IUCrData

ISSN 2414-3146

Received 28 August 2025
Accepted 5 September 2025

Edited by W. T. A. Harrison, University of Aberdeen, United Kingdom

Keywords: crystal structure; 4,4′-bridged dianilines; 4,4′-thiodianiline; shape-memory polymers and vitrimers.

CCDC reference: 2485505

Structural data: full structural data are available from iucrdata.iucr.org

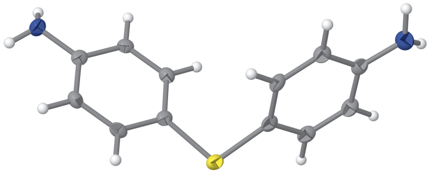
4-[(4-Aminophenyl)sulfanyl]aniline

Rao M. Uppu,[a]* Ogad A. Agu,[b] Patrick F. Mensah,[b] Guoqiang Li[c] and Frank R. Fronczek[d]

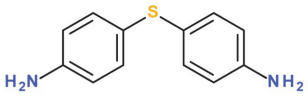
[a]Department of Environmental Toxicology, Southern University and A&M College, Baton Rouge, Louisiana 70813, USA, [b]Department of Mechanical Engineering, Southern University and A&M College, Baton Rouge, Louisiana 70813, USA, [c]Department of Mechanical and Industrial Engineering, Louisiana State University, Baton Rouge, Louisiana 70803, USA, and [d]Department of Chemistry, Louisiana State University, Baton Rouge, Louisiana, 70803, USA. *Correspondence e-mail: rao_uppu@subr.edu

The redetermined structure of the title compound, $C_{12}H_{12}N_2S$, was refined from low-temperature (100 K) single-crystal X-ray diffraction data. Although achiral, the compound crystallizes in Sohncke space group $P2_12_12_1$ in a chiral conformation distorted from idealized C_2 symmetry and the dihedral angle between the phenyl groups is 72.01 (7)°. In the extended structure, the NH_2 substituents participate in $N—H\cdots S$, $N—H\cdots N$, and $N—H\cdots\pi$ interactions, leading to a three-dimensional hydrogen-bonded array. These results highlight the role of sulfur bridges in tuning packing interactions relevant to polymer design.

3D view



Chemical scheme



Structure description

Bridged 4,4′-dianilines are important monomers for high-performance polymers. The nature of the bridging atom or functional group governs rigidity, polarity, and donor strength, which in turn affects curing kinetics, chain packing, and glass transition in dianiline-based polyimides, epoxides and related composites (Ghosh & Mittal, 1996; Sroog, 1991). Treated as *para* substituents on each aniline ring, classic Hammett/LFER considerations capture the quantitative electronic trend, namely –NH– > –O– > –S– > –CH_2– > –S(=O)– > –SO_2– (Hansch *et al.*, 1991). The sulfur bridge in the title compound imparts electronic and steric effects that modulate hydrogen bonding and curing behavior (Mazumder *et al.*, 2023). Such diamines are used in polyimides, epoxies, and dynamic polymer networks with shape-memory and vitrimer-like properties (Lendlein & Kelch, 2002; Xiao *et al.*, 2015; Winne *et al.*, 2019; Zi *et al.*, 2021).

The crystal structure of the title compound, $C_{12}H_{12}N_2S$, Fig. 1, was previously reported at room temperature based on film data (Vijayalakshmi & Srinivasan, 1973; Cambridge Structural Database refcode DAPHSD). The present study refines the structure at 100 K

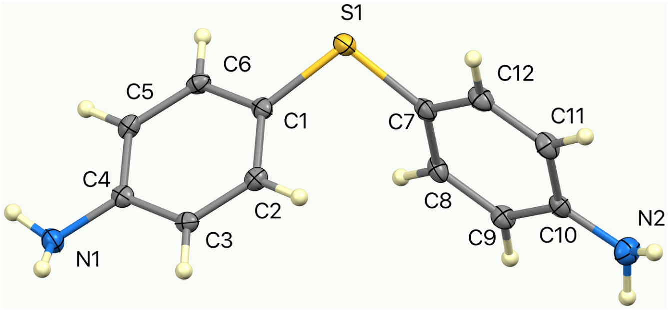


Figure 1
Molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

with modern instrumentation, providing more precise molecular geometry and intermolecular interaction details.

The molecule crystallizes in the Sohncke space group $P2_12_12_1$, adopting a chiral conformation. The phenyl groups are rotated unequally with respect to the central C—S—C plane, giving C_1 symmetry in the solid state. The dihedral angle between the C1–C6 and C7–C12 phenyl groups is 72.01 (7)°, while the individual dihedral angles with the C1—S1—C7 plane are 34.96 (8) and 52.35 (10)°, respectively. These distortions highlight the conformational flexibility of the sulfanyl bridge. The bond-angle sums at atoms N1 and N2 are 338.3 and 350.2°, respectively, suggesting that the latter atom has more sp^2 electronic character, which may correlate with the fact that the C10—N2 bond [1.377 (3) Å] is shorter than C4—N1 [1.407 (3) Å].

In the crystal, atom N1 donates a hydrogen bond (Table 1, Figs. 2, 3) to the sulfanyl sulfur atom of an adjacent molecule, while N2 accepts a hydrogen bond from a neighboring NH group. Additionally, one NH hydrogen atom is involved in an N—H$\cdots\pi$ interaction with a phenyl ring. These interactions generate a three-dimensional network of hydrogen bonds and π contacts, contributing to the stability of the packing arrangement. Graph sets for the conventional hydrogen bonds are a $C_1^1(7)$ chain in the [100] direction, a $C_2^2(9)$ chain in the [010] direction, and a $C_1^1(12)$ chain in the [001] direction.

The molecular geometry of the title compound reflects the distinctive influence of the sulfanyl bridge. The C—S—C linkage is longer and more flexible than the C—C bond in 4,4′-methylenedianiline (Bel'skii *et al.*, 1983; Gibson *et al.*, 2010; Uppu *et al.*, 2025*a*) and less bent but electronically softer than the C—O—C bridge in *N*,*N*′-[oxybis(benzene-4,1-diyl)]-diacetamide (Uppu *et al.*, 2025*b*) and 4,4′-oxydianiline (Sharma *et al.*, 2019; Uppu *et al.*, 2025*c*). In contrast, the SO_2 bridge in 4,4′-sulfonyldianiline (dapsone) (Karle & Karle, 1964; Uppu & Fronczek, 2025) introduces polarity and strong hydrogen bonding, markedly altering the packing. Thus, a systematic variation in the bridging unit (NH, O, S, CH_2, SO, SO_2) governs bond distances, torsional distortions, and intermolecular interactions, providing a framework for understanding the structure–property relationships of these technologically important dianilines.

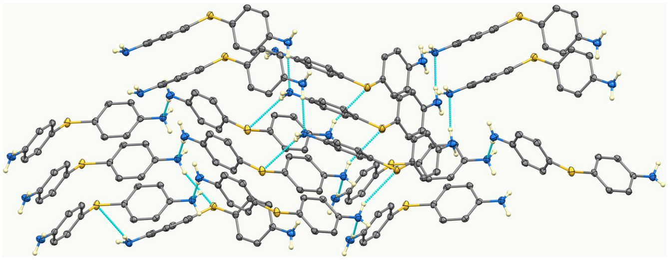


Figure 2
Hydrogen-bonding network in the title compound; only N-bound H atoms are shown.

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

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
N1—H11*N*$\cdots$S1^{i}	0.92 (3)	2.88 (3)	3.675 (2)	145 (2)
N1—H12*N*$\cdots$*Cg*2^{ii}	0.86 (3)	2.80 (3)	3.553 (2)	147 (3)
N2—H22*N*$\cdots$N1^{iii}	0.91 (3)	2.20 (3)	3.095 (3)	167 (3)

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

Synthesis and crystallization

4-[(4-Aminophenyl)sulfanyl]aniline (CAS 139–65-1) was purchased from AmBeed (Arlington Heights, IL, USA) with a reported purity of over 97% and used without further purification. Crystals suitable for X-ray analysis were grown by slow cooling hot aqueous solutions, yielding colorless needle-like crystals.

Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 2.

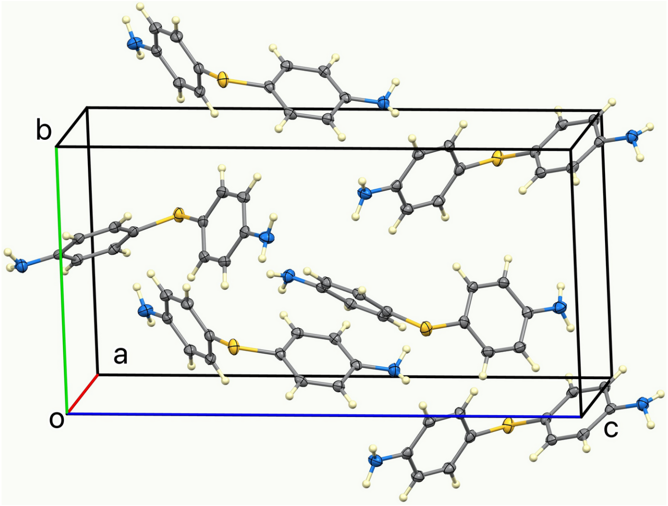


Figure 3
The unit cell of the title compound.

Funding information

Research was supported by the National Institutes of Health (NIGMS IDeA Program, Grant P20 GM103424–21), the US Department of Education (Title III), and the National Science Foundation (Grant No. 2418415 RII FEC). The diffractometer was purchased with NSF MRI award CHE–2215262.

References

Bel'skii, V. K., Rotaru, V. K. & Kruchinin, M. M. (1983). *Kristallografiya* **28**, 685–689.

Bruker (2016). *APEX5* and *SAINT* Bruker AXS Inc., Madison, Wisconsin, USA.

Ghosh, M. K. & Mittal, K. L. (1996). Editors. *Polyimides: Fundamentals and Applications*. New York: Marcel Dekker.

Gibson, E. K., Winfield, J. M., Muir, K. W., Carr, R. H., Eaglesham, A., Gavezzotti, A. & Lennon, D. (2010). *Phys. Chemi. Chem. Phys.* **12**, 3824–3833.

Hansch, C., Leo, A. & Taft, R. W. (1991). *Chem. Rev.* **91**, 165–195.

Karle, I. L. & Karle, J. (1964). *Acta Cryst.* **17**, 835–841.

Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.

Lendlein, A. & Kelch, S. (2002). *Angew. Chem. Int. Ed.* **41**, 2034–2057.

Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.

Mazumder, K., Bittrich, E., Voit, B. & Banerjee, S. (2023). *ACS Omega* **8**, 43236–43242.

Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.

Sharma, G., Anthal, S., Geetha, D. V., Al-Ostoot, F. H., Al-Gunaid, M. Q. A., Khanum, S. A., Sridhar, M. A. & Kant, R. (2019). *Rasayan J. Chem.* **12**, 2311–2317.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Sroog, C. E. (1991). *Prog. Polym. Sci.* **16**, 561–694.

Uppu, R. M., Agu, O. A., Babu, S., Mensah, P. F. & Fronczek, F. R. (2025*b*). *IUCrData* **10**, x250384.

Uppu, R. M., Agu, O. A., Mensah, P. F., Li, G. & Fronczek, F. R. (2025*a*). *CSD Communication* (CCDC 2481953). CCDC, Cambridge, England.

Uppu, R. M., Agu, O. A., Mensah, P. F., Li, G. & Fronczek, F. R. (2025*c*). *CSD Communication* (CCDC 2481952). CCDC, Cambridge, England.

Uppu, R. M. & Fronczek, F. R. (2025). *CSD Communication* (CCDC 2448841). CCDC, Cambridge, England.

Vijayalakshmi, B. K. & Srinivasan, R. (1973). *J. Cryst. Mol. Struct.* **3**, 147–155.

Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

Winne, J. M., Leibler, L. & Du Prez, F. E. (2019). *Chem. Rev.* **119**, 997–1049.

Xiao, X., Kong, D., Qiu, X., Zhang, W., Liu, Y., Zhang, S., Zhang, F., Hu, Y. & Leng, J. (2015). *Sci. Rep.* **5**, 14137.

Zi, Y., Pei, D., Wang, J., Qi, S., Tian, G. & Wu, D. (2021). *Polymers* (Basel) **13**, 3222.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{12}N_2S$
M_r	216.30
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	100
a, b, c (Å)	5.9287 (2), 9.8523 (3), 18.7766 (5)
V (Å^3)	1096.77 (6)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.34
Crystal size (mm)	0.34 × 0.06 × 0.04
Data collection	
Diffractometer	Bruker D8 Venture DUO with Photon III C14
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
$T_{\min}$, $T_{\max}$	0.727, 0.912
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13111, 2330, 2215
$R_{\rm int}$	0.043
$(\sin \theta/\lambda)_{\max}$ (Å^{-1})	0.637
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.028, 0.070, 1.07
No. of reflections	2330
No. of parameters	148
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å^{-3})	0.15, −0.23
Absolute structure	Flack x determined using 858 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.016 (9)

Computer programs: *APEX5* and *SAINT* (Bruker, 2016), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2019/1* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

IUCrData (2025). **10**, x250795 Uppu *et al.* • $C_{12}H_{12}N_2S$ **3 of 3**

full crystallographic data

IUCrData (2025). **10**, x250795 [https://doi.org/10.1107/S2414314625007953]

4-[(4-Aminophenyl)sulfanyl]aniline

Rao M. Uppu, Ogad A. Agu, Patrick F. Mensah, Guoqiang Li and Frank R. Fronczek

4-[(4-Aminophenyl)sulfanyl]aniline

Crystal data

$C_{12}H_{12}N_2S$
M_r = 216.30
Orthorhombic, $P2_12_12_1$
a = 5.9287 (2) Å
b = 9.8523 (3) Å
c = 18.7766 (5) Å
V = 1096.77 (6) Å^3
Z = 4
$F(000)$ = 456

D_x = 1.310 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 6002 reflections
θ = 5.1–79.3°
μ = 2.34 mm^{-1}
T = 100 K
Needle, colourless
0.34 × 0.06 × 0.04 mm

Data collection

Bruker D8 Venture DUO with Photon III C14 diffractometer
Radiation source: IμS 3.0 microfocus
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.727, T_{max} = 0.912
13111 measured reflections

2330 independent reflections
2215 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 79.3°, θ_{min} = 4.7°
$h = -7 \rightarrow 7$
$k = -12 \rightarrow 12$
$l = -23 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.070
S = 1.07
2330 reflections
148 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 0.160P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack x determined using 858 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.016 (9)

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. All H atoms were located in difference maps and those on C were thereafter treated as riding in geometrically idealized positions with C—H distances 0.95 Å. Coordinates of the NH hydrogen atoms were refined freely. U_{iso}(H) values were assigned as $1.2U_{\text{eq}}$ for the attached atom (1.5 for NH_2). The absolute structure (Parsons *et al.*, 2013) was determined using 858 quotients, $x = 0.016$ (9).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.02434 (8)	0.32288 (5)	0.70350 (3)	0.02444 (15)
N1	0.4024 (3)	0.46157 (19)	0.41708 (10)	0.0235 (4)
H11N	0.495 (5)	0.397 (3)	0.3971 (14)	0.035*
H21N	0.801 (5)	0.215 (3)	0.9358 (14)	0.035*
N2	0.7632 (3)	0.29720 (19)	0.91853 (11)	0.0264 (4)
H12N	0.296 (6)	0.484 (3)	0.3881 (16)	0.040*
H22N	0.878 (5)	0.359 (3)	0.9154 (15)	0.040*
C1	0.1541 (4)	0.3678 (2)	0.62144 (11)	0.0187 (4)
C2	0.3648 (3)	0.3204 (2)	0.59946 (11)	0.0190 (4)
H2	0.452849	0.265918	0.630629	0.023*
C3	0.4461 (3)	0.35248 (19)	0.53226 (11)	0.0185 (4)
H3	0.590611	0.320796	0.518102	0.022*
C4	0.3188 (4)	0.43047 (19)	0.48526 (11)	0.0182 (4)
C5	0.1109 (4)	0.4804 (2)	0.50778 (12)	0.0192 (4)
H5	0.023750	0.535640	0.476755	0.023*
C6	0.0302 (4)	0.44981 (19)	0.57538 (11)	0.0193 (4)
H6	−0.111145	0.485218	0.590355	0.023*
C7	0.2534 (4)	0.3146 (2)	0.76396 (11)	0.0208 (4)
C8	0.4022 (4)	0.4232 (2)	0.77322 (11)	0.0210 (5)
H8	0.385394	0.502546	0.744986	0.025*
C9	0.5729 (4)	0.41644 (19)	0.82279 (11)	0.0212 (5)
H9	0.673852	0.490715	0.827738	0.025*
C10	0.6002 (4)	0.3010 (2)	0.86635 (11)	0.0200 (4)
C11	0.4482 (4)	0.1934 (2)	0.85710 (11)	0.0236 (4)
H11	0.461301	0.114997	0.886228	0.028*
C12	0.2797 (4)	0.1995 (2)	0.80637 (11)	0.0234 (5)
H12	0.180799	0.124541	0.800321	0.028*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0210 (2)	0.0331 (3)	0.0192 (3)	−0.0047 (2)	0.0034 (2)	−0.0010 (2)
N1	0.0250 (10)	0.0259 (9)	0.0197 (10)	0.0004 (8)	0.0027 (8)	0.0011 (7)
N2	0.0280 (10)	0.0207 (9)	0.0303 (11)	0.0011 (8)	−0.0029 (9)	0.0037 (8)
C1	0.0200 (10)	0.0188 (9)	0.0172 (10)	−0.0034 (8)	0.0010 (8)	−0.0038 (8)
C2	0.0194 (9)	0.0168 (9)	0.0209 (11)	0.0007 (8)	−0.0022 (8)	−0.0014 (8)
C3	0.0162 (9)	0.0185 (9)	0.0207 (10)	−0.0008 (7)	0.0012 (8)	−0.0045 (7)
C4	0.0206 (10)	0.0150 (9)	0.0191 (11)	−0.0029 (7)	0.0008 (9)	−0.0040 (8)
C5	0.0198 (10)	0.0183 (9)	0.0195 (11)	0.0017 (7)	−0.0046 (9)	−0.0017 (8)
C6	0.0154 (9)	0.0198 (9)	0.0227 (11)	0.0020 (8)	−0.0012 (9)	−0.0057 (8)

C7	0.0241 (10)	0.0229 (9)	0.0154 (10)	−0.0020 (9)	0.0051 (8)	−0.0029 (8)
C8	0.0284 (11)	0.0184 (9)	0.0163 (11)	−0.0026 (8)	0.0037 (9)	0.0012 (8)
C9	0.0255 (11)	0.0170 (9)	0.0211 (11)	−0.0029 (8)	0.0024 (9)	−0.0012 (8)
C10	0.0219 (10)	0.0204 (9)	0.0176 (10)	0.0018 (8)	0.0048 (8)	−0.0024 (8)
C11	0.0305 (11)	0.0174 (9)	0.0230 (11)	−0.0002 (9)	0.0035 (9)	0.0021 (8)
C12	0.0285 (10)	0.0184 (9)	0.0233 (12)	−0.0045 (8)	0.0051 (9)	−0.0011 (8)

Geometric parameters (Å, º)

S1—C7	1.772 (2)	C4—C5	1.393 (3)
S1—C1	1.778 (2)	C5—C6	1.390 (3)
N1—C4	1.407 (3)	C5—H5	0.9500
N1—H11N	0.92 (3)	C6—H6	0.9500
N1—H12N	0.86 (3)	C7—C12	1.394 (3)
N2—C10	1.377 (3)	C7—C8	1.398 (3)
N2—H21N	0.90 (3)	C8—C9	1.376 (3)
N2—H22N	0.91 (3)	C8—H8	0.9500
C1—C6	1.393 (3)	C9—C10	1.410 (3)
C1—C2	1.397 (3)	C9—H9	0.9500
C2—C3	1.387 (3)	C10—C11	1.402 (3)
C2—H2	0.9500	C11—C12	1.382 (3)
C3—C4	1.392 (3)	C11—H11	0.9500
C3—H3	0.9500	C12—H12	0.9500
C7—S1—C1	103.60 (10)	C5—C6—C1	120.75 (19)
C4—N1—H11N	115.4 (16)	C5—C6—H6	119.6
C4—N1—H12N	112 (2)	C1—C6—H6	119.6
H11N—N1—H12N	111 (3)	C12—C7—C8	118.7 (2)
C10—N2—H21N	117.1 (18)	C12—C7—S1	119.29 (16)
C10—N2—H22N	117.3 (19)	C8—C7—S1	121.90 (16)
H21N—N2—H22N	116 (3)	C9—C8—C7	120.76 (18)
C6—C1—C2	118.9 (2)	C9—C8—H8	119.6
C6—C1—S1	117.02 (16)	C7—C8—H8	119.6
C2—C1—S1	124.03 (17)	C8—C9—C10	121.04 (19)
C3—C2—C1	120.20 (19)	C8—C9—H9	119.5
C3—C2—H2	119.9	C10—C9—H9	119.5
C1—C2—H2	119.9	N2—C10—C11	121.24 (19)
C2—C3—C4	120.95 (19)	N2—C10—C9	121.04 (19)
C2—C3—H3	119.5	C11—C10—C9	117.6 (2)
C4—C3—H3	119.5	C12—C11—C10	121.15 (19)
C3—C4—C5	118.8 (2)	C12—C11—H11	119.4
C3—C4—N1	120.41 (19)	C10—C11—H11	119.4
C5—C4—N1	120.7 (2)	C11—C12—C7	120.7 (2)
C6—C5—C4	120.4 (2)	C11—C12—H12	119.7
C6—C5—H5	119.8	C7—C12—H12	119.7
C4—C5—H5	119.8		
C7—S1—C1—C6	−146.49 (16)	C1—S1—C7—C12	−129.04 (17)

C7—S1—C1—C2	36.99 (19)	C1—S1—C7—C8	54.41 (19)
C6—C1—C2—C3	−1.3 (3)	C12—C7—C8—C9	0.6 (3)
S1—C1—C2—C3	175.15 (15)	S1—C7—C8—C9	177.12 (16)
C1—C2—C3—C4	−0.9 (3)	C7—C8—C9—C10	−1.0 (3)
C2—C3—C4—C5	2.4 (3)	C8—C9—C10—N2	−176.5 (2)
C2—C3—C4—N1	−179.57 (18)	C8—C9—C10—C11	0.3 (3)
C3—C4—C5—C6	−1.6 (3)	N2—C10—C11—C12	177.7 (2)
N1—C4—C5—C6	−179.62 (18)	C9—C10—C11—C12	0.9 (3)
C4—C5—C6—C1	−0.7 (3)	C10—C11—C12—C7	−1.4 (3)
C2—C1—C6—C5	2.1 (3)	C8—C7—C12—C11	0.7 (3)
S1—C1—C6—C5	−174.60 (15)	S1—C7—C12—C11	−175.99 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H11*N*···S1$^{\mathrm{i}}$	0.92 (3)	2.88 (3)	3.675 (2)	145 (2)
N1—H12*N*···*Cg*2$^{\mathrm{ii}}$	0.86 (3)	2.80 (3)	3.553 (2)	147 (3)
N2—H22*N*···N1$^{\mathrm{iii}}$	0.91 (3)	2.20 (3)	3.095 (3)	167 (3)

Symmetry codes: (i) *x*+1/2, −*y*+1/2, −*z*+1; (ii) −*x*+1/2, −*y*+1, *z*−1/2; (iii) −*x*+3/2, −*y*+1, *z*+1/2.