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N,N'-Bis(phenylsulfonyl)maleamide. Corrigendum

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The chemical name of the title compound in the paper by Gowda, Foro, Suchetan & Fuess [*Acta Cryst.* (2010), **E66**, o187] is corrected.

In the paper by Gowda *et al.* (2010), the chemical name given in the *Title* should be for the *trans* rather than the *cis* isomer, *i.e.* the title should be '*N,N'*-Bis(phenylsulfonyl)-fumaramide'.

References

Gowda, B. T., Foro, S., Suchetan, P. A. & Fuess, H. (2010). *Acta Cryst.* **E66**, o187.

N,N'-Bis(phenylsulfonyl)maleamide

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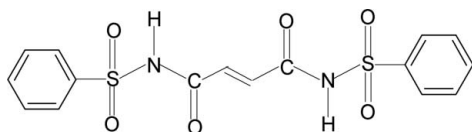
Received 13 December 2009; accepted 14 December 2009

Key indicators: single-crystal X-ray study; $T = 299$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.030; wR factor = 0.083; data-to-parameter ratio = 14.2.

Molecules of the title compound, $\text{C}_{16}\text{H}_{14}\text{N}_2\text{O}_6\text{S}_2$, show crystallographic inversion symmetry: there is one half-molecule in the asymmetric unit. The structure exhibits both intramolecular and intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For our studies of the effect of ring and the side-chain substituents on the solid-state structures of *N*-aromatic sulfonamides, see: Gowda *et al.* (2009, 2010), Suchetan *et al.* (2009).



Experimental

Crystal data

$\text{C}_{16}\text{H}_{14}\text{N}_2\text{O}_6\text{S}_2$
 $M_r = 394.41$
Monoclinic, $P2_1/c$
 $a = 8.582$ (1) Å
 $b = 5.1464$ (6) Å
 $c = 19.691$ (4) Å
 $\beta = 101.17$ (2)°

$V = 853.2$ (2) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 0.35$ mm⁻¹
 $T = 299$ K
 $0.48 \times 0.28 \times 0.22$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford

Diffraction, 2009)
 $T_{\min} = 0.850$, $T_{\max} = 0.927$
3236 measured reflections
1720 independent reflections
1500 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.009$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.083$
 $S = 1.07$
1720 reflections
121 parameters
1 restraint

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.25$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.32$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1N}\cdots\text{O2}^{\text{i}}$	0.84 (1)	2.35 (2)	3.0254 (19)	138 (2)
$\text{N1}-\text{H1N}\cdots\text{O1}^{\text{ii}}$	0.84 (1)	2.45 (2)	3.1335 (19)	139 (2)

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

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*.

PA. thanks the Council of Scientific and Industrial Research, India, for the award of a research fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5141).

References

- Gowda, B. T., Foro, S., Suchetan, P. A. & Fuess, H. (2009). *Acta Cryst.* **E65**, o2516.
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Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
Suchetan, P. A., Gowda, B. T., Foro, S. & Fuess, H. (2009). *Acta Cryst.* **E65**, o3156.

supporting information

Acta Cryst. (2010). E66, o187 [doi:10.1107/S1600536809053811]

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

B. Thimme Gowda, Sabine Foro, P. A. Suchetan and Hartmut Fues

S1. 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, 2010; Suchetan *et al.*, 2009), in the present work, the structure of *N,N'*-(Di-phenylsulfonyl)maleamide (I) has been determined (Fig. 1).

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, similar to that observed in *N,N'*-(diphenylsulfonyl)succinamide (II) (Gowda *et al.*, 2010). The molecule is bent at the S atoms with the C—SO₂—NH—C(O) torsion angle of 66.1 (2)° in (II), compared to the value of 65.2 (2)°. The dihedral angle between the benzene ring and the SO₂—NH—C(O)—C segment in the two halves of the molecule is 76.4 (1)°, compared to the corresponding angle of 77.4 (1)° in (II). 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 column like infinite chains parallel to *a*-axis (Fig. 2).

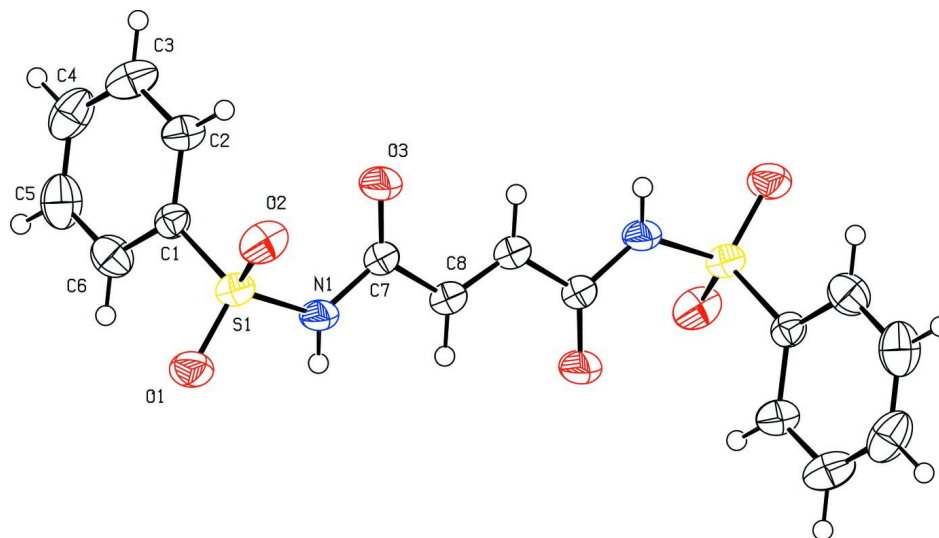
S2. Experimental

N,N'-(Diphenylsulfonyl)maleamide was prepared by refluxing a mixture of maleic anhydride (0.01 mol), benzene-sulfonamide (0.02 mol) and POCl₃ for 3hr on a water bath. The reaction mixture was allowed to cool. Ether was added to it. The solid product obtained was filtered off, washed thoroughly with ether and hot alcohol and recrystallized to the constant melting point of 255–259° C

Rod like single crystals used in the X-ray diffraction studies were obtained from a solution of the compound in DMF.

S3. Refinement

The H atom of the NH group was located in difference map and later restrained to N—H = 0.86 (1) Å. The other H atoms were positioned with idealized geometry using a riding model with C—H = 0.93 Å. All H atoms were refined with isotropic displacement parameters set to 1.2 times of the U_{eq} of the parent atom.

**Figure 1**

Molecular structure of (I), showing the atom labelling scheme and displacement ellipsoids are drawn at the 50% probability level.

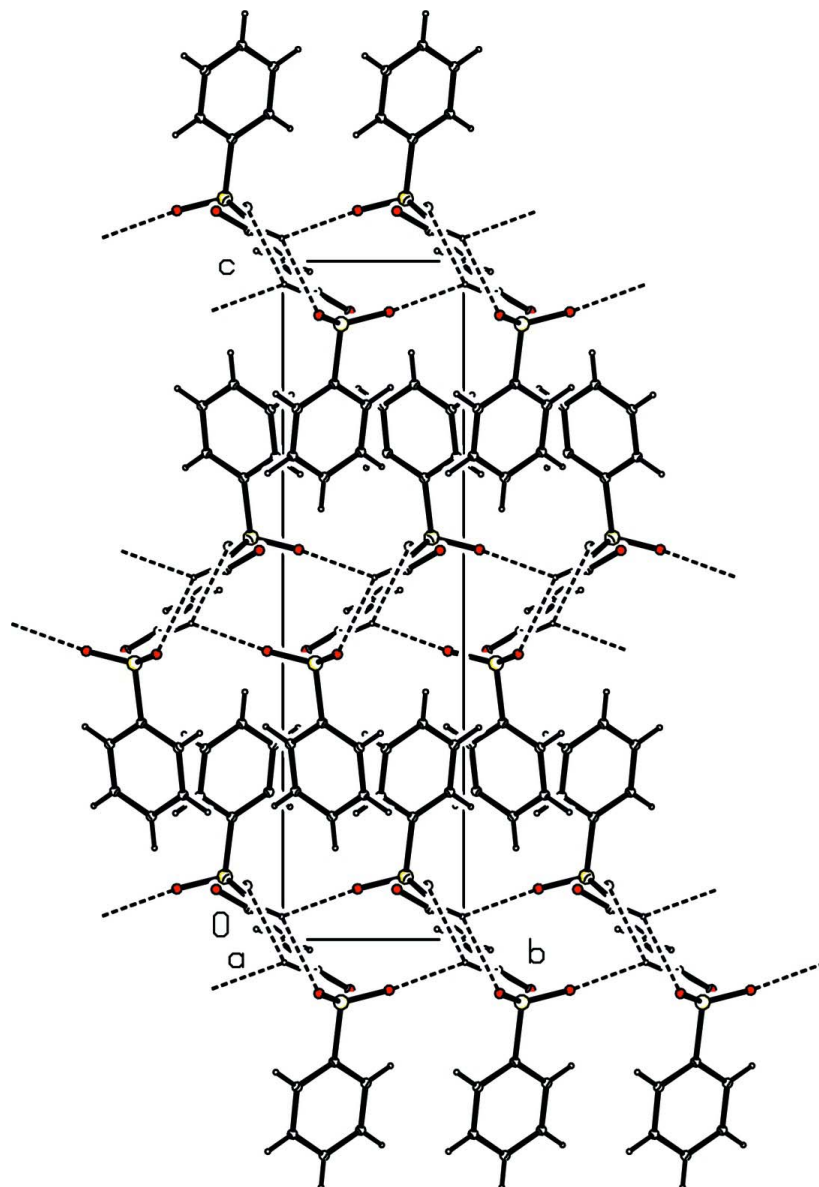


Figure 2

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

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

Crystal data

$C_{16}H_{14}N_2O_6S_2$

$M_r = 394.41$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 8.582\ (1)\ \text{\AA}$

$b = 5.1464\ (6)\ \text{\AA}$

$c = 19.691\ (4)\ \text{\AA}$

$\beta = 101.17\ (2)^\circ$

$V = 853.2\ (2)\ \text{\AA}^3$

$Z = 2$

$F(000) = 408$

$D_x = 1.535\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1915 reflections

$\theta = 2.8\text{--}27.7^\circ$

$\mu = 0.35\ \text{mm}^{-1}$

$T = 299\ \text{K}$

Rod, colourless

$0.48 \times 0.28 \times 0.22\ \text{mm}$

Data collection

Oxford Diffraction Xcalibur
diffractometer with a Sapphire CCD detector
Radiation source: fine-focus sealed tube
Graphite monochromator
Rotation method data acquisition using ω and
phi scans
Absorption correction: multi-scan
(*CrysAlis RED*; Oxford Diffraction, 2009)
 $T_{\min} = 0.850$, $T_{\max} = 0.927$

3236 measured reflections
1720 independent reflections
1500 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.009$
 $\theta_{\max} = 26.4^\circ$, $\theta_{\min} = 3.5^\circ$
 $h = -9 \rightarrow 10$
 $k = -6 \rightarrow 6$
 $l = -24 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.083$
 $S = 1.07$
1720 reflections
121 parameters
1 restraint
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
 $w = 1/[\sigma^2(F_o^2) + (0.0402P)^2 + 0.3647P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.004$
 $\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.32 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.81684 (18)	0.2173 (3)	0.31947 (8)	0.0310 (3)
C2	0.7033 (2)	0.0409 (3)	0.28846 (9)	0.0406 (4)
H2	0.6715	-0.0947	0.3139	0.049*
C3	0.6381 (2)	0.0704 (4)	0.21881 (10)	0.0539 (5)
H3	0.5618	-0.0465	0.1971	0.065*
C4	0.6857 (3)	0.2717 (4)	0.18171 (10)	0.0548 (5)
H4	0.6417	0.2894	0.1349	0.066*
C5	0.7979 (3)	0.4475 (4)	0.21310 (11)	0.0539 (5)
H5	0.8287	0.5837	0.1876	0.065*
C6	0.8651 (2)	0.4217 (4)	0.28269 (10)	0.0438 (4)
H6	0.9410	0.5393	0.3043	0.053*
C7	0.64152 (19)	0.3130 (3)	0.45450 (8)	0.0351 (4)
C8	0.57352 (19)	0.5096 (3)	0.49559 (8)	0.0370 (4)

H8	0.6360	0.6481	0.5153	0.044*
N1	0.79828 (16)	0.3588 (3)	0.45084 (8)	0.0367 (3)
H1N	0.842 (2)	0.498 (3)	0.4667 (10)	0.044*
O1	1.05692 (13)	0.3007 (3)	0.42044 (7)	0.0460 (3)
O2	0.88967 (16)	-0.0871 (2)	0.42525 (7)	0.0474 (3)
O3	0.56818 (16)	0.1304 (3)	0.42616 (7)	0.0559 (4)
S1	0.90468 (4)	0.17803 (8)	0.40734 (2)	0.03339 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0308 (7)	0.0305 (8)	0.0315 (8)	0.0033 (6)	0.0056 (6)	-0.0026 (6)
C2	0.0435 (9)	0.0360 (9)	0.0399 (9)	-0.0037 (7)	0.0019 (7)	-0.0043 (7)
C3	0.0564 (11)	0.0548 (12)	0.0431 (10)	0.0011 (10)	-0.0087 (9)	-0.0103 (9)
C4	0.0620 (12)	0.0657 (13)	0.0339 (10)	0.0213 (11)	0.0023 (9)	0.0009 (9)
C5	0.0598 (12)	0.0549 (12)	0.0502 (12)	0.0122 (10)	0.0184 (10)	0.0169 (10)
C6	0.0421 (9)	0.0382 (9)	0.0514 (11)	-0.0007 (8)	0.0100 (8)	0.0044 (8)
C7	0.0379 (8)	0.0382 (9)	0.0295 (8)	-0.0074 (7)	0.0070 (6)	-0.0050 (7)
C8	0.0398 (8)	0.0395 (9)	0.0315 (8)	-0.0077 (7)	0.0061 (7)	-0.0077 (7)
N1	0.0354 (7)	0.0335 (7)	0.0412 (8)	-0.0081 (6)	0.0077 (6)	-0.0133 (6)
O1	0.0306 (6)	0.0568 (8)	0.0481 (7)	-0.0031 (6)	0.0013 (5)	-0.0122 (6)
O2	0.0653 (8)	0.0329 (6)	0.0403 (7)	0.0037 (6)	0.0008 (6)	0.0023 (5)
O3	0.0493 (7)	0.0586 (9)	0.0639 (9)	-0.0232 (7)	0.0212 (7)	-0.0315 (7)
S1	0.0335 (2)	0.0318 (2)	0.0329 (2)	0.00033 (16)	0.00156 (15)	-0.00477 (16)

Geometric parameters (Å, °)

C1—C2	1.384 (2)	C6—H6	0.9300
C1—C6	1.385 (2)	C7—O3	1.206 (2)
C1—S1	1.7600 (16)	C7—N1	1.381 (2)
C2—C3	1.386 (3)	C7—C8	1.484 (2)
C2—H2	0.9300	C8—C8 ⁱ	1.310 (3)
C3—C4	1.375 (3)	C8—H8	0.9300
C3—H3	0.9300	N1—S1	1.6541 (15)
C4—C5	1.378 (3)	N1—H1N	0.840 (9)
C4—H4	0.9300	O1—S1	1.4288 (12)
C5—C6	1.386 (3)	O2—S1	1.4215 (13)
C5—H5	0.9300		
C2—C1—C6	121.56 (16)	C5—C6—H6	120.6
C2—C1—S1	119.29 (13)	O3—C7—N1	122.36 (16)
C6—C1—S1	119.14 (13)	O3—C7—C8	123.95 (15)
C1—C2—C3	118.68 (18)	N1—C7—C8	113.69 (14)
C1—C2—H2	120.7	C8 ⁱ —C8—C7	120.7 (2)
C3—C2—H2	120.7	C8 ⁱ —C8—H8	119.6
C4—C3—C2	120.25 (19)	C7—C8—H8	119.6
C4—C3—H3	119.9	C7—N1—S1	124.88 (11)
C2—C3—H3	119.9	C7—N1—H1N	119.4 (13)

C3—C4—C5	120.70 (18)	S1—N1—H1N	115.1 (13)
C3—C4—H4	119.7	O2—S1—O1	120.19 (8)
C5—C4—H4	119.7	O2—S1—N1	109.02 (8)
C4—C5—C6	120.08 (19)	O1—S1—N1	103.61 (7)
C4—C5—H5	120.0	O2—S1—C1	108.18 (8)
C6—C5—H5	120.0	O1—S1—C1	109.22 (8)
C1—C6—C5	118.74 (18)	N1—S1—C1	105.68 (7)
C1—C6—H6	120.6		
C6—C1—C2—C3	0.5 (3)	C8—C7—N1—S1	-178.46 (12)
S1—C1—C2—C3	-178.39 (14)	C7—N1—S1—O2	-49.95 (17)
C1—C2—C3—C4	-0.1 (3)	C7—N1—S1—O1	-179.05 (14)
C2—C3—C4—C5	-0.4 (3)	C7—N1—S1—C1	66.13 (16)
C3—C4—C5—C6	0.5 (3)	C2—C1—S1—O2	23.00 (16)
C2—C1—C6—C5	-0.3 (3)	C6—C1—S1—O2	-155.88 (14)
S1—C1—C6—C5	178.50 (14)	C2—C1—S1—O1	155.46 (13)
C4—C5—C6—C1	-0.1 (3)	C6—C1—S1—O1	-23.41 (16)
O3—C7—C8—C8 ⁱ	1.4 (3)	C2—C1—S1—N1	-93.64 (14)
N1—C7—C8—C8 ⁱ	-179.2 (2)	C6—C1—S1—N1	87.48 (14)
O3—C7—N1—S1	1.0 (3)		

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1N \cdots O2 ⁱⁱ	0.84 (1)	2.35 (2)	3.0254 (19)	138 (2)
N1—H1N \cdots O1 ⁱⁱⁱ	0.84 (1)	2.45 (2)	3.1335 (19)	139 (2)

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