1C—S1—C1A—C2A	85.3 (3)
C1A—S1—C1C—N2	−6.7 (3)	S1—C1A—C2A—C3A	61.4 (4)
C1A—S1—C1C—S2	174.60 (19)	S1—C1A—C2A—C7A	−120.0 (3)
C1B—S2—C1C—N2	106.3 (3)	C7A—C2A—C3A—C4A	0.5 (5)
C1B—S2—C1C—S1	−75.1 (2)	C1A—C2A—C3A—C4A	179.2 (3)
N2—N1—C1—O1	1.0 (5)	C2A—C3A—C4A—C5A	−0.5 (6)
N2—N1—C1—C2	−179.5 (2)	C3A—C4A—C5A—C6A	−0.3 (7)
O1—C1—C2—C3	−0.2 (5)	C4A—C5A—C6A—C7A	1.1 (6)
N1—C1—C2—C3	−179.7 (3)	C5A—C6A—C7A—C2A	−1.1 (6)
O1—C1—C2—C7	179.3 (3)	C3A—C2A—C7A—C6A	0.3 (5)
N1—C1—C2—C7	−0.1 (4)	C1A—C2A—C7A—C6A	−178.4 (3)
C7—C2—C3—C4	−0.6 (5)	C1C—S2—C1B—C2B	−61.5 (3)
C1—C2—C3—C4	179.0 (3)	S2—C1B—C2B—C3B	118.1 (4)
C2—C3—C4—C5	0.5 (6)	S2—C1B—C2B—C7B	−61.7 (4)
C3—C4—C5—C6	−0.2 (6)	C7B—C2B—C3B—C4B	0.2 (6)
C4—C5—C6—C7	0.0 (6)	C1B—C2B—C3B—C4B	−179.6 (4)
C8—O2—C7—C6	−1.5 (5)	C2B—C3B—C4B—C5B	1.6 (8)
C8—O2—C7—C2	177.1 (3)	C3B—C4B—C5B—C6B	−2.0 (10)
C5—C6—C7—O2	178.4 (3)	C4B—C5B—C6B—C7B	0.5 (9)
C5—C6—C7—C2	−0.1 (5)	C5B—C6B—C7B—C2B	1.5 (7)
C3—C2—C7—O2	−178.2 (3)	C3B—C2B—C7B—C6B	−1.8 (6)
C1—C2—C7—O2	2.3 (4)	C1B—C2B—C7B—C6B	178.0 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O2	0.86	1.94	2.625 (3)	136
C1B—H1BB···O1^{i}	0.97	2.30	3.220 (4)	159
N1—H1A···S2	0.86	2.53	2.963 (3)	112

Symmetry codes: (i) *x*, *y*−1, *z*.

Fig. 1


C4B
C3B
C5B
C1B
C2B
C6B
C7B
S2
S1
C1C
C1A
N2
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C3A
C8
N1
O2
C4A
C7
C1
C7A
O1
C2
C6
C6A
C5A
C5
C3
C4

Fig. 2