Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5′-Amino-1,3-dioxo-2′,3′-dihydro-7′*H*-spiro[indane-2,7′-thieno[3,2-*b*]pyran]-6′-carbonitrile 1′,1′-dioxide

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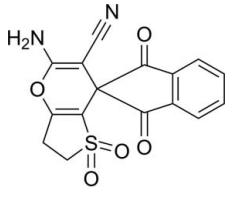
Received 7 March 2010; accepted 17 March 2010

Key indicators: single-crystal X-ray study; T = 116 K; mean σ(C–C) = 0.003 Å; R factor = 0.058; wR factor = 0.127; data-to-parameter ratio = 11.3.

The title compound, $C_{16}H_{10}N_2O_5S$, was synthesized *via* the condesation of dihydrothiophen-3(2*H*)-one 1,1-dioxide, 1*H*-indene-1,2,3-trione and malononitrile in ethanol. The 2,3-dihydrothiophene 1,1-dioxide and pyran rings adopt envelope conformations. The mean planes through the planar part of the pyran ring and the benzene ring are nearly perpendicular, forming a dihedral angle of 88.40 (7)°. The crystal packing is stabilized by intermolecular N—H···O and N—H···N hydrogen bonds with the sulfone O atom and the cyano N atom acting as acceptors.

Related literature

For the uses of thienopyranyl compounds such as thieno-[3,2-*b*]pyran derivatives as antiviral agents and α-2C adreno-receptor agonists, see: Chao *et al.* (2009); Friary *et al.* (1991). For puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{16}H_{10}N_2O_5S$
M_r = 342.32
Monoclinic, $P2_1/c$
a = 9.436 (3) Å
b = 10.602 (3) Å
c = 14.777 (4) Å
β = 99.137 (4)°
V = 1459.6 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 116 K
0.28 × 0.20 × 0.18 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2002)
T_{min} = 0.933, T_{max} = 0.956
9619 measured reflections
2549 independent reflections
1985 reflections with $I > 2\sigma(I)$
R_{int} = 0.068

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.127
S = 1.00
2549 reflections
226 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*C*···N2^{i}	0.89 (1)	2.23 (1)	3.067 (3)	157 (2)
N1—H1*D*···O2^{ii}	0.89 (1)	2.03 (1)	2.865 (2)	156 (2)

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

Data collection: *CrystalClear* (Rigaku/MSC, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge the financial support of the Natural Science Foundation of Gansu Province (No. 0916RJZA0500).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2656).

References

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Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
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Rigaku/MSC (2002). *CrystalClear*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
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supporting information

Acta Cryst. (2010). E**66**, o909 [doi:10.1107/S1600536810010019]

5′-Amino-1,3-dioxo-2′,3′-dihydro-7′*H*-spiro[indane-2,7′-thieno[3,2-*b*]pyran]-6′-carbonitrile 1′,1′-dioxide

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S1. Comment

Thienopyranyl compounds, such as thieno [3,2-b]pyran derivatives, can be used as antiviral agents (Friary *et al.*, 1991) and α-2 C adrenoreceptor agonists (Chao *et al.*, 2009). This led us to pay attention to the synthesis and bioactivity of these compounds. During the synthesis of thieno[3,2-b]pyran derivatives, the title compound, (I) was isolated and its structure was determined by X-ray diffraction. Here we report its crystal structure.

The molecular structure of (I) is shown in Fig. 1. In the molecular structure, the thiophene ring is in envelope conformation, for the deviation of C1 from the C2/C3/C4/S1 plane is 0.364 (3)Å with r.m.s. of 0.0056.

The pyran ring adopts an envelope conformation with atome C5 deviating from the C3/C4/C6/C7/O5 plane 0.228 (3) Å. According to Cremer & Pople analysis (Cremer & Pople, 1975), the puckering amplitude (Q) is 0.168 (2) Å. Its θ and φ are 103.2 (7) and 349.6 (7)°, respectively. The weighted planes of the pyran and phenyl rings are nearly perpendicular, with the dihedral angle between them 88.40 (7)°. The five membered ring of 1*H*-indene-1,3(2*H*)-dione fragment adopts an envelope conformation, for the deviation of C5 from the C9/C10/C15/C16 plane is 0.149 (3)Å with r.m.s. of 0.0033. The crystal packing is stabilized by intermolecular hydrogen bonds: N1—H1C···N2, N1—H1D···O2(Fig.2 & Table 1).

S2. Experimental

The title compound was synthesized by the reaction of dihydrothiophen-3(2*H*)-one-1,1-dioxide (1 mmol), 1*H*-indene-1,2,3-trione (1 mmol) and malononitrile (1 mmol) in 10 ml ethanol under reluxing until completion (monitored by TLC). Cooling the reaction mixture slowly gave single crystals suitable for X-ray diffraction.

S3. Refinement

The hydrogen atoms bonded to the nitrogen atom were positioned from a Fourier difference map. The N—H bond lengths were restrained to 0.90Å with an estimated standard deviation 0.01. The distance between H1C and H1D was restrained to 1.50Å with an estimated standard deviation 0.01. Other H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å, and included in the final cycles of refinement using a riding model, with $U_{iso}(H) = 1.2U_{eq}$(parent atom).

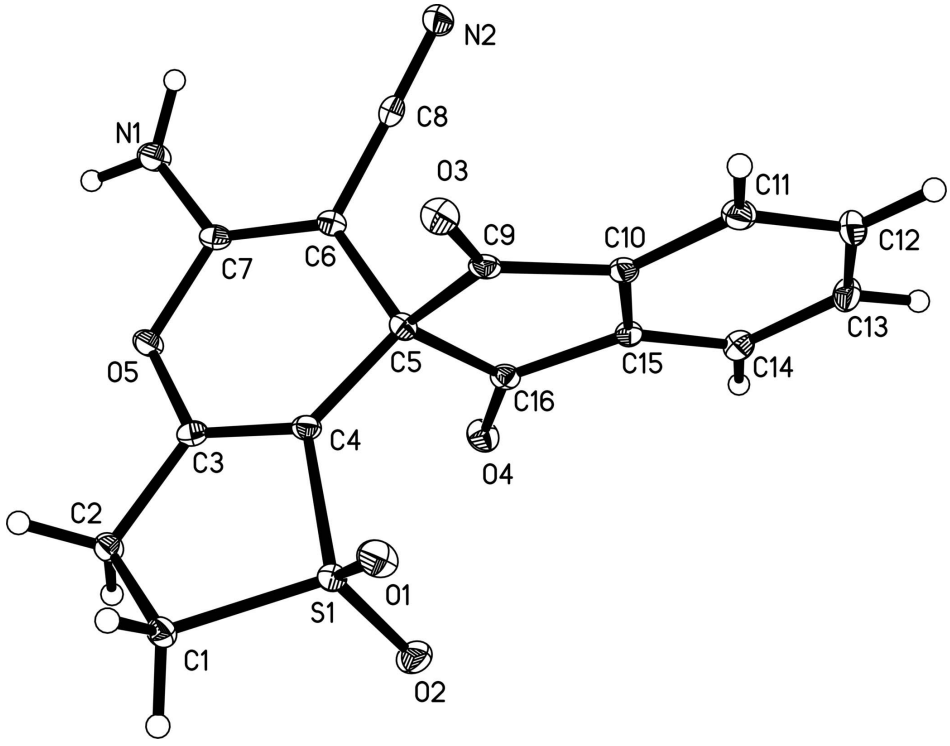

Figure 1

The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

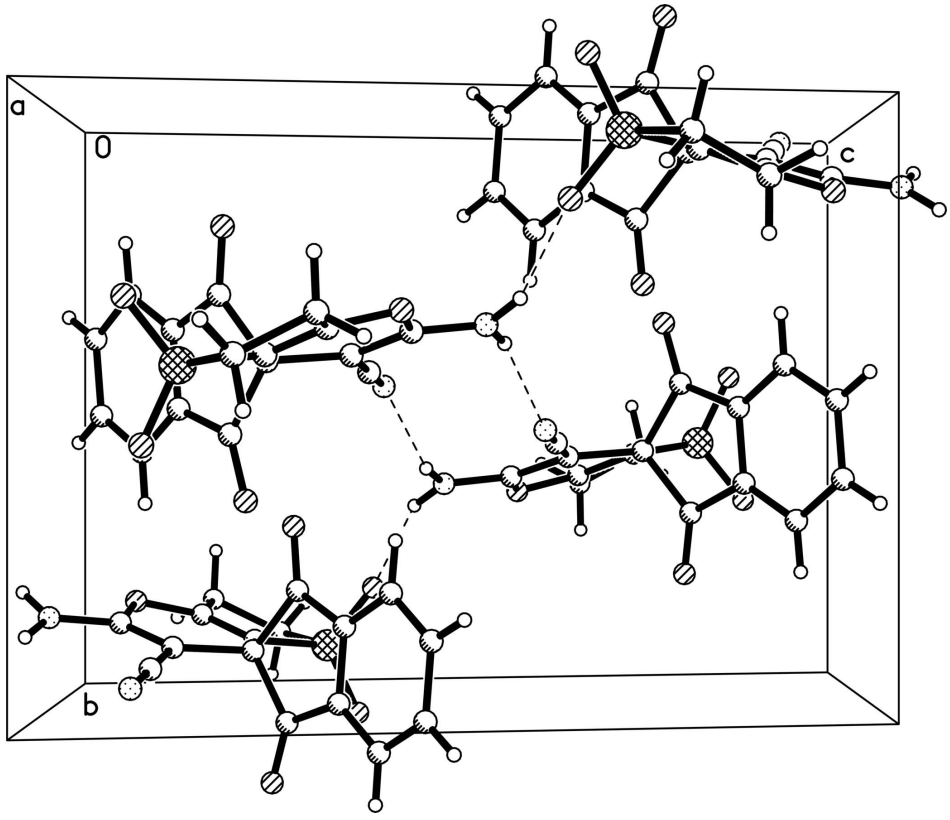

Figure 2

The packing diagram of (I). Intermolecular hydrogen bonds are shown as dashed lines.

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$b = 10.602$ (3) Å
$c = 14.777$ (4) Å
$\beta = 99.137$ (4)°
$V = 1459.6$ (6) Å^3
$Z = 4$
$F(000) = 704$
$D_x = 1.558$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5046 reflections
$\theta = 1.4$–27.9°
$\mu = 0.25$ mm^{-1}
$T = 116$ K
Prism, colorless
0.28 × 0.20 × 0.18 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Radiation source: rotating anode
Multilayer monochromator
Detector resolution: 14.63 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2002)
$T_{min} = 0.933$, $T_{max} = 0.956$
9619 measured reflections
2549 independent reflections
1985 reflections with $I > 2\sigma(I)$
$R_{int} = 0.068$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
$h = -11 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -17 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.127$
$S = 1.00$
2549 reflections
226 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0872P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.58$ e Å^{-3}
$\Delta\rho_{min} = -0.64$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.287 (14)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.97876 (6)	0.43469 (5)	0.18224 (4)	0.0160 (2)
O1	0.95541 (18)	0.55710 (13)	0.14090 (11)	0.0236 (4)
O2	0.95173 (17)	0.32826 (14)	0.12109 (11)	0.0253 (4)
O3	0.68230 (16)	0.65052 (13)	0.24233 (10)	0.0205 (4)
O4	0.68085 (16)	0.20574 (13)	0.21541 (10)	0.0216 (4)
O5	0.93203 (15)	0.34731 (13)	0.42896 (10)	0.0183 (4)
N1	0.7756 (2)	0.36526 (18)	0.52595 (13)	0.0224 (5)
N2	0.4414 (2)	0.46284 (18)	0.40031 (13)	0.0242 (5)
C1	1.1509 (2)	0.42085 (19)	0.25136 (15)	0.0170 (5)
H1A	1.2145	0.3705	0.2204	0.020*
H1B	1.1936	0.5034	0.2644	0.020*
C2	1.1251 (2)	0.35644 (19)	0.33972 (15)	0.0172 (5)
H2A	1.1471	0.2672	0.3379	0.021*
H2B	1.1854	0.3937	0.3922	0.021*
C3	0.9718 (2)	0.37524 (18)	0.34620 (14)	0.0151 (5)
C4	0.8818 (2)	0.41635 (18)	0.27348 (14)	0.0148 (5)
C5	0.7227 (2)	0.42359 (18)	0.26815 (15)	0.0149 (5)
C6	0.6933 (2)	0.41396 (18)	0.36651 (15)	0.0150 (5)
C7	0.7939 (2)	0.37715 (18)	0.43869 (14)	0.0160 (5)
C8	0.5539 (2)	0.43993 (18)	0.38449 (15)	0.0160 (5)
C9	0.6480 (2)	0.54337 (19)	0.22236 (15)	0.0158 (5)
C10	0.5243 (2)	0.50111 (19)	0.15446 (14)	0.0151 (5)
C11	0.4185 (2)	0.5739 (2)	0.10321 (15)	0.0201 (5)

H11	0.4207	0.6615	0.1074	0.024*
C12	0.3101 (2)	0.5133 (2)	0.04602 (15)	0.0233 (6)
H12	0.2375	0.5604	0.0118	0.028*
C13	0.3079 (3)	0.3814 (2)	0.03878 (15)	0.0226 (5)
H13	0.2340	0.3425	−0.0005	0.027*
C14	0.4129 (2)	0.3084 (2)	0.08852 (14)	0.0197 (5)
H14	0.4117	0.2210	0.0831	0.024*
C15	0.5215 (2)	0.36997 (18)	0.14740 (14)	0.0152 (5)
C16	0.6443 (2)	0.31490 (19)	0.20917 (14)	0.0156 (5)
H1C	0.6992 (18)	0.394 (2)	0.5484 (15)	0.036 (7)*
H1D	0.841 (2)	0.325 (2)	0.5651 (14)	0.047 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0134 (4)	0.0201 (4)	0.0148 (3)	−0.0004 (2)	0.0034 (2)	−0.0006 (2)
O1	0.0225 (10)	0.0262 (9)	0.0231 (9)	0.0053 (6)	0.0064 (7)	0.0088 (7)
O2	0.0227 (10)	0.0316 (9)	0.0226 (9)	−0.0070 (7)	0.0062 (7)	−0.0101 (7)
O3	0.0213 (10)	0.0148 (8)	0.0257 (9)	−0.0017 (6)	0.0046 (7)	−0.0003 (7)
O4	0.0219 (9)	0.0154 (8)	0.0268 (9)	0.0029 (6)	0.0016 (7)	0.0006 (7)
O5	0.0147 (9)	0.0241 (8)	0.0167 (8)	0.0048 (6)	0.0043 (6)	0.0037 (6)
N1	0.0222 (12)	0.0287 (11)	0.0171 (10)	0.0084 (9)	0.0056 (9)	0.0052 (9)
N2	0.0179 (12)	0.0353 (11)	0.0196 (11)	0.0024 (8)	0.0039 (9)	−0.0013 (8)
C1	0.0133 (12)	0.0185 (11)	0.0191 (12)	−0.0018 (9)	0.0029 (9)	−0.0009 (9)
C2	0.0152 (12)	0.0183 (10)	0.0181 (11)	0.0014 (9)	0.0025 (9)	0.0007 (9)
C3	0.0175 (12)	0.0131 (10)	0.0157 (11)	0.0008 (8)	0.0051 (9)	−0.0015 (9)
C4	0.0135 (12)	0.0162 (10)	0.0156 (11)	−0.0006 (8)	0.0053 (9)	−0.0018 (9)
C5	0.0124 (12)	0.0157 (10)	0.0167 (11)	−0.0001 (8)	0.0027 (9)	0.0002 (9)
C6	0.0141 (12)	0.0150 (10)	0.0167 (11)	0.0009 (8)	0.0047 (9)	0.0005 (9)
C7	0.0168 (12)	0.0127 (10)	0.0196 (12)	0.0011 (8)	0.0065 (9)	−0.0003 (9)
C8	0.0185 (13)	0.0163 (11)	0.0125 (11)	−0.0024 (9)	0.0005 (9)	0.0002 (8)
C9	0.0140 (12)	0.0193 (11)	0.0158 (11)	0.0014 (8)	0.0074 (9)	0.0002 (9)
C10	0.0139 (12)	0.0187 (11)	0.0136 (11)	0.0013 (9)	0.0050 (9)	0.0010 (9)
C11	0.0217 (13)	0.0201 (11)	0.0192 (12)	0.0054 (9)	0.0052 (10)	0.0012 (9)
C12	0.0215 (14)	0.0305 (12)	0.0168 (12)	0.0077 (10)	−0.0007 (10)	0.0042 (10)
C13	0.0189 (13)	0.0309 (12)	0.0169 (12)	−0.0023 (10)	−0.0008 (10)	−0.0034 (10)
C14	0.0214 (13)	0.0205 (11)	0.0175 (12)	−0.0008 (9)	0.0040 (10)	−0.0001 (9)
C15	0.0138 (12)	0.0187 (10)	0.0135 (11)	−0.0001 (8)	0.0038 (9)	−0.0001 (9)
C16	0.0143 (12)	0.0179 (11)	0.0158 (11)	−0.0012 (9)	0.0064 (9)	0.0017 (9)

Geometric parameters (Å, º)

S1—O1	1.4364 (15)	C4—C5	1.493 (3)
S1—O2	1.4428 (16)	C5—C6	1.526 (3)
S1—C4	1.756 (2)	C5—C9	1.554 (3)
S1—C1	1.782 (2)	C5—C16	1.559 (3)
O3—C9	1.205 (2)	C6—C7	1.368 (3)
O4—C16	1.207 (2)	C6—C8	1.409 (3)

O5—C3	1.367 (2)	C9—C10	1.482 (3)
O5—C7	1.371 (3)	C10—C11	1.388 (3)
N1—C7	1.334 (3)	C10—C15	1.394 (3)
N1—H1C	0.893 (9)	C11—C12	1.378 (3)
N1—H1D	0.889 (9)	C11—H11	0.9300
N2—C8	1.149 (3)	C12—C13	1.403 (3)
C1—C2	1.527 (3)	C12—H12	0.9300
C1—H1A	0.9700	C13—C14	1.374 (3)
C1—H1B	0.9700	C13—H13	0.9300
C2—C3	1.478 (3)	C14—C15	1.396 (3)
C2—H2A	0.9700	C14—H14	0.9300
C2—H2B	0.9700	C15—C16	1.477 (3)
C3—C4	1.333 (3)		

O1—S1—O2	116.12 (10)	C9—C5—C16	102.61 (17)
O1—S1—C4	111.29 (10)	C7—C6—C8	117.51 (19)
O2—S1—C4	109.41 (9)	C7—C6—C5	123.58 (19)
O1—S1—C1	112.48 (10)	C8—C6—C5	118.87 (19)
O2—S1—C1	110.42 (10)	N1—C7—C6	126.9 (2)
C4—S1—C1	95.13 (10)	N1—C7—O5	110.57 (19)
C3—O5—C7	116.39 (16)	C6—C7—O5	122.56 (18)
C7—N1—H1C	124.3 (15)	N2—C8—C6	178.7 (2)
C7—N1—H1D	119.4 (16)	O3—C9—C10	127.1 (2)
H1C—N1—H1D	116.3 (15)	O3—C9—C5	125.3 (2)
C2—C1—S1	105.81 (14)	C10—C9—C5	107.55 (16)
C2—C1—H1A	110.6	C11—C10—C15	120.68 (19)
S1—C1—H1A	110.6	C11—C10—C9	128.46 (19)
C2—C1—H1B	110.6	C15—C10—C9	110.84 (17)
S1—C1—H1B	110.6	C12—C11—C10	118.3 (2)
H1A—C1—H1B	108.7	C12—C11—H11	120.8
C3—C2—C1	106.59 (17)	C10—C11—H11	120.8
C3—C2—H2A	110.4	C11—C12—C13	120.8 (2)
C1—C2—H2A	110.4	C11—C12—H12	119.6
C3—C2—H2B	110.4	C13—C12—H12	119.6
C1—C2—H2B	110.4	C14—C13—C12	121.3 (2)
H2A—C2—H2B	108.6	C14—C13—H13	119.3
C4—C3—O5	124.2 (2)	C12—C13—H13	119.3
C4—C3—C2	119.78 (19)	C13—C14—C15	117.7 (2)
O5—C3—C2	116.05 (18)	C13—C14—H14	121.1
C3—C4—C5	124.48 (19)	C15—C14—H14	121.1
C3—C4—S1	108.20 (16)	C10—C15—C14	121.09 (19)
C5—C4—S1	126.58 (16)	C10—C15—C16	110.13 (17)
C4—C5—C6	106.25 (17)	C14—C15—C16	128.78 (19)
C4—C5—C9	116.60 (17)	O4—C16—C15	127.8 (2)
C6—C5—C9	109.32 (16)	O4—C16—C5	124.15 (19)
C4—C5—C16	112.07 (16)	C15—C16—C5	108.03 (16)
C6—C5—C16	109.94 (16)		

O1—S1—C1—C2	135.04 (14)	C3—O5—C7—C6	10.1 (3)
O2—S1—C1—C2	−93.46 (15)	C7—C6—C8—N2	59 (11)
C4—S1—C1—C2	19.47 (15)	C5—C6—C8—N2	−123 (11)
S1—C1—C2—C3	−20.47 (19)	C4—C5—C9—O3	−51.7 (3)
C7—O5—C3—C4	−7.2 (3)	C6—C5—C9—O3	68.8 (3)
C7—O5—C3—C2	173.23 (16)	C16—C5—C9—O3	−174.58 (19)
C1—C2—C3—C4	13.2 (3)	C4—C5—C9—C10	131.25 (19)
C1—C2—C3—O5	−167.28 (16)	C6—C5—C9—C10	−108.26 (18)
O5—C3—C4—C5	−7.5 (3)	C16—C5—C9—C10	8.4 (2)
C2—C3—C4—C5	172.05 (18)	O3—C9—C10—C11	−3.5 (4)
O5—C3—C4—S1	−178.14 (15)	C5—C9—C10—C11	173.4 (2)
C2—C3—C4—S1	1.4 (2)	O3—C9—C10—C15	177.91 (19)
O1—S1—C4—C3	−129.26 (15)	C5—C9—C10—C15	−5.1 (2)
O2—S1—C4—C3	101.07 (16)	C15—C10—C11—C12	0.6 (3)
C1—S1—C4—C3	−12.70 (16)	C9—C10—C11—C12	−177.8 (2)
O1—S1—C4—C5	60.3 (2)	C10—C11—C12—C13	−0.9 (3)
O2—S1—C4—C5	−69.34 (19)	C11—C12—C13—C14	0.3 (3)
C1—S1—C4—C5	176.89 (18)	C12—C13—C14—C15	0.6 (3)
C3—C4—C5—C6	16.4 (3)	C11—C10—C15—C14	0.3 (3)
S1—C4—C5—C6	−174.71 (14)	C9—C10—C15—C14	178.97 (19)
C3—C4—C5—C9	138.5 (2)	C11—C10—C15—C16	−179.47 (19)
S1—C4—C5—C9	−52.6 (2)	C9—C10—C15—C16	−0.8 (2)
C3—C4—C5—C16	−103.7 (2)	C13—C14—C15—C10	−0.9 (3)
S1—C4—C5—C16	65.2 (2)	C13—C14—C15—C16	178.8 (2)
C4—C5—C6—C7	−13.2 (3)	C10—C15—C16—O4	−173.9 (2)
C9—C5—C6—C7	−139.8 (2)	C14—C15—C16—O4	6.3 (4)
C16—C5—C6—C7	108.3 (2)	C10—C15—C16—C5	6.4 (2)
C4—C5—C6—C8	169.09 (17)	C14—C15—C16—C5	−173.4 (2)
C9—C5—C6—C8	42.5 (2)	C4—C5—C16—O4	45.5 (3)
C16—C5—C6—C8	−69.4 (2)	C6—C5—C16—O4	−72.4 (2)
C8—C6—C7—N1	−1.5 (3)	C9—C5—C16—O4	171.39 (18)
C5—C6—C7—N1	−179.2 (2)	C4—C5—C16—C15	−134.76 (18)
C8—C6—C7—O5	178.80 (17)	C6—C5—C16—C15	107.32 (18)
C5—C6—C7—O5	1.0 (3)	C9—C5—C16—C15	−8.9 (2)
C3—O5—C7—N1	−169.63 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*C*···N2^{i}	0.89 (1)	2.23 (1)	3.067 (3)	157 (2)
N1—H1*D*···O2^{ii}	0.89 (1)	2.03 (1)	2.865 (2)	156 (2)

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