

Crystal structure of *N'*-[bis(ethylsulfanyl)methylidene]-2-hydroxy-4-methoxybenzohydrazide

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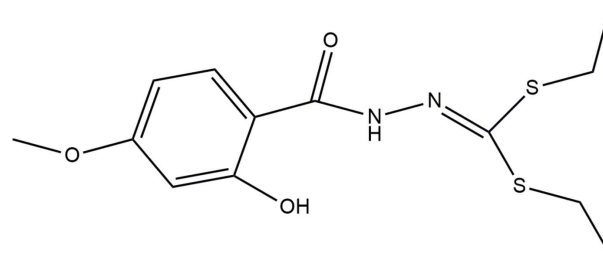
In the title compound, C₁₃H₁₈N₂O₃S₂, the amide group is in the plane of the benzoyl ring with a C–N–N–C torsion angle of 177.63 (12)°. The two dithioate groups are in an *anti* conformation [torsion angles = 173.68 (8) and –9.98 (10)°]. An intramolecular N–H···O hydrogen bond is observed. In the crystal, an O–H···O hydrogen bond and a weak C–H···O contact involving the same acceptor atom generate an S(6) ring motif and give rise to chains along [010].

Keywords: crystal structure; dithiocarbazate; hydrogen bonding; ester.

CCDC reference: 1431260

1. Related literature

For *S*-alkyl/aryl esters of dithiocarbazates that form metal complexes, see: Ali *et al.* (2008); Singh *et al.* (2010, 2012). For their biological properties, see: Bharti *et al.* (2000). For cyclization of potassium salts of *N*-(aroyl)hydrazine carbodithioates, see: Singh *et al.* (2008, 2009); Bharty *et al.* (2012). For bidentate, tridentate and multidentate esters, see: Wang *et al.* (2002); Tarafder *et al.* (2000); Ali *et al.* (2001). For related structures, see: Jasinski *et al.* (2010); Butcher *et al.* (2007); Tayamon *et al.* (2012).



2. Experimental

2.1. Crystal data

C₁₃H₁₈N₂O₃S₂

M_r = 314.41

Monoclinic, *P*₂₁/*n*

a = 8.479 (2) Å

b = 12.894 (3) Å

c = 13.843 (3) Å

β = 104.156 (10)°

V = 1467.5 (6) Å³

Z = 4

Mo *K*α radiation

μ = 0.37 mm⁻¹

T = 293 K

0.2 × 0.2 × 0.2 mm

2.2. Data collection

Rigaku Mercury 375R
diffractometer

Absorption correction: multi-scan
(*CrystalClear-SM Expert*; Rigaku,
2011)

*T*_{min} = 0.938, *T*_{max} = 1.000

12952 measured reflections

2685 independent reflections

2530 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.027

2.3. Refinement

R[*F*² > 2σ(*F*²)] = 0.029

wR(*F*²) = 0.077

S = 1.08

2685 reflections

192 parameters

H atoms treated by a mixture of
independent and constrained
refinement

Δρ_{max} = 0.28 e Å⁻³

Δρ_{min} = –0.27 e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
O2–H2A···O3 ⁱ	0.82 (2)	1.80 (2)	2.6118 (15)	177 (2)
N1–H1A···O2	0.836 (19)	1.957 (19)	2.6384 (16)	137.9 (17)
C3–H3A···O3 ⁱ	0.93	2.52	3.1975 (18)	130

Symmetry code: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$.

Data collection: *CrystalClear-SM Expert* (Rigaku, 2011); cell refinement: *CrystalClear-SM Expert*; data reduction: *CrystalClear-SM Expert*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: JJ2195).

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supporting information

Acta Cryst. (2015). E71, o967–o968 [doi:10.1107/S2056989015021271]

Crystal structure of *N'*-[bis(ethylsulfanyl)methylidene]-2-hydroxy-4-methoxybenzohydrazide

Paras Nath, Manoj K. Bharty, Rahul Chaurasia, Sanyucta Kumari and Sushil K. Gupta

S1. Comment

Nitrogen-sulfur donor chelating agents such as dithiocarbazates and their S-alkyl/aryl esters have shown interesting biological properties (Bharti *et al.* (2000)). They form large number of metal complexes with novel structural features (Ali *et al.*, 2008; Singh *et al.*, 2010; Singh *et al.*, 2012). The S-alkyl/aryl esters derived from potassium salts of N-aryldithiocarbamate have been found to be more stable towards cyclization (Singh *et al.*, 2008) and form 1,3,4-oxadiazole-2-thiones in the presence of acid or base (Singh *et al.*, 2009; Bharty *et al.*, 2012). The above esters behave as bidentate, tridentate or multidentate chelating agents with hetero donor atoms (Wang *et al.*, 2002; Tarafder *et al.*, 2000; Ali *et al.*, 2001). In view of the importance of the title compound, (**I**), herein we report its synthesis and crystal structure.

In the title compound, C₁₃H₁₈N₂O₃S₂, the sum of the angles around C9 (120.0°) and the S1/C9/S2 bond angle of 117.94 (8)° indicate a nearly planar *sp*² hybridized carbon atom (Fig. 2). The amide group is in plane to the benzoyl ring with a C8—N1—N2—C9 torsion angle of 177.63 (12)°, in contrast to the values in related structures (Jasinski *et al.* (2010); Butcher *et al.* (2007); Tayamon *et al.* (2012)). The two diethyl dithioate groups are in an *anti* conformation with respect to each other, as reflected by torsion angles C10/S1/C9/S2 of 173.68 (8)° and S1/C9/S2/C12 of –9.98 (10)°. The N2 atom in the amide linkage possesses distorted tetrahedral geometry (C9/N2/N1 = 116.59 (12)°) while the N1 atom is almost planar (sum of bond angles 359.6°). The C8—N1 and C9—N2 bond lengths (1.3448 (18) Å and 1.2837 (18) Å) lie between typical C—N and C=N values owing to the extensive delocalization of π electron density over the C9/N2/N1/C8 linkage.

In the crystal, an intermolecular O2—H2A \cdots O3 hydrogen bond and weak intermolecular C3—H3A \cdots O3 contact in bifurcated bonding arrangement (Fig. 3) generate an *S*(6) ring motif (Table 1). Intramolecular N1—H1A \cdots O2 hydrogen bonds are also observed.

S2. Experimental

Potassium 2-(2-hydroxy-4-methoxybenzoyl)hydrazinecarbodithioate was prepared by adding carbon disulfide (20.0 mmol, 1.50 mL) to a solution of 4-methoxysalicylic acid hydrazide (20.0 mmol, 3.65 g) and potassium hydroxide (20.0 mmol, 1.12 g) in ethanol (30 mL), then stirring the reaction mixture for 2 h (Fig. 1). The solid separated was filtered off, washed with ethanol and dried in *vacuo*. Ethyl iodide (20.0 mmol, 1.60 mL) was added drop-wise to a suspension of potassium 2-(2-hydroxy-4-methoxybenzoyl)hydrazinecarbodithioate (10.0 mmol, 2.96 g) in ethanol (20 mL) and stirring the reaction mixture for a period of 3–4 h. The resulting yellow solution was concentrated and acidified with dilute CH₃COOH (20% v/v) which yielded a yellow precipitate, washed with water and dried in *vacuo*. Yellow crystals of (**I**) (m.p. 427–429 K), suitable for X-ray analysis were obtained by slow evaporation of the methanol solution over a period of 9–10 days (yield 60%): Anal. Calc. for C₁₃H₁₈N₂O₃S₂ (%): C, 49.61; H, 5.77; N, 8.91; S, 20.40. Found: C, 49.24; H, 5.85; N, 8.86; S, 20.12.

S3. Refinement

The H atoms bonded to N1 and O2 were located in a difference Fourier map and refined freely; N1–H1A = 0.836 (19) Å and O2–H2A = 0.82 (2) Å. Other H atoms were positioned geometrically and allowed to ride on their parent atoms, with C–H = 0.93–0.97 Å, and with $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5U_{\text{eq}}(\text{C})$.

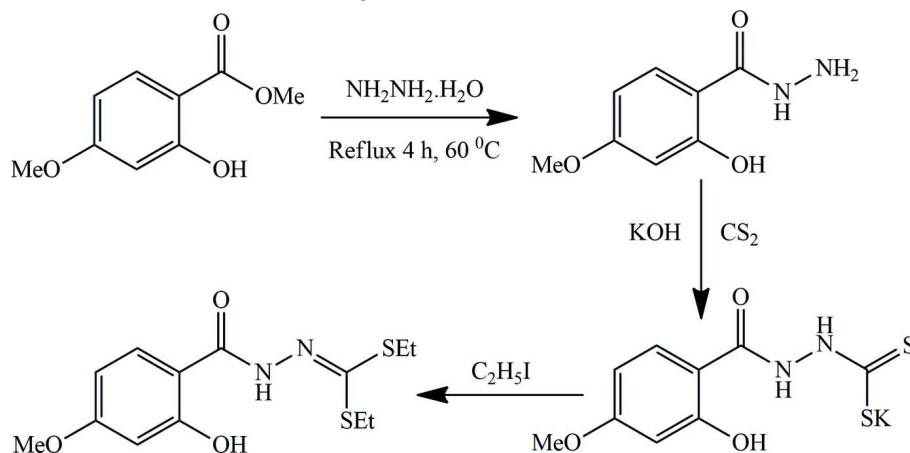


Figure 1

A reaction scheme showing the synthesis of the title compound, $\text{C}_{13}\text{H}_{18}\text{N}_2\text{O}_3\text{S}_2$.

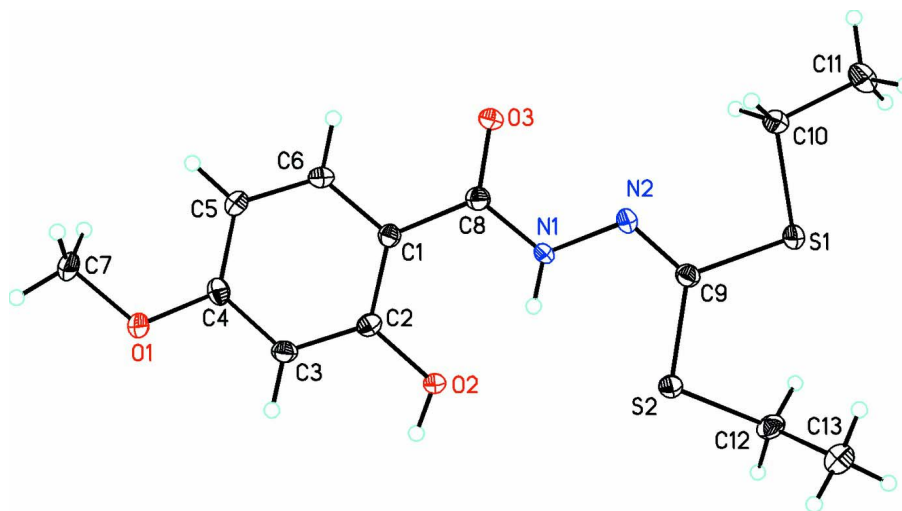


Figure 2

Molecular structure of the title compound, $\text{C}_{13}\text{H}_{18}\text{N}_2\text{O}_3\text{S}_2$, showing 50% probability displacement ellipsoids.

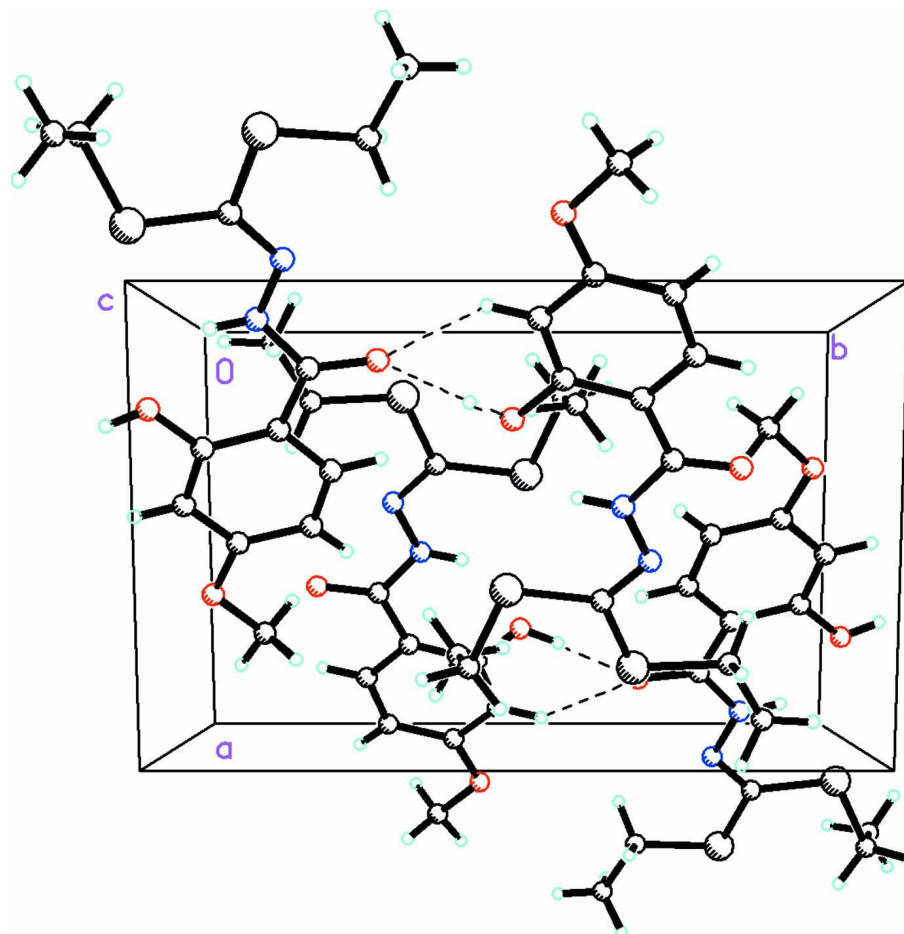


Figure 3

Molecular packing of $C_{13}H_{18}N_2O_3S_2$ viewed along the c -axis. Dashed lines indicate intermolecular hydroxyl $O—H\cdots O_{\text{carbonyl}}$ hydrogen bonds and weak phenyl $C—H\cdots O_{\text{carbonyl}}$ interactions.

***N'*-[Bis(ethylsulfanyl)methylidene]-2-hydroxy-4-methoxybenzohydrazide**

Crystal data

$C_{13}H_{18}N_2O_3S_2$

$M_r = 314.41$

Monoclinic, $P2_1/n$

$a = 8.479$ (2) Å

$b = 12.894$ (3) Å

$c = 13.843$ (3) Å

$\beta = 104.156$ (10)°

$V = 1467.5$ (6) Å³

$Z = 4$

$F(000) = 664$

$D_x = 1.423$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4529 reflections

$\theta = 3.0–27.5^\circ$

$\mu = 0.37$ mm⁻¹

$T = 293$ K

Prism, colorless

$0.2 \times 0.2 \times 0.2$ mm

Data collection

Rigaku Mercury 375R
diffractometer

Radiation source: Sealed Tube

Detector resolution: 13.6612 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*CrystalClear-SM Expert*; Rigaku, 2011)

$T_{\text{min}} = 0.938$, $T_{\text{max}} = 1.000$

12952 measured reflections

2685 independent reflections

2530 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$
 $\theta_{\text{max}} = 25.3^\circ$, $\theta_{\text{min}} = 3.0^\circ$

$h = -10 \rightarrow 10$
 $k = -15 \rightarrow 15$
 $l = -16 \rightarrow 16$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.077$
 $S = 1.08$
 2685 reflections
 192 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: mixed
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 0.8434P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.28 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.27 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. IR (selected, KBr): 3320 [$\nu(\text{O-H})$], 3276 [$\nu(\text{N-H})$], 1634 [$\nu(\text{C=O})$], 1094 [$\nu(\text{N-N})$], 876 [$\nu(\text{C=S})$] cm^{-1} .
 ^1H NMR (DMSO- d_6); δ [p.p.m.] = 12.26 (s, 1H, OH), 9.77 (s, 1H, NH), 7.80–6.40 (m, 3H, C_6H_3 , phenyl), 3.82 (s, 3H, –OCH₃), 3.06 (q, 4H, CH₂), 1.44 (t, 6H, CH₃). ^{13}C NMR (DMSO- d_6) δ [p.p.m.] = 168.3 (C4), 163.3 (C8), 162.0 (C2), 157.9 (C9), 132.1 (C6), 128.2 (C5), 106.8 (C3), 55.2 (C7), 27.1 (C10, C12), 14.4 (C11, C13).

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 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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.18898 (4)	0.33147 (3)	0.40368 (3)	0.01707 (12)
S2	0.36737 (4)	0.51413 (3)	0.34551 (3)	0.01997 (12)
O1	1.14563 (12)	0.43927 (8)	0.07886 (8)	0.0191 (2)
O2	0.73950 (13)	0.50561 (8)	0.24846 (8)	0.0175 (2)
H2A	0.775 (2)	0.5643 (17)	0.2477 (15)	0.034 (5)*
O3	0.63540 (13)	0.19012 (8)	0.25602 (8)	0.0211 (2)
N1	0.55185 (14)	0.35185 (9)	0.27860 (9)	0.0141 (2)
H1A	0.571 (2)	0.4154 (15)	0.2769 (13)	0.025 (5)*
N2	0.43294 (14)	0.31214 (9)	0.32068 (9)	0.0154 (3)
C1	0.78058 (16)	0.32991 (10)	0.20495 (10)	0.0127 (3)
C2	0.82146 (17)	0.43652 (10)	0.20485 (10)	0.0136 (3)
C3	0.94371 (17)	0.46929 (11)	0.16183 (10)	0.0147 (3)
H3A	0.9696	0.5394	0.1619	0.018*
C4	1.02795 (16)	0.39806 (11)	0.11852 (10)	0.0150 (3)
C5	0.98999 (17)	0.29255 (11)	0.11710 (10)	0.0157 (3)
H5A	1.0459	0.2447	0.0877	0.019*
C6	0.86766 (17)	0.26095 (11)	0.16032 (10)	0.0147 (3)

H6A	0.8423	0.1907	0.1596	0.018*
C7	1.23586 (18)	0.36914 (12)	0.03325 (12)	0.0214 (3)
H7A	1.3118	0.4074	0.0059	0.032*
H7B	1.1626	0.3318	-0.0190	0.032*
H7C	1.2938	0.3211	0.0822	0.032*
C8	0.65227 (16)	0.28531 (11)	0.24849 (10)	0.0139 (3)
C9	0.34330 (17)	0.37829 (11)	0.35163 (10)	0.0145 (3)
C10	0.19836 (17)	0.19372 (11)	0.37997 (11)	0.0173 (3)
H10A	0.1809	0.1812	0.3090	0.021*
H10B	0.3044	0.1666	0.4134	0.021*
C11	0.06688 (18)	0.14095 (12)	0.41920 (11)	0.0220 (3)
H11A	0.0628	0.0687	0.4021	0.033*
H11B	-0.0363	0.1725	0.3900	0.033*
H11C	0.0909	0.1483	0.4903	0.033*
C12	0.19060 (17)	0.56936 (11)	0.37838 (11)	0.0186 (3)
H12A	0.1653	0.6353	0.3444	0.022*
H12B	0.0985	0.5237	0.3543	0.022*
C13	0.2116 (2)	0.58643 (13)	0.48938 (12)	0.0253 (3)
H13A	0.1168	0.6202	0.5006	0.038*
H13B	0.3054	0.6291	0.5146	0.038*
H13C	0.2260	0.5208	0.5231	0.038*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0167 (2)	0.01427 (19)	0.0235 (2)	0.00006 (13)	0.01113 (15)	0.00050 (13)
S2	0.0224 (2)	0.01129 (19)	0.0307 (2)	0.00183 (14)	0.01520 (16)	0.00151 (14)
O1	0.0207 (5)	0.0153 (5)	0.0264 (6)	-0.0009 (4)	0.0156 (4)	-0.0009 (4)
O2	0.0195 (5)	0.0094 (5)	0.0276 (6)	-0.0009 (4)	0.0135 (4)	-0.0018 (4)
O3	0.0208 (5)	0.0106 (5)	0.0367 (6)	-0.0004 (4)	0.0161 (5)	0.0010 (4)
N1	0.0136 (6)	0.0098 (6)	0.0214 (6)	-0.0017 (5)	0.0091 (5)	0.0004 (5)
N2	0.0143 (6)	0.0147 (6)	0.0195 (6)	-0.0011 (5)	0.0085 (5)	0.0010 (5)
C1	0.0111 (6)	0.0128 (7)	0.0140 (6)	0.0004 (5)	0.0027 (5)	0.0004 (5)
C2	0.0143 (6)	0.0125 (7)	0.0135 (6)	0.0020 (5)	0.0026 (5)	-0.0002 (5)
C3	0.0171 (7)	0.0112 (6)	0.0160 (7)	-0.0008 (5)	0.0043 (5)	0.0001 (5)
C4	0.0140 (7)	0.0180 (7)	0.0137 (6)	-0.0007 (6)	0.0048 (5)	0.0023 (5)
C5	0.0163 (7)	0.0148 (7)	0.0174 (7)	0.0018 (5)	0.0069 (6)	-0.0019 (5)
C6	0.0167 (7)	0.0102 (6)	0.0173 (7)	0.0000 (5)	0.0044 (5)	-0.0005 (5)
C7	0.0212 (8)	0.0198 (7)	0.0284 (8)	0.0029 (6)	0.0162 (6)	-0.0001 (6)
C8	0.0125 (7)	0.0134 (7)	0.0154 (6)	-0.0001 (5)	0.0024 (5)	-0.0001 (5)
C9	0.0148 (7)	0.0124 (7)	0.0164 (6)	-0.0002 (5)	0.0043 (5)	0.0018 (5)
C10	0.0175 (7)	0.0136 (7)	0.0221 (7)	-0.0015 (6)	0.0073 (6)	-0.0003 (6)
C11	0.0207 (8)	0.0219 (8)	0.0242 (8)	-0.0059 (6)	0.0071 (6)	0.0020 (6)
C12	0.0170 (7)	0.0144 (7)	0.0242 (7)	0.0042 (6)	0.0048 (6)	-0.0018 (6)
C13	0.0302 (9)	0.0225 (8)	0.0259 (8)	-0.0003 (7)	0.0121 (7)	-0.0043 (6)

Geometric parameters (Å, °)

S1—C9	1.7485 (14)	C4—C5	1.397 (2)
S1—C10	1.8115 (15)	C5—C6	1.380 (2)
S2—C9	1.7678 (15)	C5—H5A	0.9300
S2—C12	1.8151 (15)	C6—H6A	0.9300
O1—C4	1.3591 (17)	C7—H7A	0.9600
O1—C7	1.4276 (17)	C7—H7B	0.9600
O2—C2	1.3588 (17)	C7—H7C	0.9600
O2—H2A	0.82 (2)	C10—C11	1.516 (2)
O3—C8	1.2430 (17)	C10—H10A	0.9700
N1—C8	1.3448 (18)	C10—H10B	0.9700
N1—N2	1.3804 (16)	C11—H11A	0.9600
N1—H1A	0.836 (19)	C11—H11B	0.9600
N2—C9	1.2837 (18)	C11—H11C	0.9600
C1—C6	1.3932 (19)	C12—C13	1.519 (2)
C1—C2	1.4176 (19)	C12—H12A	0.9700
C1—C8	1.4827 (19)	C12—H12B	0.9700
C2—C3	1.382 (2)	C13—H13A	0.9600
C3—C4	1.387 (2)	C13—H13B	0.9600
C3—H3A	0.9300	C13—H13C	0.9600
C9—S1—C10	101.15 (7)	H7B—C7—H7C	109.5
C9—S2—C12	105.35 (7)	O3—C8—N1	120.63 (13)
C4—O1—C7	117.17 (11)	O3—C8—C1	121.87 (12)
C2—O2—H2A	111.7 (14)	N1—C8—C1	117.49 (12)
C8—N1—N2	118.51 (12)	N2—C9—S1	118.17 (11)
C8—N1—H1A	118.4 (13)	N2—C9—S2	123.89 (11)
N2—N1—H1A	122.7 (13)	S1—C9—S2	117.94 (8)
C9—N2—N1	116.59 (12)	C11—C10—S1	107.85 (10)
C6—C1—C2	117.53 (12)	C11—C10—H10A	110.1
C6—C1—C8	116.99 (12)	S1—C10—H10A	110.1
C2—C1—C8	125.48 (12)	C11—C10—H10B	110.1
O2—C2—C3	120.66 (12)	S1—C10—H10B	110.1
O2—C2—C1	118.91 (12)	H10A—C10—H10B	108.4
C3—C2—C1	120.42 (13)	C10—C11—H11A	109.5
C2—C3—C4	120.25 (13)	C10—C11—H11B	109.5
C2—C3—H3A	119.9	H11A—C11—H11B	109.5
C4—C3—H3A	119.9	C10—C11—H11C	109.5
O1—C4—C3	114.98 (12)	H11A—C11—H11C	109.5
O1—C4—C5	124.37 (13)	H11B—C11—H11C	109.5
C3—C4—C5	120.65 (13)	C13—C12—S2	114.24 (11)
C6—C5—C4	118.46 (13)	C13—C12—H12A	108.7
C6—C5—H5A	120.8	S2—C12—H12A	108.7
C4—C5—H5A	120.8	C13—C12—H12B	108.7
C5—C6—C1	122.69 (13)	S2—C12—H12B	108.7
C5—C6—H6A	118.7	H12A—C12—H12B	107.6
C1—C6—H6A	118.7	C12—C13—H13A	109.5

O1—C7—H7A	109.5	C12—C13—H13B	109.5
O1—C7—H7B	109.5	H13A—C13—H13B	109.5
H7A—C7—H7B	109.5	C12—C13—H13C	109.5
O1—C7—H7C	109.5	H13A—C13—H13C	109.5
H7A—C7—H7C	109.5	H13B—C13—H13C	109.5
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C8—N1—N2—C9	177.63 (12)	C8—C1—C6—C5	179.98 (12)
C6—C1—C2—O2	-179.53 (12)	N2—N1—C8—O3	1.9 (2)
C8—C1—C2—O2	0.6 (2)	N2—N1—C8—C1	-179.09 (11)
C6—C1—C2—C3	-0.1 (2)	C6—C1—C8—O3	8.5 (2)
C8—C1—C2—C3	-179.96 (12)	C2—C1—C8—O3	-171.64 (13)
O2—C2—C3—C4	179.25 (12)	C6—C1—C8—N1	-170.50 (12)
C1—C2—C3—C4	-0.2 (2)	C2—C1—C8—N1	9.4 (2)
C7—O1—C4—C3	-179.94 (12)	N1—N2—C9—S1	179.01 (9)
C7—O1—C4—C5	-0.2 (2)	N1—N2—C9—S2	-1.42 (18)
C2—C3—C4—O1	-179.83 (12)	C10—S1—C9—N2	-6.72 (13)
C2—C3—C4—C5	0.4 (2)	C10—S1—C9—S2	173.68 (8)
O1—C4—C5—C6	179.87 (12)	C12—S2—C9—N2	170.45 (12)
C3—C4—C5—C6	-0.4 (2)	C12—S2—C9—S1	-9.98 (10)
C4—C5—C6—C1	0.1 (2)	C9—S1—C10—C11	-178.68 (10)
C2—C1—C6—C5	0.1 (2)	C9—S2—C12—C13	88.23 (12)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O2—H2 <i>A</i> \cdots O3 ⁱ	0.82 (2)	1.80 (2)	2.6118 (15)	177 (2)
N1—H1 <i>A</i> \cdots O2	0.836 (19)	1.957 (19)	2.6384 (16)	137.9 (17)
C3—H3 <i>A</i> \cdots O3 ⁱ	0.93	2.52	3.1975 (18)	130

Symmetry code: (i) $-x+3/2, y+1/2, -z+1/2$.