Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Fluoren-9-one 4-toluenesulfonylhydrazone: hydrogen-bonded $R_2^2(8)$ dimers are linked into sheets by π–π stacking interactions

Christopher Glidewell,[a]* John N. Low,[b] Janet M. S. Skakle[b] and James L. Wardell[c]

[a]School of Chemistry, University of St Andrews, St Andrews, Fife KY16 9ST, Scotland, [b]Department of Chemistry, University of Aberdeen, Meston Walk, Old Aberdeen AB24 3UE, Scotland, and [c]Instituto de Química, Departamento de Química Inorgânica, Universidade Federal do Rio de Janeiro, 21945-970 Rio de Janeiro-RJ, Brazil

Correspondence e-mail: cg@st-andrews.ac.uk

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.090
Data-to-parameter ratio = 16.5

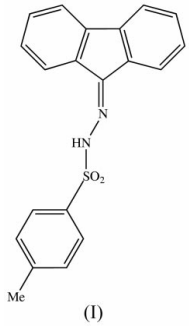
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Molecules of the title compound, $C_{20}H_{16}N_2O_2S$, are linked into centrosymmetric $R_2^2(8)$ dimers by paired N—H···O hydrogen bonds [H···O 2.14 Å, N···O 2.9951 (15) Å and N—H···O 164°]. Two distinct π–π stacking interactions link the dimers into chains along [10$\bar{1}$] and [001], respectively, hence forming (010) sheets.

Received 1 March 2004
Accepted 2 March 2004
Online 13 March 2004

Comment

4-Toluenesulfonylhydrazones, $R^1R^2C{=}NNHC_6H_4Me$, are not only important derivatives of carbonyl compounds, $R^1R^2C{=}O$, but are also very useful precursors of diazo compounds, $R^1R^2CN_2$, (Jonczyk & Wlostowska, 1978), as exemplified by the title compound, (I) (Fig. 1).



(I)

The molecules of (I) are linked by paired N—H···O=S hydrogen bonds into centrosymmetric dimers, with the reference dimer centred at ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$) (Fig. 2). The associated $R_2^2(8)$ (Bernstein *et al.*, 1995) motif has been observed previously in a

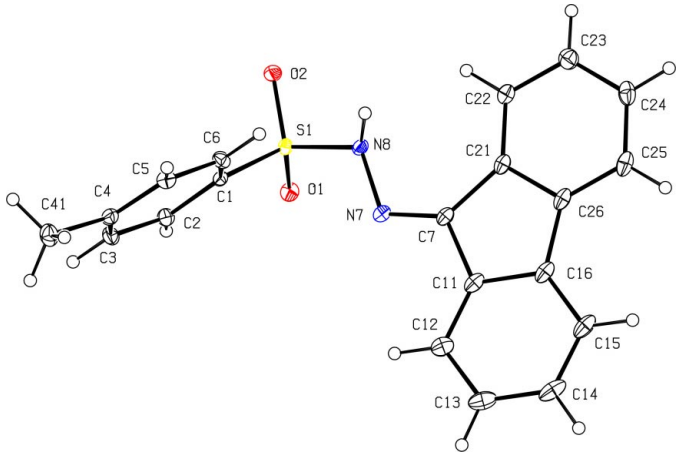


Figure 1
The molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

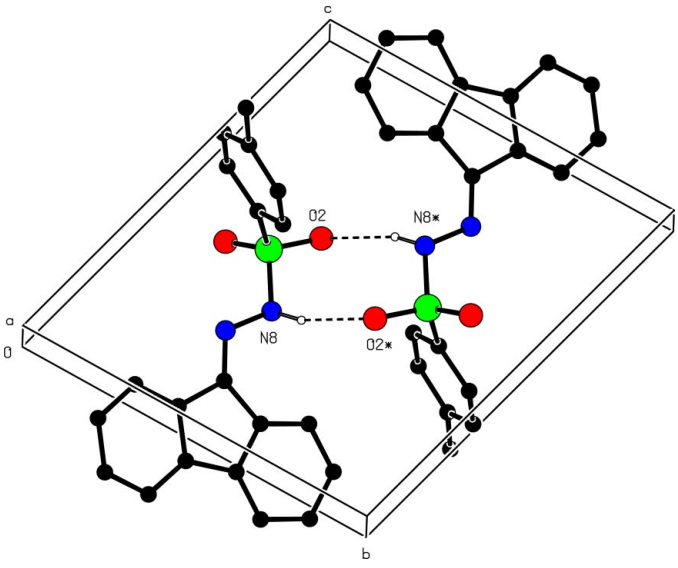


Figure 2
Part of the crystal structure of (I), showing the formation of an $R_2^2(8)$ dimer. For the sake of clarity, H atoms bonded to C atoms have been omitted. The atoms marked with an asterisk (*) are at the symmetry position $(1-x, 1-y, 1-z)$.

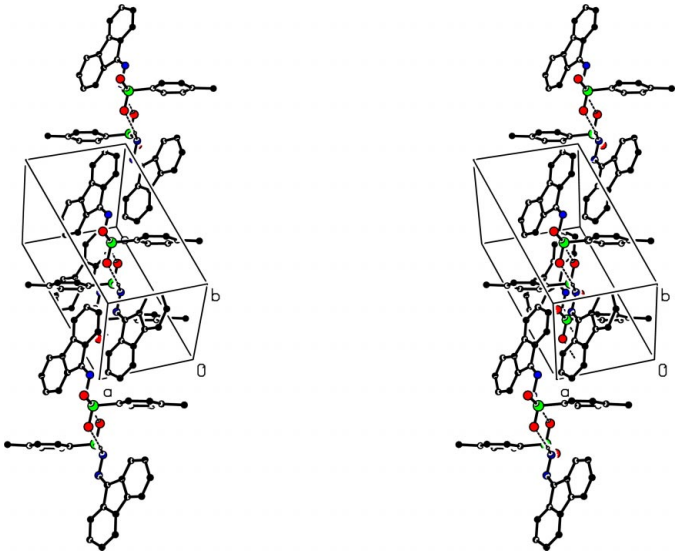


Figure 3
A stereoview of part of the crystal structure of (I), showing the formation of a $[10\bar{1}]$ chain of π-stacked dimers. For the sake of clarity, H atoms bonded to C atoms have been omitted.

number of sulfonamido species (Klug, 1968; Blaschette *et al.*, 1986; Tremayne *et al.*, 1999, 2002; Kelly *et al.*, 2002; Clark *et al.*, 2003). While there are no soft hydrogen bonds of either C—H···O or C—H···π(arene) types present in the structure of (I), the dimeric aggregates are linked into sheets by two distinct π–π stacking interactions, one involving aryl rings and the other involving the fulvene portion of the fluorenone hydrazone.

The C11–C16 aryl rings of the molecules at (x, y, z) and $(2-x, 1-y, -z)$ are parallel, with an interplanar spacing of 3.427 (2) Å; the centroid separation is 3.725 (2) Å, corresponding to a centroid offset of 1.460 (2) Å. These two molecules lie in the $R_2^2(8)$ dimers centred at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and $(\frac{3}{2}, \frac{1}{2}, -\frac{1}{2})$, respectively, so that propagation by inversion of this π–π interaction generates a chain of π-stacked dimers running parallel to the $[10\bar{1}]$ direction (Fig. 3).

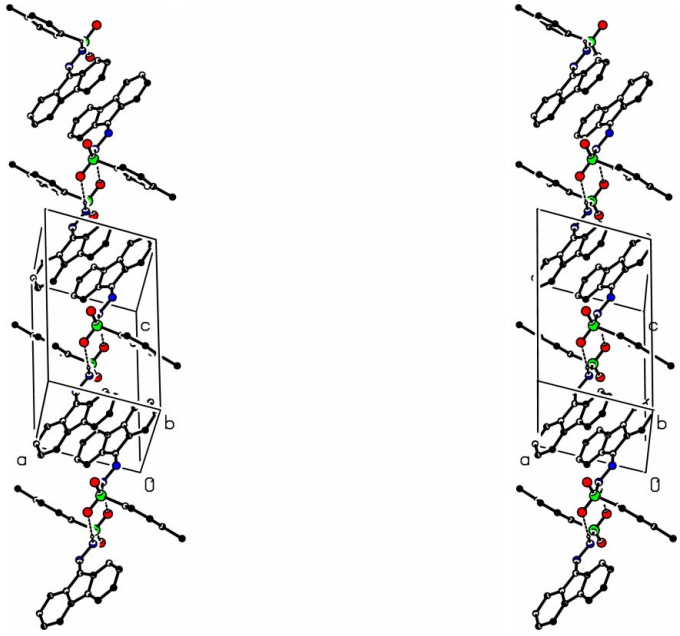


Figure 4
A stereoview of part of the crystal structure of (I), showing the formation of an [001] chain of π-stacked dimers. For the sake of clarity, H atoms bonded to C atoms have been omitted.

The fulvene-type rings (C7/C11/C16/C26/C21) of the molecules at (x, y, z) and $(1-x, 1-y, -z)$, which lie in the $R_2^2(8)$ dimers centred at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and $(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})$, respectively, are also parallel; the interplanar spacing is 3.419 (2) Å and the centroid separation is 3.451 (2) Å, corresponding to a centroid offset of only 0.473 (2) Å. Propagation by inversion of the interaction generates a second chain of π-stacked dimers, in this case running parallel to the [001] direction (Fig. 4). The combination of the [001] and $[10\bar{1}]$ chains generates an (010) sheet.

Experimental

The title compound was prepared using the published procedure of Bamford & Stevens (1952) and it was recrystallized from ethanol [m.p. 457–460 K (decomposes); literature m.p. 453–455 K (decomposes)].

Crystal data

$C_{20}H_{16}N_2O_2S$
$M_r = 348.41$
Triclinic, $P\bar{1}$
$a = 7.7487$ (2) Å
$b = 10.4290$ (3) Å
$c = 11.2007$ (3) Å
$\alpha = 71.8482$ (13)°
$\beta = 76.9553$ (17)°
$\gamma = 75.3167$ (17)°
$V = 821.34$ (4) Å^3
$Z = 2$
$D_x = 1.409$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3744 reflections
$\theta = 3.1$–27.5°
$\mu = 0.21$ mm^{-1}
$T = 120$ (2) K
Block, yellow
0.48 × 0.40 × 0.26 mm

Data collection

Nonius KappaCCD area-detector diffractometer	3744 independent reflections
φ scans, and ω scans with κ offsets	3294 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)	$R_{int} = 0.016$
$T_{min} = 0.915$, $T_{max} = 0.947$	$\theta_{max} = 27.5^\circ$
6955 measured reflections	$h = -9 \rightarrow 10$
	$k = -13 \rightarrow 13$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2 + 0.4642P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.036$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.090$	$\Delta\rho_{max} = 0.33$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -0.49$ e Å^{-3}
3744 reflections	
227 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

S1—C1	1.7569 (13)	C7—C11	1.4803 (19)
S1—O1	1.4281 (10)	C7—C21	1.485 (2)
S1—O2	1.4448 (10)	C11—C16	1.403 (2)
S1—N8	1.6375 (11)	C21—C26	1.4140 (19)
N8—N7	1.4038 (16)	C16—C26	1.467 (2)
N7—C7	1.2916 (18)		
C11—C7—N7—N8	178.55 (11)	C7—N7—N8—S1	169.89 (9)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N8—H8···O2^{i}	0.88	2.14	2.9951 (15)	164

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

All H atoms were located using difference maps and subsequently treated as riding atoms, with C—H distances of 0.95 (aromatic) or 0.98 (methyl), and an N—H distance of 0.88 Å, and with U_{iso}(H) = $1.2U_{eq}$(C,N), or $1.5U_{eq}$(C) for methyl H.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS*86 (Sheldrick, 1990); program(s) used to refine structure: *OSCAIL* and *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL*97 and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, UK; the authors thank the staff for all their help and advice. JNL thanks NCR Self-Service, Dundee, for grants which have provided computing facilities for this work. JLW thanks CNPq and FAPERJ for financial support.

References

Bamford, W. R. & Stevens, T. S. (1952). *J. Chem. Soc.* pp. 4735–4738.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Blaschette, A., Wieland, E., Schomburg, D. & Adelhelm, M. (1986). *Z. Anorg. Allg. Chem.* **533**, 7–717.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–37.
Blessing, R. H. (1997). *J. Appl. Cryst.* **30**, 421–426.
Clark, J. C., McLaughlin, M. L. & Fronczek, F. R. (2003). *Acta Cryst.* E**59**, o2005–o2006.
Ferguson, G. (1999). *PRPKAPPA*. University of Guelph, Canada.
Jonczyk, A. & Wlostowska, J. (1978). *Synth. Commun.* **8**, 569–572.
Kelly, C. J., Skakle, J. M. S., Wardell, J. L., Wardell, S. M. S. V., Low, J. N. & Glidewell, C. (2002). *Acta Cryst.* B**58**, 94–108.
Klug, H. P. (1968). *Acta Cryst.* B**24**, 792–802.
McArdle, P. (2003). *OSCAIL for Windows*. Version 10. Crystallography Centre, Chemistry Department, NUI Galway, Ireland.
Nonius (1997). *KappaCCD Server Software*. Windows 3.11 Version. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Tremayne, M., MacLean, E. J., Tang, C. C. & Glidewell, C. (1999). *Acta Cryst.* B**55**, 1068–1074.
Tremayne, M., Seaton, C. C. & Glidewell, C. (2002). *Acta Cryst.* B**58**, 823–834.

supporting information

Acta Cryst. (2004). E**60**, o520–o522 [https://doi.org/10.1107/S1600536804004878]

Fluoren-9-one 4-toluenesulfonylhydrazone: hydrogen-bonded *R*[{_2^2}](8) dimers are linked into sheets by π–π stacking interactions

Christopher Glidewell, John N. Low, Janet M. S. Skakle and James L. Wardell

Fluoren-9-one 4-toluenesulfonylhydrazone

Crystal data

$C_{20}H_{16}N_2O_2S$
$M_r = 348.41$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.7487$ (2) Å
$b = 10.4290$ (3) Å
$c = 11.2007$ (3) Å
$\alpha = 71.8482$ (13)°
$\beta = 76.9553$ (17)°
$\gamma = 75.3167$ (17)°
$V = 821.34$ (4) Å^3
$Z = 2$
$F(000) = 364$
$D_x = 1.409$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3744 reflections
$\theta = 3.1$–$27.5°$
$\mu = 0.21$ mm^{-1}
$T = 120$ K
Block, yellow
0.48 × 0.40 × 0.26 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Radiation source: rotating anode
Graphite monochromator
φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (SORTAV; Blessing, 1995, 1997)
$T_{min} = 0.915$, $T_{max} = 0.947$
6955 measured reflections
3744 independent reflections
3294 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -9 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.090$
$S = 1.06$
3744 reflections
227 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2 + 0.4642P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.49$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.49758 (4)	0.29627 (3)	0.46935 (3)	0.01486 (10)

O1	0.42730 (13)	0.19893 (10)	0.43797 (9)	0.0200 (2)
O2	0.38541 (13)	0.37025 (10)	0.55813 (9)	0.0191 (2)
N7	0.65778 (15)	0.37426 (12)	0.24099 (11)	0.0175 (2)
N8	0.53735 (15)	0.41975 (12)	0.34037 (10)	0.0170 (2)
C1	0.70124 (18)	0.21206 (14)	0.52723 (12)	0.0152 (3)
C2	0.72736 (19)	0.07160 (14)	0.58536 (13)	0.0190 (3)
C3	0.8796 (2)	0.00832 (15)	0.64325 (14)	0.0213 (3)
C4	1.00559 (19)	0.08295 (15)	0.64246 (13)	0.0198 (3)
C5	0.97835 (19)	0.22305 (15)	0.58033 (14)	0.0201 (3)
C6	0.82650 (19)	0.28867 (14)	0.52338 (13)	0.0192 (3)
C7	0.66885 (18)	0.46685 (14)	0.13309 (13)	0.0173 (3)
C11	0.79401 (19)	0.43389 (15)	0.02076 (13)	0.0203 (3)
C12	0.9210 (2)	0.31646 (16)	0.01045 (15)	0.0253 (3)
C13	1.0248 (2)	0.31484 (19)	−0.10839 (16)	0.0313 (4)
C14	0.9996 (2)	0.42802 (19)	−0.21281 (15)	0.0317 (4)
C15	0.8723 (2)	0.54628 (18)	−0.20293 (14)	0.0278 (3)
C16	0.7699 (2)	0.54903 (16)	−0.08441 (13)	0.0214 (3)
C21	0.57250 (19)	0.61144 (15)	0.08941 (13)	0.0184 (3)
C22	0.44142 (19)	0.69726 (15)	0.15144 (14)	0.0215 (3)
C23	0.3761 (2)	0.83030 (16)	0.08245 (15)	0.0264 (3)
C24	0.4379 (2)	0.87671 (16)	−0.04685 (15)	0.0273 (3)
C25	0.5645 (2)	0.79084 (16)	−0.11100 (14)	0.0253 (3)
C26	0.63292 (19)	0.65890 (15)	−0.04260 (13)	0.0203 (3)
C41	1.1667 (2)	0.01449 (17)	0.70916 (15)	0.0280 (3)
H12	0.9371	0.2391	0.0822	0.030*
H13	1.1135	0.2355	−0.1180	0.038*
H14	1.0713	0.4245	−0.2930	0.038*
H15	0.8556	0.6231	−0.2751	0.033*
H22	0.3971	0.6657	0.2396	0.026*
H23	0.2878	0.8904	0.1244	0.032*
H24	0.3927	0.9685	−0.0919	0.033*
H25	0.6037	0.8218	−0.2000	0.030*
H8	0.5552	0.4929	0.3555	0.020*
H2	0.6427	0.0196	0.5856	0.023*
H3	0.8979	−0.0876	0.6841	0.026*
H5	1.0654	0.2745	0.5770	0.024*
H6	0.8082	0.3845	0.4823	0.023*
H41A	1.1328	0.0129	0.7993	0.042*
H41B	1.2642	0.0659	0.6700	0.042*
H41C	1.2081	−0.0800	0.7017	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01527 (17)	0.01553 (17)	0.01290 (16)	−0.00454 (12)	−0.00134 (12)	−0.00203 (12)
O1	0.0209 (5)	0.0209 (5)	0.0208 (5)	−0.0083 (4)	−0.0036 (4)	−0.0055 (4)
O2	0.0182 (5)	0.0195 (5)	0.0177 (5)	−0.0023 (4)	0.0001 (4)	−0.0057 (4)
N7	0.0174 (6)	0.0213 (6)	0.0156 (6)	−0.0056 (5)	−0.0013 (4)	−0.0068 (5)

N8	0.0211 (6)	0.0172 (6)	0.0123 (5)	−0.0051 (5)	−0.0002 (4)	−0.0040 (4)
C1	0.0158 (6)	0.0170 (6)	0.0120 (6)	−0.0024 (5)	−0.0014 (5)	−0.0041 (5)
C2	0.0207 (7)	0.0172 (7)	0.0185 (7)	−0.0060 (5)	−0.0013 (5)	−0.0035 (5)
C3	0.0232 (7)	0.0162 (7)	0.0204 (7)	−0.0020 (5)	−0.0024 (5)	−0.0013 (5)
C4	0.0184 (7)	0.0231 (7)	0.0158 (6)	−0.0004 (5)	−0.0017 (5)	−0.0061 (5)
C5	0.0179 (7)	0.0223 (7)	0.0222 (7)	−0.0056 (5)	−0.0027 (5)	−0.0077 (6)
C6	0.0191 (7)	0.0157 (6)	0.0214 (7)	−0.0037 (5)	−0.0019 (5)	−0.0039 (5)
C7	0.0169 (6)	0.0236 (7)	0.0148 (6)	−0.0088 (5)	−0.0021 (5)	−0.0062 (5)
C11	0.0194 (7)	0.0303 (8)	0.0166 (7)	−0.0134 (6)	0.0001 (5)	−0.0091 (6)
C12	0.0237 (8)	0.0294 (8)	0.0271 (8)	−0.0099 (6)	−0.0009 (6)	−0.0124 (6)
C13	0.0261 (8)	0.0402 (9)	0.0369 (9)	−0.0141 (7)	0.0053 (7)	−0.0244 (8)
C14	0.0332 (9)	0.0482 (10)	0.0236 (8)	−0.0243 (8)	0.0089 (6)	−0.0199 (7)
C15	0.0323 (8)	0.0419 (9)	0.0162 (7)	−0.0235 (7)	0.0027 (6)	−0.0092 (6)
C16	0.0228 (7)	0.0317 (8)	0.0155 (7)	−0.0163 (6)	−0.0013 (5)	−0.0069 (6)
C21	0.0192 (7)	0.0244 (7)	0.0148 (6)	−0.0109 (6)	−0.0038 (5)	−0.0037 (5)
C22	0.0221 (7)	0.0260 (7)	0.0172 (7)	−0.0065 (6)	−0.0042 (5)	−0.0049 (6)
C23	0.0270 (8)	0.0266 (8)	0.0278 (8)	−0.0044 (6)	−0.0090 (6)	−0.0079 (6)
C24	0.0326 (8)	0.0249 (8)	0.0263 (8)	−0.0088 (6)	−0.0146 (6)	0.0000 (6)
C25	0.0300 (8)	0.0326 (8)	0.0168 (7)	−0.0172 (7)	−0.0072 (6)	−0.0002 (6)
C26	0.0216 (7)	0.0296 (8)	0.0142 (6)	−0.0153 (6)	−0.0033 (5)	−0.0038 (6)
C41	0.0237 (8)	0.0295 (8)	0.0274 (8)	−0.0006 (6)	−0.0092 (6)	−0.0032 (6)

Geometric parameters (Å, º)

S1—C1	1.7569 (13)	C22—H22	0.95
S1—O1	1.4281 (10)	C23—C24	1.389 (2)
S1—O2	1.4448 (10)	C23—H23	0.95
S1—N8	1.6375 (11)	C24—C25	1.385 (2)
N8—N7	1.4038 (16)	C24—H24	0.95
N7—C7	1.2916 (18)	C25—C26	1.385 (2)
C11—C12	1.381 (2)	C25—H25	0.95
C7—C11	1.4803 (19)	N8—H8	0.88
C7—C21	1.485 (2)	C1—C2	1.3876 (19)
C11—C16	1.403 (2)	C1—C6	1.3911 (19)
C21—C26	1.4140 (19)	C2—C3	1.390 (2)
C16—C26	1.467 (2)	C2—H2	0.95
C12—C13	1.394 (2)	C3—C4	1.392 (2)
C12—H12	0.95	C3—H3	0.95
C13—C14	1.388 (3)	C4—C5	1.393 (2)
C13—H13	0.95	C4—C41	1.504 (2)
C14—C15	1.388 (3)	C5—C6	1.385 (2)
C14—H14	0.95	C5—H5	0.95
C15—C16	1.389 (2)	C6—H6	0.95
C15—H15	0.95	C41—H41A	0.98
C21—C22	1.387 (2)	C41—H41B	0.98
C22—C23	1.390 (2)	C41—H41C	0.98
C12—C11—C16	121.46 (13)	N7—C7—C21	133.19 (13)

C12—C11—C7	130.27 (14)	C11—C7—C21	106.51 (12)
C16—C11—C7	108.25 (13)	C7—N7—N8	114.54 (12)
C11—C12—C13	118.00 (15)	N7—N8—S1	114.07 (9)
C11—C12—H12	121.0	N7—N8—H8	116.2
C13—C12—H12	121.0	S1—N8—H8	113.6
C14—C13—C12	120.60 (16)	O1—S1—O2	118.82 (6)
C14—C13—H13	119.7	O1—S1—N8	108.85 (6)
C12—C13—H13	119.7	O2—S1—N8	102.95 (6)
C13—C14—C15	121.61 (14)	O1—S1—C1	108.45 (6)
C13—C14—H14	119.2	O2—S1—C1	108.17 (6)
C15—C14—H14	119.2	N8—S1—C1	109.26 (6)
C14—C15—C16	118.02 (15)	C2—C1—C6	121.17 (13)
C14—C15—H15	121.0	C2—C1—S1	119.07 (10)
C16—C15—H15	121.0	C6—C1—S1	119.55 (10)
C15—C16—C11	120.29 (15)	C1—C2—C3	118.80 (13)
C15—C16—C26	130.92 (15)	C1—C2—H2	120.6
C11—C16—C26	108.77 (12)	C3—C2—H2	120.6
C22—C21—C26	119.77 (13)	C2—C3—C4	121.18 (13)
C22—C21—C7	132.65 (13)	C2—C3—H3	119.4
C26—C21—C7	107.54 (12)	C4—C3—H3	119.4
C21—C22—C23	118.84 (14)	C3—C4—C5	118.73 (13)
C21—C22—H22	120.6	C3—C4—C41	120.79 (13)
C23—C22—H22	120.6	C5—C4—C41	120.48 (13)
C24—C23—C22	121.00 (15)	C6—C5—C4	121.09 (13)
C24—C23—H23	119.5	C6—C5—H5	119.5
C22—C23—H23	119.5	C4—C5—H5	119.5
C25—C24—C23	120.84 (14)	C5—C6—C1	119.00 (13)
C25—C24—H24	119.6	C5—C6—H6	120.5
C23—C24—H24	119.6	C1—C6—H6	120.5
C26—C25—C24	118.57 (14)	C4—C41—H41A	109.5
C26—C25—H25	120.7	C4—C41—H41B	109.5
C24—C25—H25	120.7	H41A—C41—H41B	109.5
C25—C26—C21	120.93 (14)	C4—C41—H41C	109.5
C25—C26—C16	130.19 (13)	H41A—C41—H41C	109.5
C21—C26—C16	108.88 (13)	H41B—C41—H41C	109.5
N7—C7—C11	120.27 (13)		

C16—C11—C12—C13	−0.4 (2)	C12—C11—C7—C21	176.23 (14)
C7—C11—C12—C13	−178.44 (13)	C16—C11—C7—C21	−2.00 (14)
C11—C12—C13—C14	−0.4 (2)	C22—C21—C7—N7	2.4 (3)
C12—C13—C14—C15	0.4 (2)	C26—C21—C7—N7	−175.65 (14)
C13—C14—C15—C16	0.3 (2)	C22—C21—C7—C11	−179.86 (14)
C14—C15—C16—C11	−1.1 (2)	C26—C21—C7—C11	2.13 (14)
C14—C15—C16—C26	176.96 (14)	C11—C7—N7—N8	178.55 (11)
C12—C11—C16—C15	1.2 (2)	C21—C7—N7—N8	−3.9 (2)
C7—C11—C16—C15	179.58 (12)	C7—N7—N8—S1	169.89 (9)
C12—C11—C16—C26	−177.29 (12)	N7—N8—S1—O1	−57.89 (10)
C7—C11—C16—C26	1.13 (15)	N7—N8—S1—O2	175.17 (9)

C26—C21—C22—C23	−1.9 (2)	N7—N8—S1—C1	60.38 (10)
C7—C21—C22—C23	−179.72 (14)	O1—S1—C1—C2	−27.20 (13)
C21—C22—C23—C24	1.1 (2)	O2—S1—C1—C2	102.92 (11)
C22—C23—C24—C25	1.0 (2)	N8—S1—C1—C2	−145.71 (11)
C23—C24—C25—C26	−2.1 (2)	O1—S1—C1—C6	158.00 (11)
C24—C25—C26—C21	1.3 (2)	O2—S1—C1—C6	−71.89 (12)
C24—C25—C26—C16	−178.06 (14)	N8—S1—C1—C6	39.49 (12)
C22—C21—C26—C25	0.8 (2)	C6—C1—C2—C3	1.7 (2)
C7—C21—C26—C25	179.07 (12)	S1—C1—C2—C3	−173.04 (10)
C22—C21—C26—C16	−179.79 (12)	C1—C2—C3—C4	−0.7 (2)
C7—C21—C26—C16	−1.48 (15)	C2—C3—C4—C5	−1.1 (2)
C15—C16—C26—C25	1.4 (3)	C2—C3—C4—C41	177.93 (13)
C11—C16—C26—C25	179.61 (14)	C3—C4—C5—C6	1.9 (2)
C15—C16—C26—C21	−178.00 (14)	C41—C4—C5—C6	−177.11 (13)
C11—C16—C26—C21	0.23 (15)	C4—C5—C6—C1	−0.9 (2)
C12—C11—C7—N7	−5.6 (2)	C2—C1—C6—C5	−0.9 (2)
C16—C11—C7—N7	176.12 (12)	S1—C1—C6—C5	173.81 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N8—H8···O2^{i}	0.88	2.14	2.9951 (15)	164

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.