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ISSN 2414-3146

2-(Phenylsulfanyl)aniline

Velabo Mdluli, James A. Golen and David R. Manke*

Department of Chemistry and Biochemistry, University of Massachusetts Dartmouth, 285 Old Westport Road, North Dartmouth, MA 02747, USA. *Correspondence e-mail: dmanke@umassd.edu

Received 25 December 2015
Accepted 29 December 2015

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

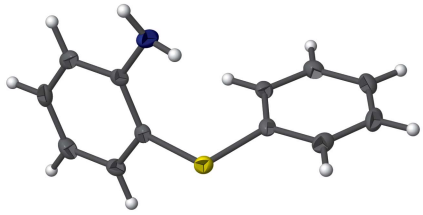
Keywords: crystal structure; anilines; 2-arylthioanilines; hydrogen bonding.

CCDC reference: 1444623

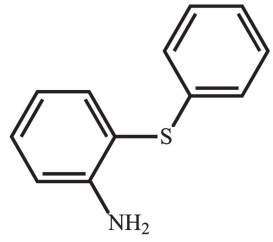
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{12}H_{11}NS$, the aniline and phenyl rings have a skewed conformation with a dihedral angle of 81.31 (7)°. There is a short intramolecular N–H···S contact enclosing an *S*(5) ring motif. In the crystal, molecules are linked *via* N–H···S hydrogen bonds, forming chains along [10$\bar{3}$]. The chains are linked *via* N—H···π and C—H···π interactions, forming layers parallel to plane (010). No π–π interactions are noted between the layers.

3D view



Chemical scheme



Structure description

2-(Arylsulfanyl)anilines have potential as pharmaceuticals, and herein we report the crystal structure of the parent 2-(phenylsulfanyl)aniline. In the title compound, Fig. 1, the aniline and phenyl rings have a skewed conformation with a dihedral angle of 81.31 (7)° and the C2—S1—C7 angle is 105.42 (10)°. This varies slightly from the values for 2-(*p*-tolylsulfanyl)aniline, where the corresponding dihedral angle is 87.80 (7)° and the C—S—C angle is 103.21 (12)° (Betz *et al.*, 2011). There is a short intramolecular N1—H1*B*···S1 contact forming an *S*(5) ring motif (Table 1).

In the crystal, molecules are linked *via* N1—H1*A*···S1 hydrogen bonds, forming chains along [10$\bar{3}$]. The chains are linked by N—H···π and C—H···π interactions, forming layers that lie parallel to plane (010); Table 1 and Fig. 2. No π–π interactions are noted between the layers.

Though other 2-arylsulfanylanilines demonstrate intramolecular N—H···S hydrogen bonding, the observed intermolecular interactions are N—H···N hydrogen bonds (Yao *et al.*, 2012; Beppu *et al.*, 2014; Sellmann *et al.*, 1999; Yuan *et al.*, 2008). The structure of 2-[(4-methylphenyl)sulfanyl]aniline has been reported (Betz *et al.*, 2011), as has that of another 2-arylthioaniline, 2-[(4-bromophenyl)sulfanyl]-4-nitroaniline (Yao *et al.*, 2012).

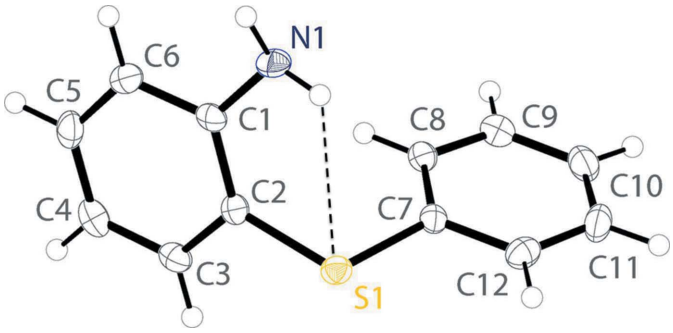


Figure 1
Molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level. The short intramolecular N—H···S contact is shown as a dashed line (see Table 1).

Synthesis and crystallization

A commercial sample (Tokyo Chemical Industries) of the title compound was used for crystallization. Single crystals suitable for X-ray diffraction studies were grown by slow evaporation of a hexanes solution.

Refinement

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

Acknowledgements

Support from the National Science Foundation (CHE-1429086) is gratefully acknowledge.

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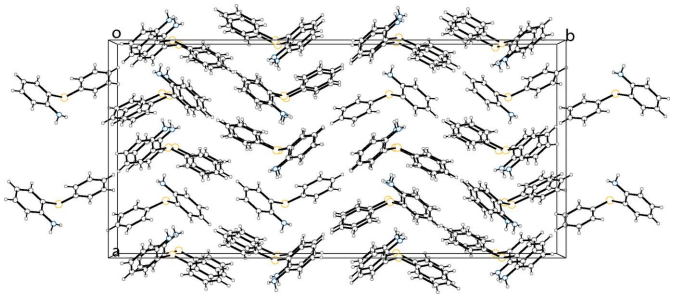

Figure 2
A view along the *c* axis of the crystal packing of the title compound, with hydrogen bonds shown as dashed lines (see Table 1).

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

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C7–C12 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···S1	0.86 (1)	2.61 (3)	3.054 (2)	113 (2)
N1—H1*A*···S1^{i}	0.86 (1)	2.73 (1)	3.580 (2)	174 (2)
N1—H1*B*···*Cg*1^{ii}	0.86 (1)	2.87 (3)	3.510 (2)	132 (2)
C6—H6···*Cg*2^{i}	0.95	2.72	3.506 (2)	141
C9—H9···*Cg*1^{iii}	0.95	2.90	3.606 (2)	132

Symmetry codes: (i) $x-\frac{1}{4}, -y+\frac{5}{4}, z+\frac{3}{4}$; (ii) $x-\frac{1}{4}, -y+\frac{5}{4}, z-\frac{1}{4}$; (iii) $x+\frac{1}{4}, -y+\frac{5}{4}, z+\frac{1}{4}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{11}NS$
M_r	201.28
Crystal system, space group	Orthorhombic, *Fdd*2
Temperature (K)	120
a, *b*, *c* (Å)	17.7430 (7), 37.3075 (19), 6.1420 (2)
V (Å^3)	4065.7 (3)
Z	16
Radiation type	Mo *Kα*
μ (mm^{-1})	0.27
Crystal size (mm)	0.4 × 0.2 × 0.2
Data collection	
Diffractometer	Bruker D8 Venture CMOS diffractometer
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.717, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14523, 1862, 1776
R_{int}	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.603
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.023, 0.055, 1.10
No. of reflections	1862
No. of parameters	134
No. of restraints	3
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, −0.16
Absolute structure	Flack *x* determined using 779 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.04 (3)

Computer programs: *APEX2* (Bruker, 2014), *SAINT* (Bruker, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), OLEX2 (Dolomanov *et al.*, 2009), *OLEX2* (Dolomanov *et al.*, 2009), *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2016). **1**, x152489 [doi:10.1107/S241431461502489X]

2-(Phenylsulfanyl)aniline

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2-(Phenylsulfanyl)aniline

Crystal data

$C_{12}H_{11}NS$
M_r = 201.28
Orthorhombic, *Fdd*2
Hall symbol: F 2 -2d
a = 17.7430 (7) Å
b = 37.3075 (19) Å
c = 6.1420 (2) Å
V = 4065.7 (3) Å^3
Z = 16
F(000) = 1696
D_x = 1.315 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 7209 reflections
θ = 3.2–25.3°
μ = 0.27 mm^{-1}
T = 120 K
Block, colourless
0.4 × 0.2 × 0.2 mm

Data collection

Bruker D8 Venture CMOS diffractometer
Radiation source: fine-focus sealed tube
TRIUMPH monochromator
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)
T_{min} = 0.717, T_{max} = 0.745
14523 measured reflections
1862 independent reflections
1776 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 25.4°, θ_{min} = 3.2°
h = −21→21
k = −44→44
l = −7→7

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.055
S = 1.10
1862 reflections
134 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0293P)^2 + 1.8762P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack *x* determined using 779 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.04 (3)

Special details

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.24353 (3)	0.61620 (2)	0.24971 (10)	0.01900 (14)
N1	0.15876 (11)	0.61631 (5)	0.6825 (3)	0.0238 (4)
C1	0.20904 (11)	0.64429 (6)	0.6541 (4)	0.0175 (5)
C2	0.25623 (10)	0.64606 (5)	0.4712 (3)	0.0169 (5)
C3	0.30828 (12)	0.67388 (5)	0.4495 (4)	0.0206 (5)
H3	0.3399	0.6748	0.3249	0.025*
C4	0.31437 (13)	0.70019 (6)	0.6072 (4)	0.0256 (5)
H4	0.3500	0.7191	0.5920	0.031*
C5	0.26753 (13)	0.69856 (6)	0.7883 (4)	0.0245 (5)
H5	0.2711	0.7165	0.8973	0.029*
C6	0.21570 (12)	0.67112 (6)	0.8121 (4)	0.0209 (5)
H6	0.1843	0.6705	0.9373	0.025*
C7	0.28473 (12)	0.57490 (6)	0.3348 (4)	0.0171 (5)
C8	0.32540 (11)	0.57064 (5)	0.5250 (4)	0.0194 (5)
H8	0.3286	0.5897	0.6272	0.023*
C9	0.36152 (12)	0.53829 (6)	0.5658 (4)	0.0239 (5)
H9	0.3902	0.5354	0.6953	0.029*
C10	0.35599 (13)	0.51019 (6)	0.4184 (4)	0.0267 (5)
H10	0.3815	0.4883	0.4457	0.032*
C11	0.31329 (12)	0.51427 (6)	0.2318 (4)	0.0271 (5)
H11	0.3082	0.4948	0.1331	0.033*
C12	0.27773 (13)	0.54671 (6)	0.1877 (4)	0.0230 (5)
H12	0.2489	0.5496	0.0585	0.028*
H1A	0.1217 (10)	0.6211 (6)	0.767 (4)	0.028*
H1B	0.1497 (15)	0.6036 (6)	0.568 (3)	0.037 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0204 (2)	0.0204 (2)	0.0162 (2)	0.0016 (2)	−0.0004 (2)	0.0009 (2)
N1	0.0230 (10)	0.0262 (10)	0.0222 (11)	−0.0040 (8)	0.0085 (8)	−0.0004 (9)
C1	0.0157 (10)	0.0181 (10)	0.0186 (11)	0.0045 (8)	−0.0003 (9)	0.0051 (9)
C2	0.0149 (9)	0.0161 (10)	0.0198 (12)	0.0032 (7)	−0.0016 (9)	0.0007 (9)
C3	0.0181 (10)	0.0205 (10)	0.0233 (12)	0.0007 (8)	0.0027 (9)	0.0052 (10)
C4	0.0252 (12)	0.0176 (11)	0.0339 (14)	−0.0032 (9)	−0.0025 (11)	0.0027 (10)
C5	0.0324 (12)	0.0167 (10)	0.0245 (15)	0.0062 (9)	−0.0057 (10)	−0.0030 (10)
C6	0.0196 (10)	0.0245 (12)	0.0187 (11)	0.0084 (9)	0.0006 (9)	0.0023 (9)
C7	0.0144 (10)	0.0158 (11)	0.0212 (11)	−0.0020 (8)	0.0037 (9)	−0.0009 (9)
C8	0.0213 (10)	0.0172 (10)	0.0197 (11)	−0.0036 (8)	0.0006 (10)	−0.0005 (9)
C9	0.0244 (11)	0.0241 (11)	0.0233 (12)	−0.0007 (9)	−0.0001 (10)	0.0034 (10)
C10	0.0285 (12)	0.0176 (11)	0.0339 (14)	0.0021 (9)	0.0063 (11)	0.0032 (10)
C11	0.0300 (11)	0.0196 (11)	0.0318 (14)	−0.0033 (9)	0.0069 (11)	−0.0088 (11)
C12	0.0215 (11)	0.0275 (12)	0.0202 (12)	−0.0029 (9)	0.0005 (9)	−0.0031 (9)

Geometric parameters (Å, º)

S1—C2	1.772 (2)	C5—C6	1.384 (3)
S1—C7	1.784 (2)	C6—H6	0.9500
N1—C1	1.384 (3)	C7—C8	1.383 (3)
N1—H1A	0.857 (7)	C7—C12	1.392 (3)
N1—H1B	0.862 (7)	C8—H8	0.9500
C1—C2	1.403 (3)	C8—C9	1.389 (3)
C1—C6	1.400 (3)	C9—H9	0.9500
C2—C3	1.396 (3)	C9—C10	1.388 (3)
C3—H3	0.9500	C10—H10	0.9500
C3—C4	1.383 (3)	C10—C11	1.382 (4)
C4—H4	0.9500	C11—H11	0.9500
C4—C5	1.390 (3)	C11—C12	1.391 (3)
C5—H5	0.9500	C12—H12	0.9500
C2—S1—C7	105.42 (10)	C5—C6—C1	120.8 (2)
C1—N1—H1A	114.4 (16)	C5—C6—H6	119.6
C1—N1—H1B	115.7 (19)	C8—C7—S1	124.12 (17)
H1A—N1—H1B	118 (3)	C8—C7—C12	120.5 (2)
N1—C1—C2	121.4 (2)	C12—C7—S1	115.22 (17)
N1—C1—C6	120.4 (2)	C7—C8—H8	120.2
C6—C1—C2	118.13 (19)	C7—C8—C9	119.5 (2)
C1—C2—S1	120.60 (16)	C9—C8—H8	120.2
C3—C2—S1	118.58 (16)	C8—C9—H9	119.8
C3—C2—C1	120.4 (2)	C10—C9—C8	120.4 (2)
C2—C3—H3	119.6	C10—C9—H9	119.8
C4—C3—C2	120.8 (2)	C9—C10—H10	120.1
C4—C3—H3	119.6	C11—C10—C9	119.7 (2)
C3—C4—H4	120.6	C11—C10—H10	120.1
C3—C4—C5	118.9 (2)	C10—C11—H11	119.8
C5—C4—H4	120.6	C10—C11—C12	120.4 (2)
C4—C5—H5	119.5	C12—C11—H11	119.8
C6—C5—C4	121.0 (2)	C7—C12—H12	120.3
C6—C5—H5	119.5	C11—C12—C7	119.4 (2)
C1—C6—H6	119.6	C11—C12—H12	120.3
S1—C2—C3—C4	172.78 (17)	C4—C5—C6—C1	−0.1 (3)
S1—C7—C8—C9	−173.59 (16)	C6—C1—C2—S1	−172.52 (16)
S1—C7—C12—C11	174.84 (17)	C6—C1—C2—C3	0.1 (3)
N1—C1—C2—S1	9.5 (3)	C7—S1—C2—C1	−78.46 (18)
N1—C1—C2—C3	−177.8 (2)	C7—S1—C2—C3	108.74 (16)
N1—C1—C6—C5	177.9 (2)	C7—C8—C9—C10	−1.0 (3)
C1—C2—C3—C4	0.0 (3)	C8—C7—C12—C11	−1.2 (3)
C2—S1—C7—C8	−7.2 (2)	C8—C9—C10—C11	−1.1 (3)
C2—S1—C7—C12	176.93 (16)	C9—C10—C11—C12	1.9 (3)
C2—C1—C6—C5	−0.1 (3)	C10—C11—C12—C7	−0.8 (3)
C2—C3—C4—C5	−0.1 (3)	C12—C7—C8—C9	2.1 (3)

C3—C4—C5—C6	0.2 (3)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the C1–C6 and C7–C12 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···S1	0.86 (1)	2.61 (3)	3.054 (2)	113 (2)
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