

1165 reflections	Scattering factors from
116 parameters	Stewart, Davidson &
All H atoms refined	Simpson (1965) (H)
$w = 1/\sigma^2(F)$	and Creagh & McAuley
$(\Delta/\sigma)_{\max} < 0.01$	(1992) (C, N, O)
$\Delta\rho_{\max} = 0.24 \text{ e } \text{\AA}^{-3}$	
$\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$	

Table 1. Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

O1—C7	1.234 (2)	C2—C3	1.423 (2)
O2—C7	1.266 (2)	C3—C4	1.374 (3)
N1—C2	1.360 (2)	C3—C7	1.514 (2)
N1—C6	1.348 (2)	C4—C5	1.398 (3)
N2—C2	1.322 (2)	C5—C6	1.355 (3)
C2—N1—C6	122.5 (2)	O1—C7—C3	117.4 (2)
O1—C7—O2	125.6 (2)	O2—C7—C3	116.9 (2)

Table 2. Hydrogen bonds and significant C—H...O interactions in 2-aminonicotinic acid at 296 K ( $\text{\AA}$ ,  $^\circ$ )

D—H...A	D—H	H...A	D...A	D—H...A
N1—H1...O2 <sup>i</sup>	0.96 (2)	1.70 (2)	2.652 (2)	174 (2)
N2—H2...O1 <sup>j</sup>	0.88 (2)	1.93 (2)	2.807 (2)	173 (2)
N2—H3...O2	0.94 (3)	1.88 (3)	2.651 (2)	137 (2)
C4—H4...O1 <sup>ii</sup>	0.97 (2)	2.87 (2)	3.713 (2)	146 (1)
C5—H5...O2 <sup>iii</sup>	0.91 (2)	3.18 (2)	3.847 (3)	131 (2)
C6—H6...O1 <sup>iv</sup>	1.02 (2)	3.28 (2)	3.506 (3)	94 (1)

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

Table 3. First- and second-level graph-set descriptors involving hydrogen bonds designated a–c as described in the text

	a	b	c
a	C(6)	C <sub>2</sub> <sup>2</sup> (6) [R <sub>2</sub> <sup>2</sup> (8)]	C <sub>2</sub> <sup>1</sup> (6)
b		C(6)	C <sub>2</sub> <sup>2</sup> (6)
c			S(6)

Scan widths were  $(1.50 + 0.35 \tan \theta)^\circ$  in  $\omega$ , with a background/scan time-ratio of 0.5. The data were corrected for Lorentz and polarization effects. The Laue group assignment, systematic absences and intensity statistics were consistent with centrosymmetry indicated space group  $P2_1/c$  (No. 14) and since refinement proceeded well it was adopted. Fourier difference methods were used to locate the initial H-atom positions. Refined C—H and N—H distances are given in Table 2;  $U_{\text{iso}}$  for H atoms ranged from 0.038 (6) to 0.055 (7)  $\text{\AA}^2$ . The maximum effect of extinction was 13.1% of  $F_o$  for 002. The maximum positive residual peak was located near the midpoint of the C3—C7 bond; the maximum negative peak was located near the center of the pyridine ring.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1991). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1989). Program(s) used to solve structure: *MITHRIL* (Gilmore, 1984). Program(s) used to refine structure: *TEXSAN*. Molecular graphics: *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *TEXSAN*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1064). Services for accessing these data are described at the back of the journal.

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*Acta Cryst.* (1997). **C53**, 1429–1432

## Polysulfonylamines. LXXXVII.† Bis-(benzenesulfonamido) Sulfone–Dichloromethane (1/0.5)

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## Abstract

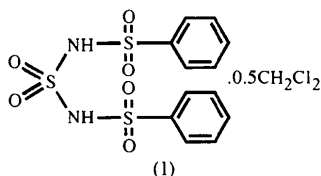
Bis(benzenesulfonamido) sulfone,  $\text{C}_{12}\text{H}_{12}\text{N}_2\text{O}_6\text{S}_3$ , forms strands in the solid state that are made up from two independent molecules linked by four independent N—H...O hydrogen bonds. In addition, the structure displays numerous C—H...O interactions. The bond

† Part LXXXVI: Weitze, Blaschette & Jones (1997).

distances and angles closely resemble those in sulfamide and bis(benzenesulfonyl)amine. The CH<sub>2</sub>Cl<sub>2</sub> solvate molecule is disordered.

### Comment

Crystals of the previously unknown title compound, (1), formed adventitiously *via* unspecified protolysis and condensation processes in a reaction mixture containing Ph<sub>3</sub>GeCl and AgN(SO<sub>2</sub>F)<sub>2</sub> (Hiemisch, 1996). Although several related substances O<sub>2</sub>S[N(Y)—SO<sub>2</sub>—X]<sub>2</sub> have been described (*e.g.* Meuwsen & Papenfuss, 1962; Nannelli, Failli & Moeller, 1965; Roesky & Hoff, 1968; Gandel'sman, Dronkina, Nazaretyan & Yagupol'skii, 1972; Roesky, Diehl, Krebs & Hein, 1979), no associated structure could be located in the Cambridge Structural Database (Allen & Kennard, 1993).



The asymmetric unit of (1) consists of two independent but closely similar O<sub>2</sub>S(NHSO<sub>2</sub>Ph)<sub>2</sub> molecules, hereafter denoted as A and A', and a severely disordered molecule of dichloromethane. Molecule A is depicted in Fig. 1. Neglecting the tilt of the phenyl rings, the idealized point-group symmetry of both molecules is C<sub>2</sub>. Related structures are those of the parent compound sulfamide, O<sub>2</sub>S(NH<sub>2</sub>)<sub>2</sub>, which displays crystallographic C<sub>2</sub> symmetry (Belaj, Kratky, Nachbaur & Popitsch, 1987), and of bis(benzenesulfonyl)amine, (PhSO<sub>2</sub>)<sub>2</sub>NH, featuring an approximately C<sub>2</sub> symmetric (CSO<sub>2</sub>)<sub>2</sub>NH fragment (Cotton & Stokely, 1970). In general, the bond lengths and angles of (1) are in good agreement with the corresponding parameters of O<sub>2</sub>S(NH<sub>2</sub>)<sub>2</sub> and (PhSO<sub>2</sub>)<sub>2</sub>NH. Including both independent molecules of (1), the S—N, S—O and S—C distances lie in the ranges 1.622 (3)–1.663 (3), 1.411 (2)–1.432 (2) and 1.741 (3)–1.753 (3) Å, respectively, while the S—N—S angles range from 122.7 (2) to 127.3 (2)°. The S atoms possess distorted tetrahedral geometry (see Table 2). The tilt of the phenyl rings is quantified by the torsion angles N1—S1—C11—C12 and N2—S3—C21—C22, which are 74.2 (3) and –89.2 (3)° for A, and 69.9 (3) and –86.6 (3)° for A'.

The molecules are linked by strong N—H···O hydrogen bonds into [AAA'A']<sub>∞</sub> strands extending in the [011] direction (Fig. 2). The strand sequence may be viewed as alternating centrosymmetric homodimers (A)<sub>2</sub> and (A')<sub>2</sub>, both characterized by an N1—H1···O1 motif of graph set N<sub>1</sub> = D[R<sub>2</sub><sup>2</sup>(8)] (Bernstein, Davis, Shimoni & Chang, 1995). Adjacent non-equivalent homodimers are further connected by N2—H2···O2 hydrogen bonds forming a motif of graph set N<sub>2</sub> = R<sub>2</sub><sup>2</sup>(12). Details

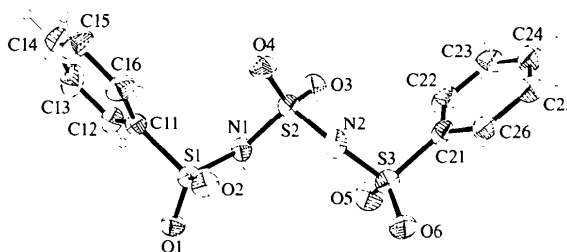


Fig. 1. One of the two independent molecules of the title compound. Ellipsoids represent 40% probability levels. H-atom radii are arbitrary.

of the four independent N—H···O bonds are shown in Table 2; they employ all four independent N—H donors and four independent O acceptors belonging to the sulfonyl groups O1—S1—O2, leaving free four O acceptors in each molecule.

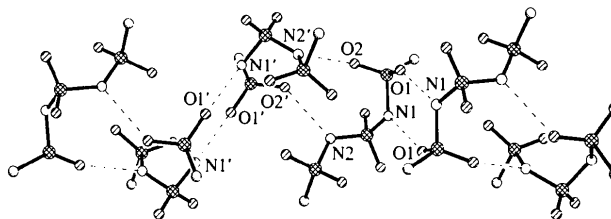


Fig. 2. Part of the hydrogen-bonded chain of the title compound (see text). Radii are arbitrary. H atoms have been omitted for clarity. Hydrogen bonds are indicated by dashed lines. Phenyl rings are represented by the *ipso*-C atoms.

In addition to these strong hydrogen bonds there are numerous C—H···O sequences, both intra- and intermolecular, that match the accepted geometric criteria for hydrogen bonds (Desiraju, 1996); instructive examples are included in Table 2. It is possible that the dichloromethane also forms C—H···O hydrogen bonds, but in view of the disorder no unambiguous information is available.

### Experimental

Crystals of solvate (1) originated fortuitously from an attempted silver salt metathesis as follows (Hiemisch, 1996): AgN(SO<sub>2</sub>F)<sub>2</sub>·C<sub>6</sub>H<sub>6</sub> (1.08 g, 2.95 mmol) in benzene (10 ml) was added to Ph<sub>3</sub>GeCl (1.00 g, 2.95 mmol) in benzene (10 ml) at ambient temperature. The mixture was refluxed for 6 h, then AgCl was removed by filtration (0.36 g, 86% of the stoichiometric quantity) and the benzene evaporated *in vacuo*. After redissolving the solid residue in CH<sub>2</sub>Cl<sub>2</sub> (10 ml), petroleum ether was added to produce a permanent turbidity and the solution then cooled to 253 K for several days, when a small crop of colourless crystals separated. A suitable crystal was removed from the mother liquor and without delay subjected to the low-temperature structure determination.

**Crystal data**C<sub>12</sub>H<sub>12</sub>N<sub>2</sub>O<sub>6</sub>S<sub>3</sub>·0.5CH<sub>2</sub>Cl<sub>2</sub>*M<sub>r</sub>* = 418.88

Triclinic

*P* $\bar{1}$ *a* = 11.6191 (14) Å*b* = 12.576 (2) Å*c* = 13.474 (2) Å $\alpha$  = 106.666 (10)° $\beta$  = 100.155 (8)° $\gamma$  = 103.946 (10)°*V* = 1765.7 (4) Å<sup>3</sup>*Z* = 4*D<sub>x</sub>* = 1.576 Mg m<sup>-3</sup>*D<sub>m</sub>* not measuredMo *K*α radiation $\lambda$  = 0.71073 Å

Cell parameters from 63 reflections

 $\theta$  = 5.0–12.5° $\mu$  = 0.603 mm<sup>-1</sup>*T* = 173 (2) K

Prism

0.24 × 0.20 × 0.20 mm

Colourless

**Data collection**Siemens *P4* diffractometer $\omega$  scans

Absorption correction:

 $\psi$  scans (*XEMP*; Siemens, 1994a)*T<sub>min</sub>* = 0.814, *T<sub>max</sub>* = 0.906

8740 measured reflections

6042 independent reflections

3723 reflections with

*I* > 2σ(*I*)**Refinement**Refinement on *F*<sup>2</sup> $R[F^2 > 2\sigma(F^2)] = 0.041$  $wR(F^2) = 0.094$ *S* = 0.856

6042 reflections

481 parameters

H atoms treated by a

mixture of independent

and constrained refinement

*R<sub>int</sub>* = 0.027 $\theta_{\max}$  = 25°*h* = -13 → 13*k* = -13 → 5*l* = -16 → 15

3 standard reflections

every 247 reflections

intensity decay: none

 $w = 1/[\sigma^2(F_o^2) + (0.049P)^2]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} = -0.103$  $\Delta\rho_{\max} = 0.425 \text{ e \AA}^{-3}$  $\Delta\rho_{\min} = -0.368 \text{ e \AA}^{-3}$ 

Extinction correction: none

Scattering factors from

*International Tables for Crystallography* (Vol. C)

Table 1. Selected geometric parameters (Å, °)

S1—O1	1.432 (2)	S1'—O1'	1.430 (2)
S1—O2	1.432 (2)	S1'—O2'	1.426 (2)
S1—N1	1.653 (3)	S1'—N1'	1.660 (3)
S1—C11	1.741 (3)	S1'—C11'	1.753 (3)
S2—O3	1.411 (2)	S2'—O3'	1.413 (2)
S2—O4	1.412 (2)	S2'—O4'	1.416 (2)
S2—N2	1.623 (3)	S2'—N2'	1.622 (3)
S2—N1	1.639 (3)	S2'—N1'	1.645 (3)
S3—O5	1.418 (2)	S3'—O5'	1.418 (3)
S3—O6	1.422 (2)	S3'—O6'	1.423 (2)
S3—N2	1.660 (3)	S3'—N2'	1.663 (3)
S3—C21	1.747 (4)	S3'—C21'	1.745 (4)
O1—S1—O2	119.57 (13)	O1'—S1'—O2'	119.57 (14)
O1—S1—N1	104.36 (13)	O1'—S1'—N1'	103.99 (14)
O2—S1—N1	108.49 (14)	O2'—S1'—N1'	109.03 (14)
O1—S1—C11	109.01 (15)	O1'—S1'—C11'	109.89 (15)
O2—S1—C11	109.37 (14)	O2'—S1'—C11'	107.8 (2)
N1—S1—C11	105.0 (2)	N1'—S1'—C11'	105.70 (14)
O3—S2—O4	123.2 (2)	O3'—S2'—O4'	122.6 (2)
O3—S2—N2	108.0 (2)	O3'—S2'—N2'	108.25 (14)
O4—S2—N2	105.63 (15)	O4'—S2'—N2'	106.37 (15)
O3—S2—N1	105.27 (14)	O3'—S2'—N1'	105.4 (2)
O4—S2—N1	106.98 (15)	O4'—S2'—N1'	106.10 (14)
N2—S2—N1	106.8 (2)	N2'—S2'—N1'	107.4 (2)
O5—S3—O6	121.1 (2)	O5'—S3'—O6'	121.7 (2)
O5—S3—N2	107.8 (2)	O5'—S3'—N2'	107.3 (2)

O6—S3—N2	104.15 (15)	O6'—S3'—N2'	103.5 (2)
O5—S3—C21	109.4 (2)	O5'—S3'—C21'	109.7 (2)
O6—S3—C21	108.9 (2)	O6'—S3'—C21'	109.0 (2)
N2—S3—C21	104.1 (2)	N2'—S3'—C21'	104.0 (2)
S2—N1—S1	124.8 (2)	S2'—N1'—S1'	122.7 (2)
S2—N2—S3	126.8 (2)	S2'—N2'—S3'	127.3 (2)

Table 2. Hydrogen-bonding 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—H1...O1'	0.73 (2)	2.10 (2)	2.819 (3)	172 (4)
N1'—H1'...O1''	0.74 (2)	2.17 (2)	2.911 (4)	175 (4)
N2—H2...O2'	0.72 (2)	2.11 (2)	2.830 (3)	174 (4)
N2'—H2'...O2	0.74 (2)	2.13 (2)	2.868 (3)	174 (4)
C22—H22...O3	0.95	2.72	3.242 (5)	115
C22'—H22'...O3'	0.95	2.65	3.195 (4)	117
C26'—H26'...O1	0.95	2.71	3.564 (4)	151
C12—H12...O6''	0.95	2.46	3.217 (4)	137
C12'—H12'...O6''	0.95	2.58	3.483 (5)	159

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

NH H atoms were refined freely except that N—H distances were restrained to be approximately equal; other H atoms were refined using a riding model. The dichloromethane molecule is disordered over two sites, which were restrained to approximately equal bond lengths and angles. Residual electron density in the solvent region probably indicates that the disorder is still more complicated.

Data collection: *XSCANS* (Fait, 1991). Cell refinement: *XSCANS*. Data reduction: *XSCANS*. Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *XP* (Siemens, 1994b). Software used to prepare material for publication: *SHELXL93*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FG1336). Services for accessing these data are described at the back of the journal.

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*Acta Cryst.* (1997). **C53**, 1432–1434

### 5-Iodo-2-[iodo(5-iodo-1,3,3-trimethyl-2-indolinylidene)methyl]-1,3,3-trimethyl-3H-indolium Perchlorate: a Highly Overcrowded Cyanine Dye

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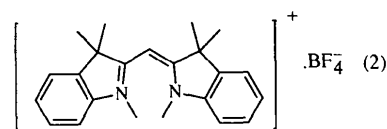
#### Abstract

The title compound, C<sub>23</sub>H<sub>24</sub>I<sub>3</sub>N<sub>2</sub><sup>+</sup>·ClO<sub>4</sub><sup>-</sup>, adopts a *di-cis* conformation in which the indolenine end groups are mutually rotated; the interplanar angle is 50.2(1)°. There are secondary contacts (I···I and I···O) involving the terminal iodo substituents and the O atoms of the perchlorate.

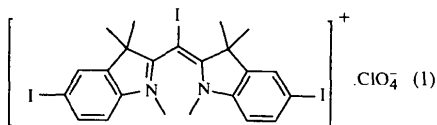
#### Comment

Cyanine dyes are promising components of non-linear optical materials (Nalwa, 1993). In order to design a specific cyanine dye we are interested in the effects of structural modifications on the conformational behaviour, the light absorption and other properties of the ground state.

In the cations of symmetrical monomethine cyanines, bulky terminal heterocyclic groups *E, E'* (see scheme below) and/or voluminous chain substituents *X* produce large steric interactions in the planar *di-trans* conformation (Tyutyulkov, Fabian, Mehlhorn, Dietz & Tadjer, 1991). These are relieved by conversion into twisted *di-cis* forms according to models (Grahn, 1979) and calculations (AM1) (Grahn, Johannes, Rheinheimer, Knieriem & Würthwein, 1995).



1. I<sub>2</sub>, Ag<sub>2</sub>SO<sub>4</sub>
2. NaClO<sub>4</sub>



The end groups of the cation of the cyanine dye 2-[(1,3,3-trimethyl-2-indolinylidene)methyl]-1,3,3-trimethyl-3H-indolium tetrafluoroborate, (2), are bulky. As expected, the calculated structure (Grahn *et al.*, 1995) exhibits planar indolenine end groups that are mutually rotated by an interplanar angle of 44.4°. In accordance with these results, the cation of (2) adopts a twisted *di-cis* conformation both in solution (Grahn *et al.*, 1995) and in the crystalline state (Allmann & Debaerdemaker, 1976). In the crystal, the indolenine end groups are almost planar (mean deviations 0.02 and 0.01 Å) and are mutually rotated by 43°.

According to AM1 calculations (Grahn *et al.*, 1995) the overcrowding in the cation of (2) should be enhanced by the introduction of large substituents such as bromine or iodine. We have prepared the 10-bromo and the 10-iodo derivative of cyanine (2), which also adopt the twisted *di-cis* conformation in solution (Grahn *et al.*, 1995), but could not obtain suitable single crystals. We did, however, succeed in obtaining single crystals of the title compound, the triiodo derivative (1), and report here its structure.

The indolenine end groups of (1) are indeed more mutually twisted than those of (2). The interplanar angle is increased to 50.2(1)° (calculated: 55.6°), whereas the central angle C2—C10—C2' is reduced from 130.3 in (2) to 124.5(4)° in (1). The methine bonds C10—C2 and C10—C2' of (2) [1.385(4) and 1.395(4) Å] are similar to those of (1) [1.392(6) and 1.398(6) Å].

Besides the primary I—C bonds involving the phenyl rings [2.097(4) and 2.101(5) Å], two types of secondary contact involving iodine are found: (i) each terminal I