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N,*N*′-Bis(phenylsulfonyl)succinamide

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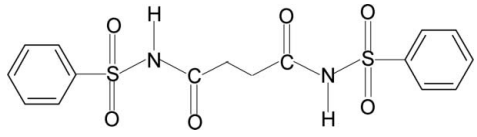
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.080; data-to-parameter ratio = 14.5.

In the crystal structure of the title compound, $C_{16}H_{16}N_2O_6S_2$, the conformation of the N—C bonds in the C—SO_2—NH—C(O)—C segments have *gauche* torsions with respect to the S═O bonds, while the conformations of the N—H and C═O bonds in the amide fragments are *trans* to each other and the amide O atom is *anti* to the H atoms attached to the adjacent C atom. The molecule is bent at the S atom with a C—SO_2—NH—C(O) torsion angle of 65.2 (2)°. The molecule lies about a centre of inversion. The dihedral angle between the benzene ring and the SO_2—NH—C(O)—C_2 segment in the two halves of the molecule is 77.4 (1)°. The structure exhibits both intramolecular and intermolecular hydrogen bonds. A series of N—H···O(S) hydrogen bonds links the molecules into infinite chains.

Related literature

For our studies of the effect of ring and side-chain substituents on the solid state structures of *N*-aromatic sulfonamides, see: Gowda *et al.* (2009*a*,*b*); Suchetan *et al.* (2009)



Experimental

Crystal data

$C_{16}H_{16}N_2O_6S_2$
M_r = 396.43
Monoclinic, $P2_1/c$
a = 8.7800 (5) Å
b = 5.1590 (3) Å
c = 19.622 (1) Å
β = 101.255 (5)°
V = 871.71 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 299 K
0.32 × 0.20 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
T_{min} = 0.898, T_{max} = 0.973
3275 measured reflections
1751 independent reflections
1427 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.080
S = 1.05
1751 reflections
121 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O2^{i}	0.80 (2)	2.39 (2)	3.042 (2)	139 (2)
N1—H1N···O1^{ii}	0.80 (2)	2.46 (2)	3.093 (2)	137 (2)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2185).

References

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supplementary materials

Acta Cryst. (2010). E**66**, o181 [**doi:10.1107/S1600536809053537**]

N,*N*'-Bis(phenylsulfonyl)succinamide

B. T. Gowda, S. Foro, P. A. Suchetan and H. Fuess

Comment

Diaryl acylsulfonamides are known as potent antitumor agents against a broad spectrum of human tumor xenografts in nude mice. As part of a study of the effect of ring and the side chain substituents on the solid state structures of *N*-aromatic sulfonamides (Gowda *et al.*, 2009*a,b*; Suchetan *et al.*, 2009), in the present work, the structure of *N*,*N*-(diphenylsulfonyl)succinamide has been determined (Fig.1).

The conformation of the N—C bonds in both the C—SO_2—NH—C(O)—C segments have *gauche* torsions with respect to the S═O bonds, while the conformations of N—H and C=O bonds in the amide fragments are *trans* to each other and the amide O atoms are *anti* to the H atoms attached to the adjacent C atoms. The molecule is bent at the S atoms with the C—SO_2—NH—C(O) torsion angle of 65.2 (2)°. The dihedral angle between the benzene ring and the SO_2—NH—C(O)—C_2 segment in the two halves of the molecule is 77.4 (1)°. The structure exhibits both the intramolecular and intermolecular hydrogen bonds. The series of N—H···O(S) hydrogen bonds (Table 1) link the molecules into infinite chains (Fig. 2).

Experimental

N,*N*-(Diphenylsulfonyl)succinamide was prepared by refluxing a mixture of succinic anhydride (0.01 mol) with benzenesulfonamide (0.02 mol) and POCl3 for 1 hr on a water bath. The reaction mixture was allowed to cool and added ether to it. The solid product obtained was filtered, washed thoroughly with ether and hot alcohol. The compound was recrystallized to the constant melting point (235–237° C).

Rod like single crystals used in the X-ray diffraction studies were obtained from a slow evaporation of a solution of the compound in methyl ethyl ketone at room temperature.

Refinement

The H atom of the NH group was located in difference map and later restrained to N—H = 0.86 (2) Å. The other H atoms were positioned with idealized geometry using a riding model [C—H = 0.93—0.97 Å]. All H atoms were refined with isotropic displacement parameters (set to 1.2 times of the U_{eq} of the parent atom).

Figures

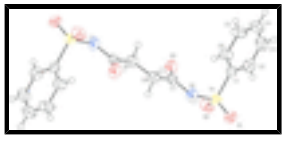

Fig. 1. Molecular structure of (I), showing the atom labelling scheme and displacement ellipsoids are drawn at the 50% probability level. Symmetry code for unlabelled part of the molecule: -x, -y, -z.

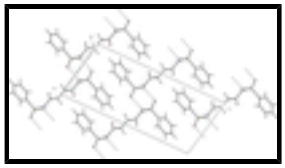

Fig. 2. Molecular packing of (I) with hydrogen bonding shown as dashed lines.

N,N'-Bis(phenylsulfonyl)succinamide

Crystal data

$C_{16}H_{16}N_2O_6S_2$	$F(000) = 412$
$M_r = 396.43$	$D_x = 1.510$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2246 reflections
$a = 8.7800$ (5) Å	$\theta = 2.8–27.8°$
$b = 5.1590$ (3) Å	$\mu = 0.34$ mm^{-1}
$c = 19.622$ (1) Å	$T = 299$ K
$\beta = 101.255$ (5)°	Rod, colourless
$V = 871.71$ (8) Å^3	0.32 × 0.20 × 0.08 mm
$Z = 2$	

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector	1751 independent reflections
Radiation source: fine-focus sealed tube	1427 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.015$
Rotation method data acquisition using ω and phi scans	$\theta_{max} = 26.4°$, $\theta_{min} = 3.5°$
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)	$h = -10\rightarrow9$
$T_{min} = 0.898$, $T_{max} = 0.973$	$k = -4\rightarrow6$
3275 measured reflections	$l = -19\rightarrow24$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.032$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.080$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2 + 0.3671P]$ where $P = (F_o^2 + 2F_c^2)/3$
1751 reflections	$(\Delta/\sigma)_{max} < 0.001$
121 parameters	$\Delta\rho_{max} = 0.29$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.29$ e Å^{-3}

Special details

Experimental. CrysAlis RED (Oxford Diffraction, 2009) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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}
C1	0.31653 (19)	0.7383 (3)	0.31933 (9)	0.0331 (4)
C2	0.3666 (2)	0.9450 (4)	0.28431 (11)	0.0470 (5)
H2	0.4429	1.0571	0.3070	0.056*
C3	0.3010 (3)	0.9812 (5)	0.21518 (12)	0.0578 (6)
H3	0.3334	1.1185	0.1908	0.069*
C4	0.1877 (3)	0.8148 (5)	0.18224 (11)	0.0604 (6)
H4	0.1440	0.8401	0.1356	0.072*
C5	0.1385 (3)	0.6118 (5)	0.21760 (11)	0.0588 (6)
H5	0.0613	0.5013	0.1949	0.071*
C6	0.2028 (2)	0.5703 (4)	0.28671 (10)	0.0437 (5)
H6	0.1703	0.4323	0.3108	0.052*
C7	0.1467 (2)	0.8280 (3)	0.45506 (8)	0.0336 (4)
C8	0.0833 (2)	1.0277 (4)	0.49737 (9)	0.0381 (4)
H8A	0.0889	1.1968	0.4764	0.046*
H8B	0.1470	1.0324	0.5437	0.046*
O1	0.55295 (14)	0.8013 (3)	0.42093 (7)	0.0479 (4)
O2	0.38326 (17)	0.4210 (2)	0.42254 (7)	0.0486 (4)
O3	0.07266 (16)	0.6510 (3)	0.42511 (7)	0.0526 (4)
S1	0.40186 (5)	0.68656 (9)	0.40706 (2)	0.03488 (15)
N1	0.30125 (18)	0.8647 (3)	0.45214 (8)	0.0380 (4)
H1N	0.343 (2)	0.998 (3)	0.4659 (11)	0.046*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0342 (9)	0.0330 (9)	0.0317 (8)	0.0039 (7)	0.0057 (7)	−0.0025 (7)
C2	0.0467 (11)	0.0420 (11)	0.0524 (12)	−0.0011 (9)	0.0102 (9)	0.0036 (9)
C3	0.0679 (14)	0.0579 (14)	0.0506 (12)	0.0151 (12)	0.0187 (11)	0.0188 (11)
C4	0.0701 (15)	0.0726 (16)	0.0348 (10)	0.0272 (13)	0.0015 (10)	0.0049 (11)
C5	0.0599 (13)	0.0637 (14)	0.0441 (11)	0.0025 (11)	−0.0112 (10)	−0.0104 (11)

C6	0.0460 (11)	0.0411 (11)	0.0413 (10)	−0.0029 (9)	0.0019 (8)	−0.0039 (8)
C7	0.0380 (9)	0.0341 (9)	0.0287 (8)	−0.0058 (8)	0.0061 (7)	−0.0016 (7)
C8	0.0380 (10)	0.0381 (10)	0.0383 (9)	−0.0070 (8)	0.0076 (8)	−0.0082 (8)
O1	0.0324 (7)	0.0617 (9)	0.0473 (8)	−0.0024 (6)	0.0023 (6)	−0.0128 (7)
O2	0.0680 (9)	0.0346 (7)	0.0405 (7)	0.0043 (7)	0.0036 (6)	0.0010 (6)
O3	0.0482 (8)	0.0533 (9)	0.0593 (9)	−0.0200 (7)	0.0177 (7)	−0.0259 (7)
S1	0.0359 (2)	0.0342 (3)	0.0328 (2)	0.00061 (19)	0.00258 (17)	−0.00498 (18)
N1	0.0367 (8)	0.0361 (9)	0.0413 (8)	−0.0091 (7)	0.0084 (6)	−0.0141 (7)

Geometric parameters (Å, °)

C1—C6	1.381 (3)	C6—H6	0.9300
C1—C2	1.386 (3)	C7—O3	1.205 (2)
C1—S1	1.7586 (17)	C7—N1	1.382 (2)
C2—C3	1.379 (3)	C7—C8	1.497 (2)
C2—H2	0.9300	C8—C8^{i}	1.514 (3)
C3—C4	1.376 (3)	C8—H8A	0.9700
C3—H3	0.9300	C8—H8B	0.9700
C4—C5	1.372 (3)	O1—S1	1.4294 (13)
C4—H4	0.9300	O2—S1	1.4196 (14)
C5—C6	1.380 (3)	S1—N1	1.6471 (16)
C5—H5	0.9300	N1—H1N	0.800 (15)
C6—C1—C2	121.56 (17)	O3—C7—N1	121.63 (16)
C6—C1—S1	119.32 (14)	O3—C7—C8	124.62 (16)
C2—C1—S1	119.11 (14)	N1—C7—C8	113.75 (14)
C3—C2—C1	118.7 (2)	C7—C8—C8^{i}	112.14 (18)
C3—C2—H2	120.6	C7—C8—H8A	109.2
C1—C2—H2	120.6	C8^{i}—C8—H8A	109.2
C4—C3—C2	120.1 (2)	C7—C8—H8B	109.2
C4—C3—H3	119.9	C8^{i}—C8—H8B	109.2
C2—C3—H3	119.9	H8A—C8—H8B	107.9
C5—C4—C3	120.6 (2)	O2—S1—O1	120.02 (9)
C5—C4—H4	119.7	O2—S1—N1	109.12 (8)
C3—C4—H4	119.7	O1—S1—N1	103.98 (8)
C4—C5—C6	120.4 (2)	O2—S1—C1	108.12 (8)
C4—C5—H5	119.8	O1—S1—C1	109.01 (8)
C6—C5—H5	119.8	N1—S1—C1	105.68 (8)
C5—C6—C1	118.57 (19)	C7—N1—S1	125.40 (12)
C5—C6—H6	120.7	C7—N1—H1N	119.9 (15)
C1—C6—H6	120.7	S1—N1—H1N	113.4 (15)
C6—C1—C2—C3	−0.3 (3)	C2—C1—S1—O2	−155.96 (15)
S1—C1—C2—C3	178.83 (16)	C6—C1—S1—O1	155.23 (15)
C1—C2—C3—C4	0.3 (3)	C2—C1—S1—O1	−23.93 (17)
C2—C3—C4—C5	0.1 (4)	C6—C1—S1—N1	−93.53 (16)
C3—C4—C5—C6	−0.5 (4)	C2—C1—S1—N1	87.30 (16)
C4—C5—C6—C1	0.4 (3)	O3—C7—N1—S1	2.2 (3)
C2—C1—C6—C5	0.0 (3)	C8—C7—N1—S1	−177.07 (13)
S1—C1—C6—C5	−179.17 (16)	O2—S1—N1—C7	−50.87 (18)

O3—C7—C8—C8^{i}	3.9 (3)	O1—S1—N1—C7	179.93 (15)
N1—C7—C8—C8^{i}	−176.81 (19)	C1—S1—N1—C7	65.19 (17)
C6—C1—S1—O2	23.21 (17)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O2^{ii}	0.80 (2)	2.39 (2)	3.042 (2)	139 (2)
N1—H1N···O1^{iii}	0.80 (2)	2.46 (2)	3.093 (2)	137 (2)

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

Fig. 1

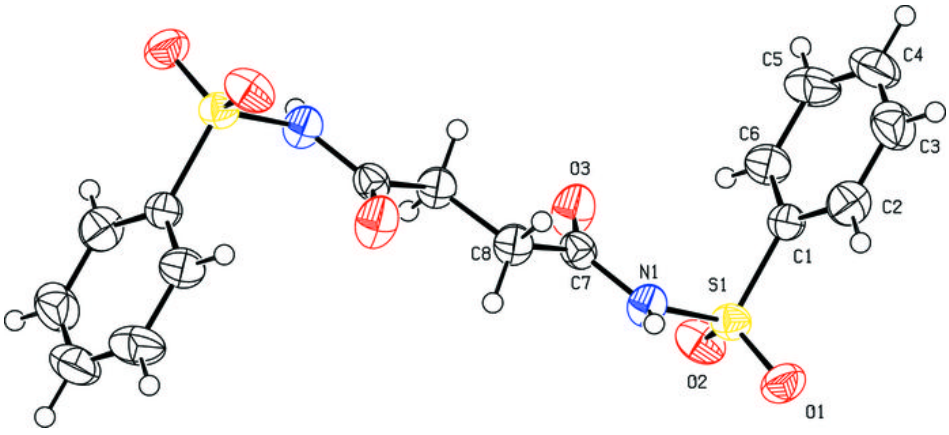
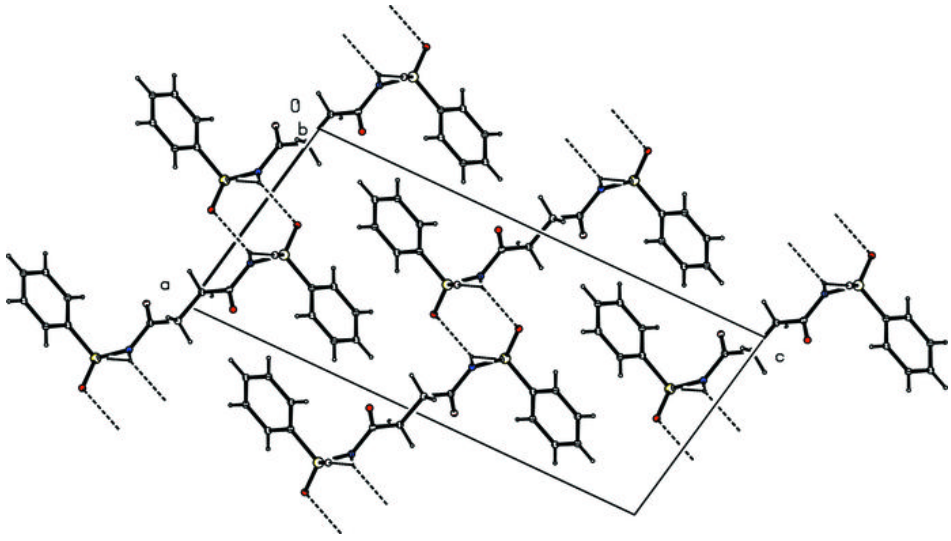
Fig. 2