

# Dipropylammonium 4-aminobenzenesulfonate

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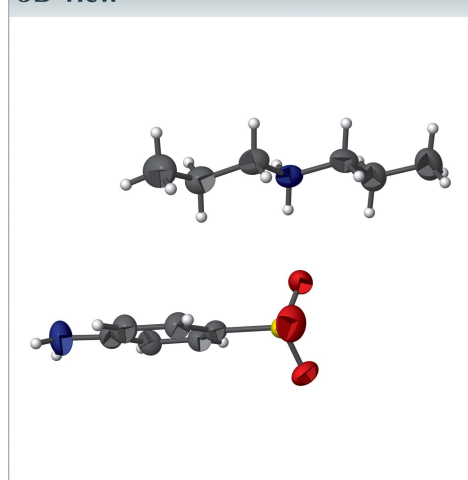
Keywords: crystal structure; hydrogen bonds; sulfanilate.

CCDC reference: 2004571

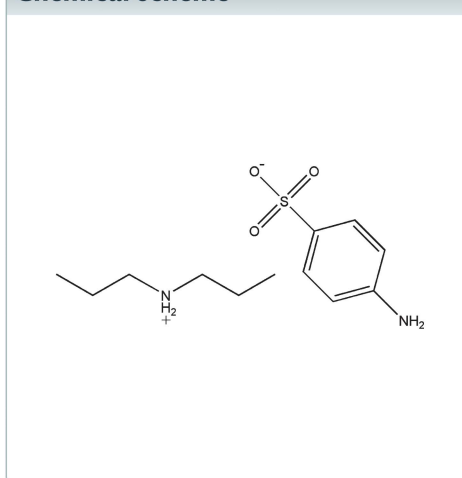
Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

In the title molecular salt,  $\text{NH}_2(\text{C}_3\text{H}_7)_2^+ \cdot [\text{NH}_2\text{C}_6\text{H}_4\text{SO}_3]^-$ , the cation displays an extended conformation. In the crystal, anion-to-anion  $\text{N}-\text{H} \cdots \text{O}$  and  $\text{N}-\text{H} \cdots (\text{O}, \text{O})$  hydrogen bonds generate (101) layers. Cation-to-anion  $\text{N}-\text{H} \cdots \text{O}$  hydrogen bonds connect the layers into a three-dimensional network.

## 3D view



## Chemical scheme

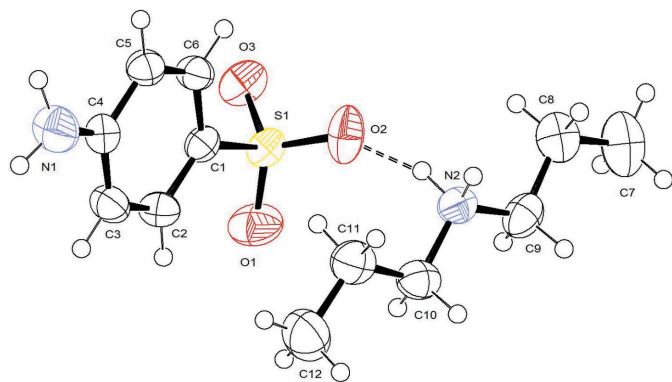


## Structure description

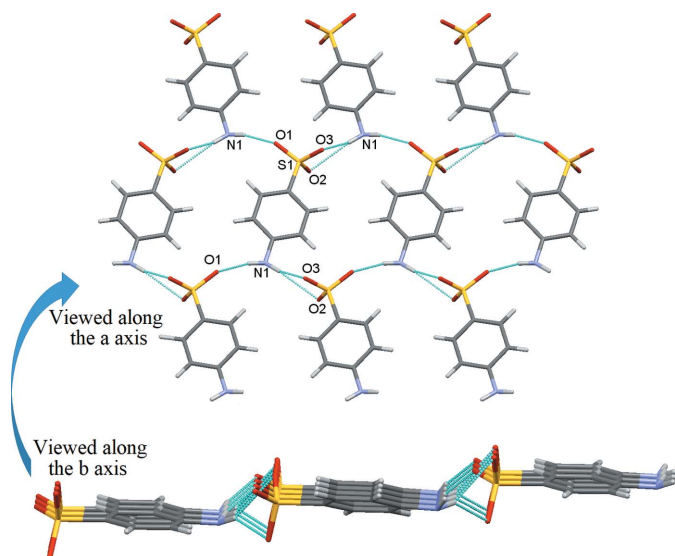
Some sulfanilate-based compounds have high optical non-linearity and may be candidates for applications in optoelectronics and photonics in combination with organic cations such as guanidinium (Russell *et al.*, 1994), triethylammonium (Li *et al.*, 2007), diisopropylammonium (Sarr *et al.*, 2016) and cyclohexylammonium (Kama *et al.*, 2019). As part of our ongoing studies in this area (Sarr *et al.*, 2016), we now describe the synthesis and crystal structure of the title molecular salt, which crystallizes in the non-centrosymmetric space group  $Pn$ .

The asymmetric unit, shown in Fig. 1, consists of one dipropylammonium  $\text{NH}_2(\text{C}_3\text{H}_7)_2^+$  cation and one 4-aminobenzenesulfonate  $[\text{NH}_2\text{C}_6\text{H}_4\text{SO}_3]^-$  anion. The cation adopts an extended structure with a minimum torsion angle of  $174.7 (4)^\circ$  for  $\text{N}2-\text{C}10-\text{C}11-\text{C}12$ . The involvement of the oxygen atoms of the sulfonate group in the anion as hydrogen-bond acceptors is manifested in a slight difference in the  $\text{S}-\text{O}$  bond lengths [ $\text{S}1-\text{O}1 = 1.446 (2)$ ,  $\text{S}1-\text{O}2 = 1.454 (2)$ ,  $\text{S}1-\text{O}3 = 1.449 (2)$  Å]; these data are consistent with those in sulfanilate anions previously reported (Sarr *et al.*, 2016; Kama *et al.*, 2019).

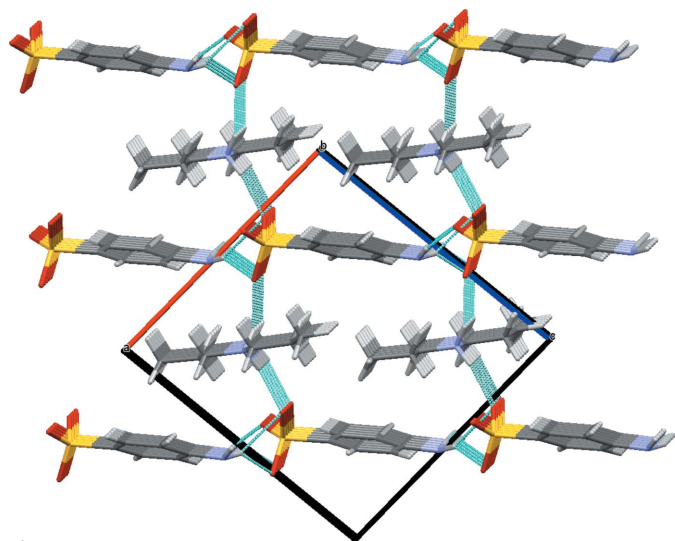
In the extended structure, each sulfanilate anion interacts with four neighbours *via* simple  $\text{N}-\text{H} \cdots \text{O}$  and bifurcated  $\text{N}-\text{H} \cdots (\text{O}, \text{O})$  hydrogen bonds (Table 1) to generate (101) layers (Fig. 2). The dipropylammonium cations play the role of bridges between the infinite anion layers *via* cation-to-anion  $\text{N}-\text{H} \cdots \text{O}$  hydrogen bonds (Fig. 3) to generate a



**Figure 1**  
The asymmetric unit with displacement ellipsoids drawn at the 50% probability level. The N2–H2B···O2 hydrogen bond is shown as a dashed line.



**Figure 2**  
A perspective view of an infinite layer, viewed along the *a* and *b* axes.



**Figure 3**  
The packing viewed along [010].

**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>
N1–H1A···O2 <sup>i</sup>	0.90 (2)	2.39 (3)	3.196 (4)	149 (4)
N1–H1A···O3 <sup>i</sup>	0.90 (2)	2.49 (3)	3.313 (4)	153 (4)
N1–H1B···O1 <sup>iii</sup>	0.88 (2)	2.08 (2)	2.940 (4)	165 (4)
N2–H2A···O3 <sup>iii</sup>	0.91 (2)	1.91 (2)	2.801 (3)	164 (3)
N2–H2B···O2	0.90 (2)	1.95 (3)	2.786 (3)	154 (3)

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

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	$C_6H_{16}N^+ \cdot C_6H_6NO_3S^-$
$M_r$	274.38
Crystal system, space group	Monoclinic, <i>Pn</i>
Temperature (K)	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	10.2564 (7), 6.5369 (5), 10.9683 (9)
$\beta$ (°)	95.067 (7)
<i>V</i> (Å <sup>3</sup> )	732.50 (10)
<i>Z</i>	2
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.22
Crystal size (mm)	0.38 × 0.28 × 0.19
Data collection	
Diffractometer	Agilent Xcalibur, Sapphire2
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2008)
$T_{min}$ , $T_{max}$	0.669, 0.746
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	21351, 4018, 3387
$R_{int}$	0.149
$(\sin \theta/\lambda)_{max}$ (Å <sup>-1</sup> )	0.699
Refinement	
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , $S$	0.039, 0.097, 1.17
No. of reflections	4018
No. of parameters	181
No. of restraints	13
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ , $\Delta\rho_{min}$ (e Å <sup>-3</sup> )	0.21, -0.28
Absolute structure	Flack (1983)
Absolute structure parameter	0.09 (6)

Computer programs: *SHELXT* (Sheldrick, 2015), *SHELXL97* (Sheldrick, 2008), *OLEX2* (Dolomanov *et al.*, 2009) *ORTEP-3 for Windows* (Farrugia, 2012) *Mercury* (Macrae *et al.*, 2020), *OLEX2* (Dolomanov *et al.*, 2009), *WinGX* (Farrugia, 2012), *PLATON* (Spek, 2020), *enCIFer* (Allen *et al.*, 2004).

three-dimensional network. Each sulfanilate anion is thus surrounded by four anions and two cations.

### Synthesis and crystallization

A 1:2 mixture of sulfanilic acid (1.00 g, 5.80 mmol) and dipropylamine (1.16 g, 11.50 mmol) was dissolved in water and the colourless solution obtained was stirred for an hour. After a few days of evaporation in an oven at 333 K, some yellowish crystals were collected from the solution and then dried in air. The IR spectrum and peak assignments are given in the supporting information.

## Refinement

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

## Acknowledgements

The authors thank the Laboratoire de Chimie Minérale et Analytique, Département de Chimie, Faculté des Sciences et Techniques, Université Cheikh Anta Diop de Dakar, Sénégal, the Laboratoire de Chimie et de Physique des Matériaux (LCPM) de l'Université Assane Seck de Ziguinchor (UASZ), Sénégal and the Service Commun d'Analyse par Diffraction des Rayons X, Université de Bretagne Occidentale, France for financial support.

## References

- Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). *J. Appl. Cryst.* **37**, 335–338.
- Bruker (2008). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Kama, A. B., Génois, R., Massuyeau, F., Sidibé, M., Diop, C. A. K. & Gautier, R. (2019). *Mater. Lett.* **241**, 6–9.
- Li, J., Liang, Z.-P. & Guo, H.-M. (2007). *Acta Cryst.* **E63**, o2884.
- 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.
- Russell, V. A., Etter, M. C. & Ward, M. D. (1994). *Chem. Mater.* **6**, 1206–1217.
- Sarr, B., Diop, C. A. K., Diop, L., Blanchard, F. & Michaud, F. (2016). *IUCrData*, **1**, x161545.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Spek, A. L. (2020). *Acta Cryst.* **E76**, 1–11.

## full crystallographic data

*IUCrData* (2020). 5, x200659 [https://doi.org/10.1107/S2414314620006598]

## Dipropylammonium 4-aminobenzenesulfonate

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## Dipropylazanium 4-aminobenzenesulfonate

*Crystal data*

$C_6H_{16}N^+ \cdot C_6H_6NO_3S^-$

$M_r = 274.38$

Monoclinic,  $Pn$

$a = 10.2564$  (7) Å

$b = 6.5369$  (5) Å

$c = 10.9683$  (9) Å

$\beta = 95.067$  (7)°

$V = 732.50$  (10) Å<sup>3</sup>

$Z = 2$

$F(000) = 296$

$D_x = 1.244$  Mg m<sup>-3</sup>

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

Cell parameters from 38522 reflections

$\theta = 3.5\text{--}37.4^\circ$

$\mu = 0.22$  mm<sup>-1</sup>

$T = 293$  K

Block, clear light colourless

$0.38 \times 0.28 \times 0.19$  mm

*Data collection*

Agilent Xcalibur, Sapphire2  
diffractometer

Graphite monochromator

$\omega$  scans

Absorption correction: multi-scan  
(SADABS; Bruker, 2008)

$T_{\min} = 0.669$ ,  $T_{\max} = 0.746$

21351 measured reflections

4018 independent reflections

3387 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.149$

$\theta_{\max} = 29.8^\circ$ ,  $\theta_{\min} = 6.4^\circ$

$h = -13 \rightarrow 14$

$k = -9 \rightarrow 9$

$l = -15 \rightarrow 15$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.097$

$S = 1.17$

4018 reflections

181 parameters

13 restraints

34 constraints

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

$w = 1/[\sigma^2(F_o^2) + (0.P)^2 + 0.0621P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.003$

$\Delta\rho_{\max} = 0.21$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.28$  e Å<sup>-3</sup>

Absolute structure: Flack (1983)

Absolute structure parameter: 0.09 (6)

*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  $F^2 > 2\sigma(F^2)$  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. The C-bound H atoms were geometrically placed and refined as riding atoms. The N-bound H atoms were located in difference maps and their positions were freely refined.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2799 (2)	0.3112 (4)	0.2052 (2)	0.0367 (5)
C2	0.2417 (3)	0.1097 (4)	0.2172 (3)	0.0445 (6)
H2	0.265741	0.011733	0.161908	0.053*
C3	0.1673 (3)	0.0538 (4)	0.3118 (3)	0.0478 (6)
H3	0.142230	-0.082099	0.319082	0.057*
C4	0.1296 (3)	0.1968 (4)	0.3958 (2)	0.0422 (6)
C5	0.1670 (3)	0.4010 (4)	0.3810 (3)	0.0437 (6)
H5	0.141106	0.500353	0.434520	0.052*
C6	0.2419 (3)	0.4561 (4)	0.2879 (2)	0.0413 (6)
H6	0.267171	0.591786	0.280253	0.050*
N1	0.0600 (3)	0.1413 (5)	0.4919 (3)	0.0648 (8)
O1	0.3872 (3)	0.2145 (4)	0.0083 (2)	0.0685 (7)
O2	0.4990 (2)	0.4606 (4)	0.1461 (2)	0.0629 (6)
O3	0.3054 (2)	0.5583 (3)	0.02517 (18)	0.0554 (6)
H1A	0.012 (4)	0.243 (5)	0.520 (4)	0.088 (14)*
H1B	0.018 (3)	0.024 (5)	0.488 (4)	0.072 (12)*
C7	0.9403 (4)	0.6507 (8)	0.1124 (4)	0.0829 (12)
H7A	0.909563	0.612015	0.030421	0.124*
H7B	1.021641	0.582605	0.135713	0.124*
H7C	0.953392	0.796103	0.116045	0.124*
C8	0.8400 (3)	0.5899 (5)	0.1991 (3)	0.0614 (9)
H8A	0.867832	0.640996	0.280284	0.074*
H8B	0.757055	0.654361	0.172644	0.074*
C9	0.8201 (3)	0.3642 (5)	0.2060 (3)	0.0530 (7)
H9A	0.901763	0.299306	0.235920	0.064*
H9B	0.794755	0.311445	0.124654	0.064*
C10	0.6895 (3)	0.0913 (5)	0.3018 (3)	0.0516 (8)
H10A	0.768416	0.021660	0.334665	0.062*
H10B	0.663027	0.033385	0.221981	0.062*
C11	0.5834 (4)	0.0585 (5)	0.3850 (3)	0.0591 (8)
H11A	0.507946	0.140033	0.355995	0.071*
H11B	0.613660	0.106484	0.466270	0.071*
C12	0.5419 (4)	-0.1628 (7)	0.3930 (5)	0.0802 (12)
H12A	0.512348	-0.211830	0.312830	0.120*

H12B	0.472165	-0.173525	0.445549	0.120*
H12C	0.614985	-0.243529	0.425863	0.120*
N2	0.7169 (2)	0.3125 (4)	0.2888 (2)	0.0435 (5)
S1	0.37479 (6)	0.38949 (10)	0.08711 (6)	0.04080 (17)
H2A	0.734 (3)	0.372 (4)	0.364 (2)	0.064 (10)*
H2B	0.644 (2)	0.382 (4)	0.264 (3)	0.069 (12)*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0348 (12)	0.0419 (13)	0.0332 (11)	0.0043 (10)	0.0018 (9)	0.0014 (9)
C2	0.0517 (17)	0.0382 (13)	0.0438 (14)	0.0021 (11)	0.0060 (12)	-0.0044 (11)
C3	0.0528 (16)	0.0376 (13)	0.0533 (16)	-0.0064 (12)	0.0073 (13)	-0.0001 (12)
C4	0.0381 (13)	0.0457 (14)	0.0427 (13)	-0.0032 (11)	0.0033 (11)	0.0007 (11)
C5	0.0461 (15)	0.0431 (14)	0.0427 (14)	-0.0006 (11)	0.0087 (12)	-0.0080 (10)
C6	0.0455 (14)	0.0349 (12)	0.0437 (14)	-0.0006 (10)	0.0049 (12)	-0.0033 (10)
N1	0.072 (2)	0.0622 (18)	0.0641 (18)	-0.0099 (15)	0.0292 (16)	0.0007 (14)
O1	0.0877 (17)	0.0627 (14)	0.0594 (13)	0.0110 (13)	0.0303 (12)	-0.0067 (12)
O2	0.0394 (11)	0.0936 (17)	0.0546 (12)	-0.0071 (11)	-0.0020 (10)	0.0245 (12)
O3	0.0606 (13)	0.0637 (13)	0.0416 (11)	0.0157 (11)	0.0023 (10)	0.0158 (10)
C7	0.066 (2)	0.116 (3)	0.065 (2)	-0.023 (2)	0.0032 (19)	0.010 (2)
C8	0.061 (2)	0.073 (2)	0.0502 (17)	-0.0077 (17)	0.0041 (16)	0.0003 (15)
C9	0.0443 (16)	0.069 (2)	0.0448 (15)	0.0084 (14)	0.0000 (13)	-0.0059 (13)
C10	0.058 (2)	0.0487 (17)	0.0464 (16)	0.0045 (13)	-0.0052 (14)	-0.0062 (12)
C11	0.062 (2)	0.0575 (19)	0.0567 (18)	0.0025 (16)	-0.0017 (16)	0.0008 (15)
C12	0.075 (3)	0.068 (2)	0.096 (3)	-0.010 (2)	0.000 (2)	0.012 (2)
N2	0.0454 (12)	0.0454 (13)	0.0383 (11)	0.0061 (11)	-0.0038 (9)	-0.0062 (10)
S1	0.0402 (3)	0.0483 (3)	0.0339 (3)	0.0074 (3)	0.0033 (2)	0.0044 (3)

*Geometric parameters (Å, °)*

C1—C2	1.384 (3)	C7—C8	1.515 (5)
C1—C6	1.391 (3)	C8—H8A	0.9700
C1—S1	1.763 (3)	C8—H8B	0.9700
C2—H2	0.9300	C8—C9	1.492 (5)
C2—C3	1.390 (4)	C9—H9A	0.9700
C3—H3	0.9300	C9—H9B	0.9700
C3—C4	1.391 (4)	C9—N2	1.493 (4)
C4—C5	1.402 (4)	C10—H10A	0.9700
C4—N1	1.373 (4)	C10—H10B	0.9700
C5—H5	0.9300	C10—C11	1.496 (5)
C5—C6	1.378 (4)	C10—N2	1.483 (4)
C6—H6	0.9300	C11—H11A	0.9700
N1—H1A	0.90 (2)	C11—H11B	0.9700
N1—H1B	0.88 (2)	C11—C12	1.513 (5)
O1—S1	1.446 (2)	C12—H12A	0.9600
O2—S1	1.454 (2)	C12—H12B	0.9600
O3—S1	1.449 (2)	C12—H12C	0.9600

C7—H7A	0.9600	N2—H2A	0.91 (2)
C7—H7B	0.9600	N2—H2B	0.90 (2)
C7—H7C	0.9600		
C2—C1—C6	119.2 (2)	C8—C9—N2	111.2 (2)
C2—C1—S1	121.7 (2)	H9A—C9—H9B	108.0
C6—C1—S1	119.1 (2)	N2—C9—H9A	109.4
C1—C2—H2	120.0	N2—C9—H9B	109.4
C1—C2—C3	120.0 (3)	H10A—C10—H10B	108.1
C3—C2—H2	120.0	C11—C10—H10A	109.5
C2—C3—H3	119.3	C11—C10—H10B	109.5
C2—C3—C4	121.4 (3)	N2—C10—H10A	109.5
C4—C3—H3	119.3	N2—C10—H10B	109.5
C3—C4—C5	117.9 (2)	N2—C10—C11	110.7 (3)
N1—C4—C3	121.6 (3)	C10—C11—H11A	108.9
N1—C4—C5	120.4 (3)	C10—C11—H11B	108.9
C4—C5—H5	119.6	C10—C11—C12	113.3 (3)
C6—C5—C4	120.7 (2)	H11A—C11—H11B	107.7
C6—C5—H5	119.6	C12—C11—H11A	108.9
C1—C6—H6	119.6	C12—C11—H11B	108.9
C5—C6—C1	120.8 (2)	C11—C12—H12A	109.5
C5—C6—H6	119.6	C11—C12—H12B	109.5
C4—N1—H1A	114 (3)	C11—C12—H12C	109.5
C4—N1—H1B	118 (3)	H12A—C12—H12B	109.5
H1A—N1—H1B	113 (4)	H12A—C12—H12C	109.5
H7A—C7—H7B	109.5	H12B—C12—H12C	109.5
H7A—C7—H7C	109.5	C9—N2—H2A	112 (2)
H7B—C7—H7C	109.5	C9—N2—H2B	109 (2)
C8—C7—H7A	109.5	C10—N2—C9	115.5 (2)
C8—C7—H7B	109.5	C10—N2—H2A	110.4 (19)
C8—C7—H7C	109.5	C10—N2—H2B	111 (2)
C7—C8—H8A	108.9	H2A—N2—H2B	98 (3)
C7—C8—H8B	108.9	O1—S1—C1	107.05 (13)
H8A—C8—H8B	107.7	O1—S1—O2	113.52 (17)
C9—C8—C7	113.2 (3)	O1—S1—O3	112.81 (14)
C9—C8—H8A	108.9	O2—S1—C1	106.52 (12)
C9—C8—H8B	108.9	O3—S1—C1	106.58 (12)
C8—C9—H9A	109.4	O3—S1—O2	109.88 (15)
C8—C9—H9B	109.4		
C1—C2—C3—C4	0.1 (4)	C6—C1—S1—O1	-173.8 (2)
C2—C1—C6—C5	0.1 (4)	C6—C1—S1—O2	64.5 (2)
C2—C1—S1—O1	5.8 (3)	C6—C1—S1—O3	-52.8 (2)
C2—C1—S1—O2	-116.0 (2)	N1—C4—C5—C6	177.1 (3)
C2—C1—S1—O3	126.7 (2)	C7—C8—C9—N2	-177.9 (3)
C2—C3—C4—C5	1.1 (4)	C8—C9—N2—C10	179.9 (3)
C2—C3—C4—N1	-177.7 (3)	C11—C10—N2—C9	-179.1 (3)
C3—C4—C5—C6	-1.7 (4)	N2—C10—C11—C12	174.7 (3)

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C4—C5—C6—C1	1.2 (4)	S1—C1—C2—C3	179.8 (2)
C6—C1—C2—C3	-0.7 (4)	S1—C1—C6—C5	179.6 (2)

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*Hydrogen-bond geometry (Å, °)*

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<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>
N1—H1A···O2 <sup>i</sup>	0.90 (2)	2.39 (3)	3.196 (4)	149 (4)
N1—H1A···O3 <sup>i</sup>	0.90 (2)	2.49 (3)	3.313 (4)	153 (4)
N1—H1B···O1 <sup>ii</sup>	0.88 (2)	2.08 (2)	2.940 (4)	165 (4)
N2—H2A···O3 <sup>iii</sup>	0.91 (2)	1.91 (2)	2.801 (3)	164 (3)
N2—H2B···O2	0.90 (2)	1.95 (3)	2.786 (3)	154 (3)

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