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4-Azidomethyl-7-methyl-2-oxo-2H-chromene-6-sulfonyl azide

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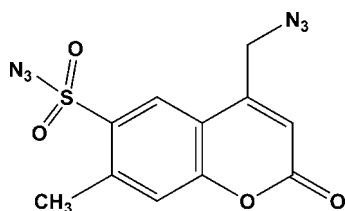
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Key indicators: single-crystal X-ray study; $T = 292$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.041; wR factor = 0.102; data-to-parameter ratio = 15.5.

In the title compound, $\text{C}_{11}\text{H}_8\text{N}_6\text{O}_4\text{S}$, the plane of the coumarin aromatic ring is twisted by $17.2(2)^\circ$ with respect to the plane of the azide group bound to the methylene substituent, whereas it is twisted by $83.2(2)^\circ$ to the plane of the azide attached to the sulfonyl group. The crystal structure is stabilized by weak $\text{C}-\text{H}\cdots\text{O}$ interactions, leading to the formation of dimers with $R_2^2(12)$ graph-set motifs. These dimers are further linked by weak $\text{S}-\text{O}\cdots\pi$ and $\pi-\pi$ contacts [centroid-centroid distance = $3.765(2)$ Å], leading to the formation of a layered structure.

Related literature

For azides, see: Scriven & Turnbull (1988); Amblard *et al.* (2009). For 4-azidomethylcoumarin derivatives, see: Melavanki *et al.* (2008, 2009, 2010); Naik & Kulkarni (2010); Basanagouda *et al.* (2010). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$\text{C}_{11}\text{H}_8\text{N}_6\text{O}_4\text{S}$
 $M_r = 320.29$
 Orthorhombic, *Fdd2*
 $a = 13.5452(12)$ Å
 $b = 27.952(3)$ Å
 $c = 14.1107(13)$ Å

$V = 5342.5(9)$ Å³
 $Z = 16$
 Mo $K\alpha$ radiation
 $\mu = 0.27$ mm⁻¹
 $T = 292$ K
 $0.24 \times 0.16 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008)
 $T_{\min} = 0.891$, $T_{\max} = 0.973$

11344 measured reflections
 3124 independent reflections
 2677 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.102$
 $S = 1.05$
 3124 reflections
 201 parameters
 7 restraints

H-atom parameters constrained
 $\Delta\rho_{\max} = 0.26$ e Å⁻³
 $\Delta\rho_{\min} = -0.21$ e Å⁻³
 Absolute structure: Flack (1983),
 1438 Friedel pairs
 Flack parameter: 0.09 (8)

Table 1

Hydrogen-bond geometry (Å, °).

Cg is the centroid of the C5–C10 ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C8}-\text{H8}\cdots\text{O2}^{\text{i}}$	0.93	2.52	3.416 (3)	161
$\text{S1}-\text{O4}\cdots\text{Cg}^{\text{ii}}$	1.42 (1)	2.96 (1)	3.931 (2)	128

Symmetry codes: (i) $-x + 1, -y + 2, z$; (ii) $x - \frac{1}{2}, -y + \frac{7}{2}, z - \frac{3}{2}$.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINTE* (Bruker, 2004); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2607).

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4-Azidomethyl-7-methyl-2-oxo-2H-chromene-6-sulfonyl azide

Mahantesha Basanagouda, Susanta K. Nayak, T. N. Guru Row and Manohar V. Kulkarni

S1. Comment

The Chemistry of azides has been the subject of intensive investigations during the last 50 years because of its importance in preparative heterocyclic chemistry (Scriven *et al.*, 1988). The Cu(I)-catalyzed 1,3-dipolar cycloaddition reaction between alkynes and azides has been suitable for the synthesis of a large number of modified nucleosides, nucleotides and oligonucleotides with a broad range of applications (Amblard *et al.*, 2009). 4-Azidomethylcoumarin derivatives have aroused increasing interest because of their photophysical properties (Melavanki *et al.*, 2008, 2009, 2010; Naik *et al.*, 2010) and antimicrobial activities (Basanagouda *et al.*, 2010). As a part of our study on synthesis of biological active compounds, We report the crystal structure of 4-Azidomethyl-7-methyl-coumarin-6-sulfonyl azide.

The title compound (I), the molecular conformation (Fig.1) is preferred with the plane of the coumarin aromatic ring is $17.2(2)^\circ$ with respect to the plane of azide of methylene substituent whereas it is $83.2(2)^\circ$ to the plane of azide of sulfonyl group. The molecular arrangement is stabilized by the formation of dimer through C—H \cdots O interactions with $R_2^2(12)$ ring motif (Bernstein *et al.*, 1995)(Fig. 2). Further, it is stabilized by S=O $\cdots\pi$ (Table 1, Cg being the centroid of the C5-C10 ring) and slipped π - π interaction (symmetry code $(-1/4 + x, 7/4 - y, 1/4 + z)$ with centroid to centroid distance = $3.765(2)$ Å, interplanar distance = $3.564(1)$ Å and an offset angle of 18.8° , which form a layered structure (Fig. 2).

S2. Experimental

The 4-Bromomethyl-7-methyl-coumarin-6-sulfonyl chloride (3.51 g, 0.01 mol) was taken in acetone (20 ml) in a round bottom flask. To this, solution of sodium azide(1.56 g, 0.024 mol) in water (6 ml) was added drop wise with stirring. The stirring was continued for 10 h. Then the reaction mixture was poured on to crushed ice (100 g). The separated solid was filtered and recrystallized from benzene to obtain a colorless solid in 62% yield, m.p. 132–133 °C; IR (KBr) cm^{-1} 1722 (C=O), 2130 (N_3 , azido); ^1H NMR (CDCl_3 , 300 MHz, TMS): δ 2.73 (s, 3H, C7— CH_3), 4.62 (s, 2H, C4— CH_2), 6.64 (s, 1H, C3—H), 7.31 (s, 1H, C8—H), 8.30 (s, 1H, C5—H); LC—MS: 321 ($M+1$). Anal. Calcd for $\text{C}_{11}\text{H}_8\text{N}_6\text{O}_4\text{S}$ (%): Calcd. C, 41.25; H, 2.52; N, 26.24. Found C, 41.15; H, 2.46; N, 26.21.

S3. Refinement

All H atoms were fixed geometrically and treated as riding with C—H = 0.93Å (aromatic), 0.96Å (methyl) or 0.97Å (methylene) with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{Cmethyl})$.

Rigid bond restraints on the ellipsoids were used for both azide groups.

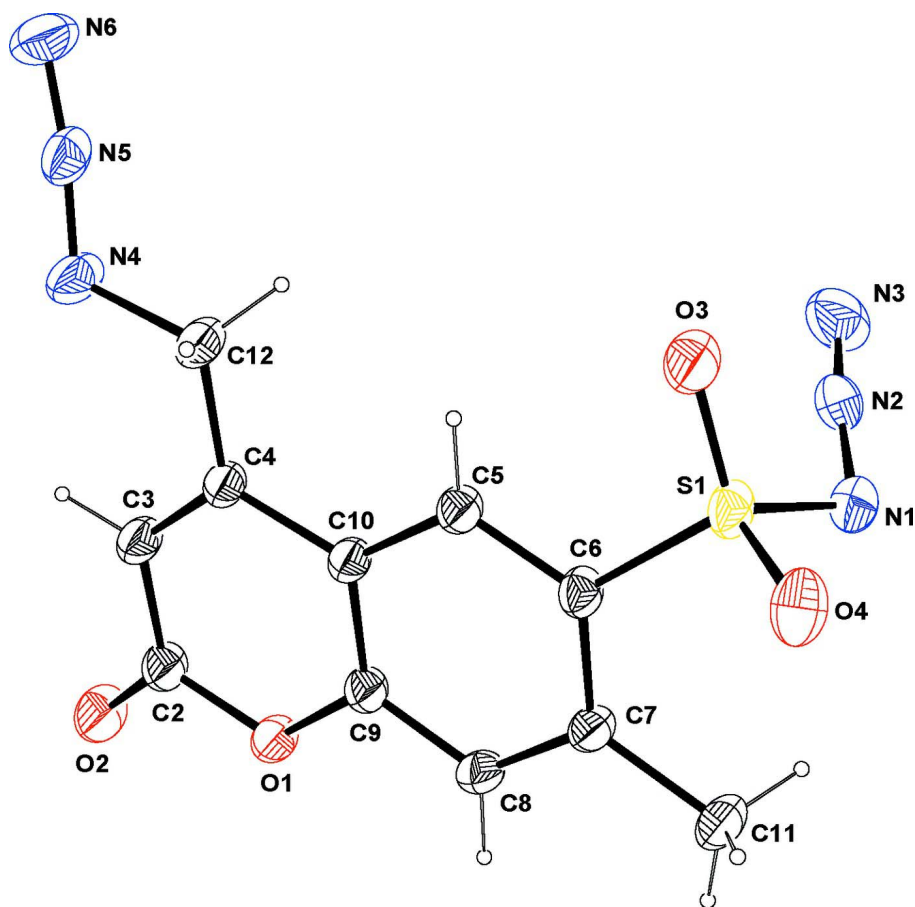


Figure 1

Molecular view of (I) with the atom labeling scheme. Ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

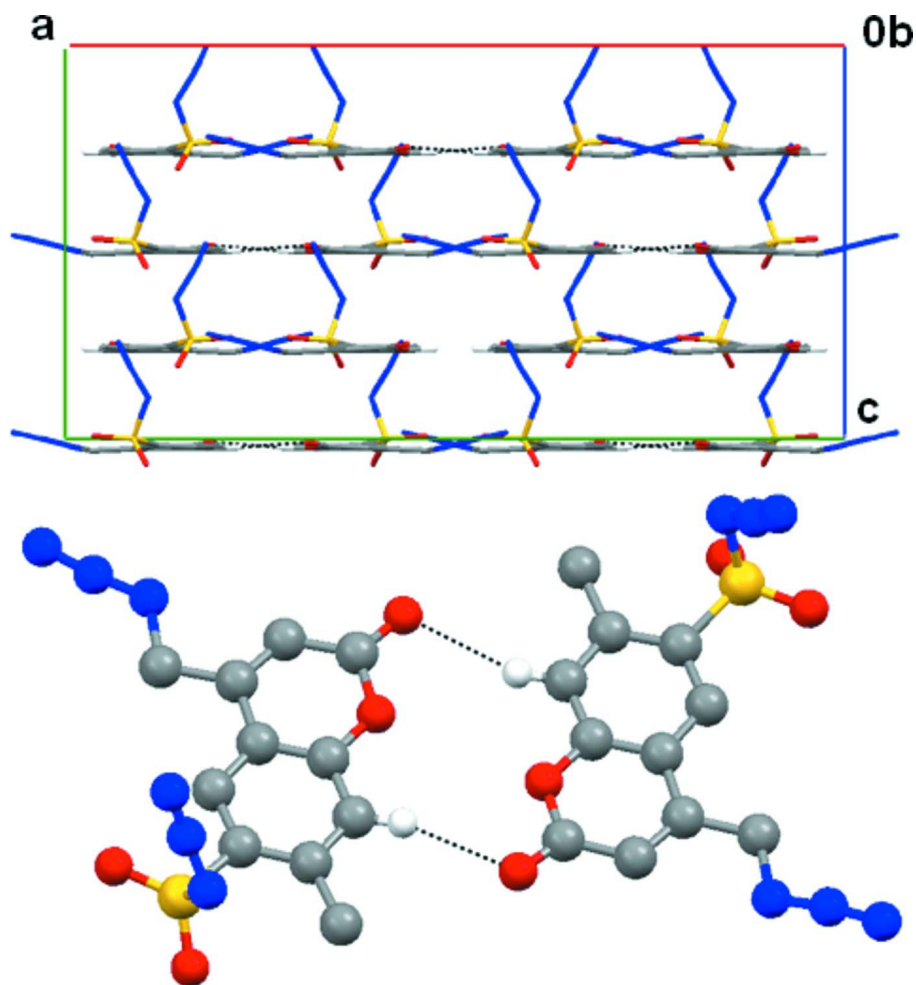


Figure 2

Molecular packing showing the layered structure stabilized by π - π and $\text{S}=\text{O}\cdots\pi$ contacts and the dimer formation through $\text{C}-\text{H}\cdots\text{O}$ intermolecular interactions. H atoms not involved in hydrogen bonding have been omitted for clarity

4-Azidomethyl-7-methyl-2-oxo-2H-chromene-6-sulfonyl azide

Crystal data

$\text{C}_{11}\text{H}_8\text{N}_6\text{O}_4\text{S}$

$M_r = 320.29$

Orthorhombic, $Fdd2$

Hall symbol: $F\ 2\ -2d$

$a = 13.5452\ (12)\ \text{\AA}$

$b = 27.952\ (3)\ \text{\AA}$

$c = 14.1107\ (13)\ \text{\AA}$

$V = 5342.5\ (9)\ \text{\AA}^3$

$Z = 16$

$F(000) = 2624$

$D_x = 1.593\ \text{Mg m}^{-3}$

Melting point: 406 K

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 400 reflections

$\theta = 1.0\text{--}28.0^\circ$

$\mu = 0.27\ \text{mm}^{-1}$

$T = 292\ \text{K}$

Hexagonal, pale yellow

$0.24 \times 0.16 \times 0.10\ \text{mm}$

Data collection

Bruker SMART APEX CCD diffractometer	11344 measured reflections
Radiation source: fine-focus sealed tube	3124 independent reflections
Graphite monochromator	2677 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.025$
Absorption correction: multi-scan (SADABS; Sheldrick, 2008)	$\theta_{\text{max}} = 28.0^\circ$, $\theta_{\text{min}} = 2.2^\circ$
$T_{\text{min}} = 0.891$, $T_{\text{max}} = 0.973$	$h = -17 \rightarrow 0$
	$k = -36 \rightarrow 0$
	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.041$	$w = 1/[\sigma^2(F_o^2) + (0.0532P)^2 + 3.5426P]$
$wR(F^2) = 0.102$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{\text{max}} = 0.001$
3124 reflections	$\Delta\rho_{\text{max}} = 0.26 \text{ e } \text{\AA}^{-3}$
201 parameters	$\Delta\rho_{\text{min}} = -0.21 \text{ e } \text{\AA}^{-3}$
7 restraints	Absolute structure: Flack (1983), 1438 Friedel pairs
Primary atom site location: structure-invariant direct methods	Absolute structure parameter: 0.09 (8)
Secondary atom site location: difference Fourier map	

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.85568 (4)	0.83758 (2)	0.50177 (5)	0.04317 (17)
O1	0.47627 (11)	0.93758 (5)	0.47959 (14)	0.0462 (4)
O2	0.31442 (12)	0.93929 (6)	0.49151 (18)	0.0610 (6)
O3	0.83522 (13)	0.78772 (6)	0.5081 (2)	0.0663 (6)
O4	0.92870 (14)	0.85453 (7)	0.43818 (16)	0.0598 (5)
N1	0.89734 (14)	0.85727 (8)	0.60674 (18)	0.0507 (5)
N2	0.86115 (15)	0.83563 (8)	0.67677 (19)	0.0511 (6)
N3	0.8356 (2)	0.81892 (11)	0.7443 (3)	0.0727 (8)
N4	0.37159 (16)	0.76434 (8)	0.4783 (2)	0.0643 (8)
N5	0.36677 (14)	0.72360 (8)	0.4993 (2)	0.0494 (5)
N6	0.35192 (18)	0.68477 (9)	0.5172 (3)	0.0715 (8)
C2	0.38675 (17)	0.91435 (8)	0.4834 (2)	0.0439 (6)
C3	0.38818 (17)	0.86301 (8)	0.4776 (2)	0.0436 (6)
H3	0.3284	0.8467	0.4752	0.052*
C4	0.47186 (17)	0.83767 (7)	0.47560 (17)	0.0370 (5)

C5	0.65857 (15)	0.84097 (8)	0.48129 (17)	0.0372 (5)
H5	0.6634	0.8078	0.4815	0.045*
C6	0.74334 (15)	0.86865 (8)	0.48503 (18)	0.0368 (5)
C7	0.74063 (16)	0.91904 (8)	0.48102 (17)	0.0366 (5)
C8	0.64872 (16)	0.94005 (8)	0.47701 (18)	0.0397 (6)
H8	0.6439	0.9732	0.4741	0.048*
C9	0.56344 (16)	0.91278 (8)	0.47726 (18)	0.0371 (5)
C10	0.56574 (15)	0.86284 (7)	0.47717 (17)	0.0354 (5)
C11	0.83110 (18)	0.95033 (9)	0.4850 (2)	0.0507 (7)
H11A	0.8697	0.9457	0.4287	0.076*
H11B	0.8698	0.9420	0.5395	0.076*
H11C	0.8114	0.9833	0.4893	0.076*
C12	0.47394 (17)	0.78398 (8)	0.4712 (2)	0.0482 (7)
H12A	0.5036	0.7738	0.4119	0.058*
H12B	0.5138	0.7716	0.5227	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0256 (2)	0.0409 (3)	0.0630 (4)	0.0027 (2)	-0.0001 (3)	-0.0076 (3)
O1	0.0301 (7)	0.0290 (7)	0.0796 (13)	0.0036 (6)	-0.0053 (9)	0.0013 (8)
O2	0.0330 (8)	0.0437 (9)	0.1064 (17)	0.0092 (7)	-0.0043 (12)	-0.0052 (11)
O3	0.0391 (9)	0.0387 (9)	0.1212 (18)	0.0081 (7)	-0.0105 (13)	-0.0100 (12)
O4	0.0346 (9)	0.0800 (14)	0.0647 (12)	0.0016 (9)	0.0090 (9)	-0.0099 (11)
N1	0.0365 (11)	0.0561 (13)	0.0595 (14)	-0.0065 (9)	-0.0045 (10)	0.0077 (11)
N2	0.0321 (11)	0.0519 (14)	0.0693 (16)	0.0087 (10)	-0.0030 (11)	0.0056 (12)
N3	0.0538 (14)	0.0844 (19)	0.080 (2)	0.0118 (13)	0.0103 (15)	0.0282 (17)
N4	0.0326 (10)	0.0369 (11)	0.123 (3)	-0.0022 (8)	-0.0061 (13)	0.0063 (13)
N5	0.0336 (9)	0.0501 (13)	0.0645 (14)	-0.0067 (8)	-0.0001 (11)	-0.0062 (13)
N6	0.0595 (15)	0.0435 (13)	0.111 (3)	-0.0128 (11)	0.0026 (15)	0.0127 (15)
C2	0.0319 (11)	0.0366 (12)	0.0631 (17)	0.0037 (8)	-0.0045 (11)	-0.0015 (12)
C3	0.0293 (10)	0.0351 (11)	0.0662 (17)	-0.0035 (8)	-0.0032 (11)	0.0006 (11)
C4	0.0292 (10)	0.0308 (10)	0.0511 (14)	-0.0019 (8)	-0.0037 (10)	-0.0017 (11)
C5	0.0299 (10)	0.0315 (10)	0.0502 (15)	0.0013 (8)	-0.0011 (10)	-0.0032 (10)
C6	0.0271 (9)	0.0356 (10)	0.0476 (13)	0.0018 (8)	-0.0006 (10)	-0.0048 (10)
C7	0.0346 (11)	0.0318 (10)	0.0433 (14)	-0.0053 (8)	0.0007 (10)	-0.0012 (10)
C8	0.0382 (11)	0.0271 (10)	0.0540 (15)	-0.0019 (8)	-0.0027 (12)	0.0018 (10)
C9	0.0293 (11)	0.0326 (11)	0.0495 (13)	0.0025 (8)	-0.0036 (10)	0.0000 (10)
C10	0.0284 (10)	0.0306 (10)	0.0473 (13)	-0.0019 (8)	-0.0023 (10)	-0.0003 (9)
C11	0.0356 (11)	0.0391 (12)	0.077 (2)	-0.0089 (9)	0.0015 (14)	-0.0030 (14)
C12	0.0310 (11)	0.0321 (10)	0.0814 (19)	-0.0031 (9)	-0.0035 (12)	-0.0037 (12)

Geometric parameters (Å, °)

S1—O4	1.417 (2)	C4—C12	1.502 (3)
S1—O3	1.4237 (18)	C5—C6	1.386 (3)
S1—N1	1.678 (3)	C5—C10	1.399 (3)
S1—C6	1.768 (2)	C5—H5	0.9300

O1—C9	1.370 (3)	C6—C7	1.410 (3)
O1—C2	1.376 (3)	C7—C8	1.378 (3)
O2—C2	1.208 (3)	C7—C11	1.507 (3)
N1—N2	1.258 (3)	C8—C9	1.384 (3)
N2—N3	1.116 (4)	C8—H8	0.9300
N4—N5	1.178 (3)	C9—C10	1.396 (3)
N4—C12	1.495 (3)	C11—H11A	0.9600
N5—N6	1.133 (3)	C11—H11B	0.9600
C2—C3	1.438 (3)	C11—H11C	0.9600
C3—C4	1.337 (3)	C12—H12A	0.9700
C3—H3	0.9300	C12—H12B	0.9700
C4—C10	1.453 (3)		
O4—S1—O3	120.17 (13)	C7—C6—S1	121.23 (16)
O4—S1—N1	102.39 (12)	C8—C7—C6	116.80 (19)
O3—S1—N1	109.36 (14)	C8—C7—C11	119.3 (2)
O4—S1—C6	110.61 (12)	C6—C7—C11	123.9 (2)
O3—S1—C6	108.77 (11)	C7—C8—C9	121.3 (2)
N1—S1—C6	104.26 (11)	C7—C8—H8	119.4
C9—O1—C2	121.45 (17)	C9—C8—H8	119.4
N2—N1—S1	113.88 (19)	O1—C9—C8	116.16 (18)
N3—N2—N1	173.0 (3)	O1—C9—C10	121.68 (19)
N5—N4—C12	115.0 (2)	C8—C9—C10	122.1 (2)
N6—N5—N4	172.8 (3)	C9—C10—C5	117.18 (19)
O2—C2—O1	116.5 (2)	C9—C10—C4	117.67 (19)
O2—C2—C3	126.3 (2)	C5—C10—C4	125.13 (19)
O1—C2—C3	117.18 (19)	C7—C11—H11A	109.5
C4—C3—C2	122.8 (2)	C7—C11—H11B	109.5
C4—C3—H3	118.6	H11A—C11—H11B	109.5
C2—C3—H3	118.6	C7—C11—H11C	109.5
C3—C4—C10	119.02 (19)	H11A—C11—H11C	109.5
C3—C4—C12	123.1 (2)	H11B—C11—H11C	109.5
C10—C4—C12	117.89 (19)	N4—C12—C4	110.29 (18)
C6—C5—C10	120.1 (2)	N4—C12—H12A	109.6
C6—C5—H5	119.9	C4—C12—H12A	109.6
C10—C5—H5	119.9	N4—C12—H12B	109.6
C5—C6—C7	122.3 (2)	C4—C12—H12B	109.6
C5—C6—S1	116.36 (17)	H12A—C12—H12B	108.1
O4—S1—N1—N2	-160.77 (19)	S1—C6—C7—C11	3.5 (4)
O3—S1—N1—N2	-32.3 (2)	C6—C7—C8—C9	0.2 (4)
C6—S1—N1—N2	83.9 (2)	C11—C7—C8—C9	-177.3 (2)
C9—O1—C2—O2	175.3 (2)	C2—O1—C9—C8	-177.7 (2)
C9—O1—C2—C3	-4.6 (4)	C2—O1—C9—C10	1.0 (4)
O2—C2—C3—C4	-175.0 (3)	C7—C8—C9—O1	175.7 (2)
O1—C2—C3—C4	4.8 (4)	C7—C8—C9—C10	-3.0 (4)
C2—C3—C4—C10	-1.4 (4)	O1—C9—C10—C5	-175.7 (2)
C2—C3—C4—C12	179.0 (3)	C8—C9—C10—C5	2.9 (3)

C10—C5—C6—C7	-2.6 (4)	O1—C9—C10—C4	2.5 (3)
C10—C5—C6—S1	174.00 (18)	C8—C9—C10—C4	-178.8 (2)
O4—S1—C6—C5	134.2 (2)	C6—C5—C10—C9	-0.1 (3)
O3—S1—C6—C5	0.2 (3)	C6—C5—C10—C4	-178.3 (2)
N1—S1—C6—C5	-116.4 (2)	C3—C4—C10—C9	-2.3 (4)
O4—S1—C6—C7	-49.1 (2)	C12—C4—C10—C9	177.4 (2)
O3—S1—C6—C7	176.8 (2)	C3—C4—C10—C5	175.8 (2)
N1—S1—C6—C7	60.3 (2)	C12—C4—C10—C5	-4.5 (4)
C5—C6—C7—C8	2.6 (4)	N5—N4—C12—C4	-161.8 (3)
S1—C6—C7—C8	-173.89 (19)	C3—C4—C12—N4	-5.1 (4)
C5—C6—C7—C11	179.9 (3)	C10—C4—C12—N4	175.3 (2)

Hydrogen-bond geometry (Å, °)

Cg is the centroid of the C5–C10 ring.

<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>
C8—H8...O2 ⁱ	0.93	2.52	3.416 (3)	161
S1—O4...Cg ⁱⁱ	1.42 (1)	2.96 (1)	3.931 (2)	128

Symmetry codes: (i) $-x+1, -y+2, z$; (ii) $x-1/4, -y+7/4, z-3/4$.