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4-Nitro-*N*-phenylbenzenesulfonamide

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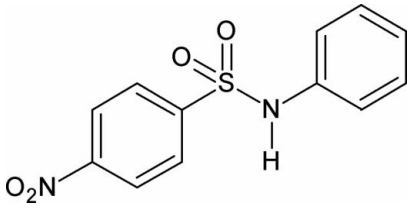
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.037; wR factor = 0.086; data-to-parameter ratio = 8.1.

In the title compound, $C_{12}H_{10}N_2O_4S$, the dihedral angle between the aromatic rings is 36.19 (18)°. In the crystal, N—H···O hydrogen bonds link the molecules into $C(4)$ chains running along the a axis.

Related literature

For studies on the effects of substituents on the structures and other aspects of *N*-(aryl)-amides, see: Alkan *et al.* (2011); Gowda & Weiss (1994); Shahwar *et al.* (2012), of *N*-arylsulfonamides, see: Chaithanya *et al.* (2012); Gowda *et al.* (2003) and of *N*-chloroarylsulfonamides, see: Gowda *et al.* (2005); Shetty & Gowda (2004).



Experimental

Crystal data

$C_{12}H_{10}N_2O_4S$
M_r = 278.28
Monoclinic, Cc
a = 5.1948 (4) Å
b = 12.8089 (9) Å
c = 18.682 (1) Å
β = 93.419 (7)°
V = 1240.88 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 293 K
0.36 × 0.32 × 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} = 0.908, T_{max} = 0.979
2074 measured reflections
1421 independent reflections
1311 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.086
S = 1.20
1421 reflections
175 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack (1983), 282 Friedel pairs
Flack parameter: 0.09 (12)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1^{i}	0.85 (2)	2.28 (2)	3.094 (4)	162 (4)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2009); 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: BT6832).

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Acta Cryst. (2012). E**68**, o2872 [https://doi.org/10.1107/S1600536812037798]

4-Nitro-*N*-phenylbenzenesulfonamide

U. Chaithanya, Sabine Foro and B. Thimme Gowda

S1. Comment

As a part of our studies on the substituent effects on the structures and other aspects of *N*-(aryl)-amides (Alkan *et al.*, 2011; Gowda & Weiss, 1994; Shahwar *et al.*, 2012); *N*-arylsulfonamides (Chaithanya *et al.*, 2012; Gowda *et al.*, 2003) and *N*-chloroarylsulfonamides (Gowda *et al.*, 2005; Shetty & Gowda, 2004),in the present work, the crystal structure of *N*-(phenyl)-4-nitrobenzenesulfonamide has been determined (Fig. 1).

The conformation of the N—C bond in the —SO_2—NH—C segment has *gauche* torsions with respect to the S═O bonds (Fig.1). The molecule is twisted at the S—N bond with the torsional angle of 61.89 (32)°, compared to the value of -72.83 (15)° in *N*-(phenyl)-2-nitrobenzenesulfonamide (I)(Chaithanya *et al.*, 2012).

The dihedral angle between the sulfonyl and the anilino rings is 36.19 (18)°, compared to the value of 59.55 (7)° in (I).

In the crystal, the intermolecular N—H···O hydrogen bond interactions link the molecules into C(4) chains. Part of the crystal structure is shown in Fig. 2.

S2. Experimental

The title compound was prepared by treating 4-nitrobenzenesulfonylchloride with aniline in the stoichiometric ratio and boiling the reaction mixture for 15 minutes. The reaction mixture was then cooled to room temperature and added to ice cold water (100 ml). The resultant solid *N*-(phenyl)-4-nitrobenzenesulfonamide was filtered under suction and washed thoroughly with cold water and dilute HCl to remove the excess sulfonylchloride and aniline, respectively. It was then recrystallized to constant melting point from dilute ethanol. The purity of the compound was checked and characterized by its infrared spectra.

Plate like colourless single crystals of the title compound used in X-ray diffraction studies were grown in ethanolic solution by slow evaporation of the solvent at room temperature.

S3. Refinement

H atoms bonded to C were positioned with idealized geometry using a riding model with C—H = 0.93 Å. The coordinates of the amino H atom were refined with the N—H distance restrained to 0.86 (2) Å. All H atoms were refined with isotropic displacement parameters set at 1.2 U_{eq} of the parent atom.

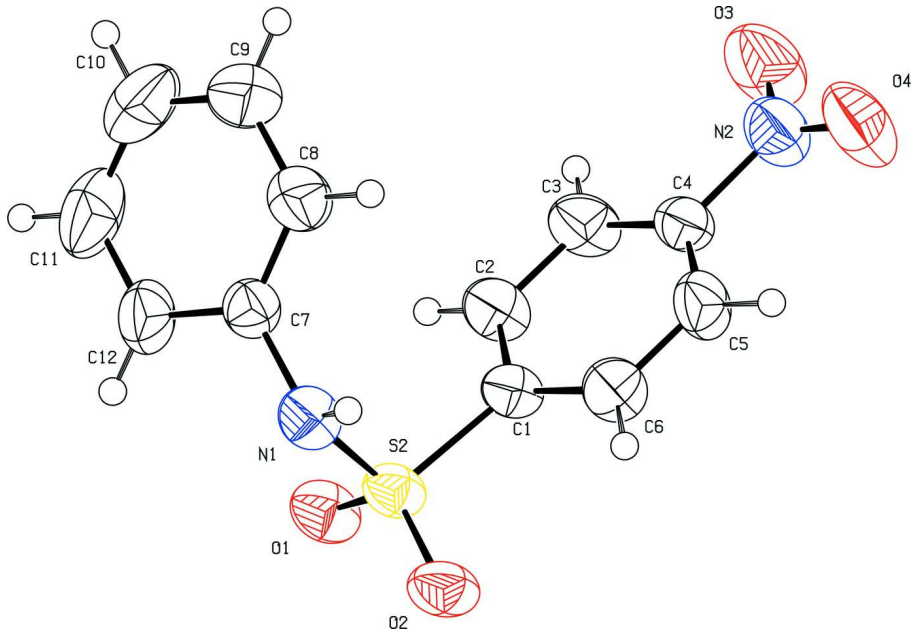

Figure 1

Molecular structure of the title compound, showing the atom labelling scheme and with displacement ellipsoids drawn at the 50% probability level.

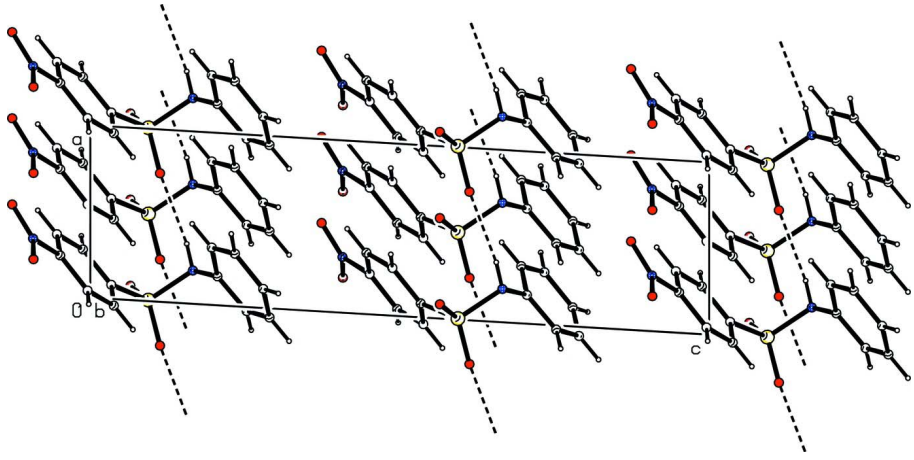

Figure 2

Molecular packing of the title compound with hydrogen bonding shown as dashed lines.

4-Nitro-*N*-phenylbenzenesulfonamide

Crystal data

$C_{12}H_{10}N_2O_4S$
M_r = 278.28
Monoclinic, *Cc*
Hall symbol: C -2yc
a = 5.1948 (4) Å
b = 12.8089 (9) Å
c = 18.682 (1) Å
β = 93.419 (7)°
V = 1240.88 (15) Å^3
Z = 4
F(000) = 576
D_x = 1.490 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1242 reflections
θ = 3.2–27.6°
μ = 0.27 mm^{-1}

T = 293 K
Plate, colourless
0.36 × 0.32 × 0.08 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 scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
T_{min} = 0.908, T_{max} = 0.979
2074 measured reflections
1421 independent reflections
1311 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 25.3°, θ_{min} = 3.2°
$h = -6 \rightarrow 3$
$k = -5 \rightarrow 15$
$l = -22 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.086
S = 1.20
1421 reflections
175 parameters
3 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.032P)^2 + 0.9798P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack (1983), 282 Friedel pairs
Absolute structure parameter: 0.09 (12)

Special details

Experimental. Absorption correction: 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	0.0817 (7)	0.9140 (3)	0.0338 (2)	0.0425 (9)
C2	−0.0381 (8)	1.0097 (3)	0.0379 (2)	0.0535 (11)
H2	−0.1700	1.0195	0.0688	0.064*
C3	0.0406 (8)	1.0907 (3)	−0.0044 (2)	0.0570 (12)
H3	−0.0381	1.1558	−0.0026	0.068*
C4	0.2345 (8)	1.0741 (3)	−0.0487 (2)	0.0457 (9)
C5	0.3565 (9)	0.9789 (3)	−0.0540 (3)	0.0569 (11)
H5	0.4883	0.9697	−0.0849	0.068*
C6	0.2773 (8)	0.8980 (3)	−0.0120 (2)	0.0533 (11)
H6	0.3550	0.8328	−0.0146	0.064*
C7	0.1676 (8)	0.9283 (3)	0.2053 (2)	0.0457 (9)

C8	0.3323 (9)	1.0099 (3)	0.1962 (3)	0.0604 (12)
H8	0.4631	1.0034	0.1646	0.072*
C9	0.3052 (12)	1.1013 (4)	0.2335 (3)	0.0762 (15)
H9	0.4186	1.1564	0.2277	0.091*
C10	0.1108 (13)	1.1109 (4)	0.2793 (3)	0.0826 (17)
H10	0.0895	1.1734	0.3036	0.099*
C11	−0.0527 (11)	1.0291 (5)	0.2895 (3)	0.0825 (16)
H11	−0.1833	1.0358	0.3211	0.099*
C12	−0.0235 (9)	0.9362 (4)	0.2526 (2)	0.0658 (13)
H12	−0.1322	0.8800	0.2599	0.079*
N1	0.1932 (7)	0.8315 (2)	0.16574 (19)	0.0491 (8)
H1N	0.346 (5)	0.817 (3)	0.156 (2)	0.059*
N2	0.3232 (8)	1.1618 (3)	−0.0926 (2)	0.0624 (10)
O1	−0.2542 (5)	0.82835 (19)	0.11253 (16)	0.0535 (8)
O2	0.0826 (6)	0.71539 (19)	0.06472 (17)	0.0569 (8)
O3	0.2037 (8)	1.2437 (3)	−0.0919 (2)	0.0907 (13)
O4	0.5135 (8)	1.1485 (3)	−0.1263 (2)	0.0894 (13)
S2	0.00585 (16)	0.81293 (6)	0.09388 (7)	0.0445 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.037 (2)	0.0366 (16)	0.054 (2)	0.0000 (16)	0.0048 (17)	0.0008 (16)
C2	0.045 (2)	0.0422 (19)	0.076 (3)	0.0090 (18)	0.024 (2)	0.0009 (19)
C3	0.055 (3)	0.038 (2)	0.080 (3)	0.0115 (19)	0.017 (2)	0.005 (2)
C4	0.048 (2)	0.0387 (18)	0.051 (2)	−0.0031 (17)	0.0065 (18)	0.0020 (16)
C5	0.061 (3)	0.054 (2)	0.058 (3)	0.005 (2)	0.027 (2)	0.003 (2)
C6	0.054 (3)	0.042 (2)	0.066 (3)	0.0123 (19)	0.018 (2)	−0.0004 (19)
C7	0.047 (2)	0.0451 (19)	0.045 (2)	0.0006 (18)	0.0039 (18)	0.0022 (17)
C8	0.061 (3)	0.058 (2)	0.064 (3)	−0.006 (2)	0.016 (2)	−0.002 (2)
C9	0.104 (5)	0.051 (2)	0.074 (3)	−0.008 (3)	0.009 (3)	0.000 (2)
C10	0.104 (5)	0.078 (3)	0.066 (3)	0.017 (3)	0.004 (3)	−0.025 (3)
C11	0.072 (4)	0.115 (4)	0.062 (3)	0.007 (4)	0.022 (3)	−0.024 (3)
C12	0.061 (3)	0.087 (3)	0.051 (3)	−0.014 (2)	0.020 (2)	−0.007 (2)
N1	0.0428 (19)	0.0479 (18)	0.057 (2)	0.0060 (16)	0.0083 (16)	0.0036 (15)
N2	0.068 (3)	0.054 (2)	0.067 (3)	0.0027 (19)	0.016 (2)	0.0115 (17)
O1	0.0344 (15)	0.0529 (16)	0.074 (2)	−0.0013 (12)	0.0104 (14)	0.0027 (13)
O2	0.0585 (19)	0.0351 (13)	0.078 (2)	0.0002 (12)	0.0166 (16)	−0.0035 (12)
O3	0.109 (3)	0.0544 (18)	0.112 (3)	0.020 (2)	0.038 (3)	0.0257 (18)
O4	0.095 (3)	0.071 (2)	0.108 (3)	0.0060 (19)	0.053 (3)	0.027 (2)
S2	0.0383 (5)	0.0369 (4)	0.0592 (5)	−0.0003 (5)	0.0108 (4)	0.0004 (5)

Geometric parameters (Å, º)

C1—C2	1.379 (5)	C8—C9	1.375 (6)
C1—C6	1.383 (5)	C8—H8	0.9300
C1—S2	1.773 (4)	C9—C10	1.366 (7)
C2—C3	1.382 (5)	C9—H9	0.9300

C2—H2	0.9300	C10—C11	1.369 (8)
C3—C4	1.358 (5)	C10—H10	0.9300
C3—H3	0.9300	C11—C12	1.387 (7)
C4—C5	1.380 (5)	C11—H11	0.9300
C4—N2	1.480 (5)	C12—H12	0.9300
C5—C6	1.376 (5)	N1—S2	1.628 (4)
C5—H5	0.9300	N1—H1N	0.85 (2)
C6—H6	0.9300	N2—O4	1.215 (5)
C7—C8	1.368 (6)	N2—O3	1.220 (5)
C7—C12	1.371 (5)	O1—S2	1.429 (3)
C7—N1	1.454 (5)	O2—S2	1.429 (3)

C2—C1—C6	121.1 (3)	C10—C9—C8	119.7 (5)
C2—C1—S2	119.7 (3)	C10—C9—H9	120.1
C6—C1—S2	118.9 (3)	C8—C9—H9	120.1
C1—C2—C3	119.1 (4)	C9—C10—C11	120.4 (5)
C1—C2—H2	120.5	C9—C10—H10	119.8
C3—C2—H2	120.5	C11—C10—H10	119.8
C4—C3—C2	119.1 (3)	C10—C11—C12	120.0 (5)
C4—C3—H3	120.4	C10—C11—H11	120.0
C2—C3—H3	120.4	C12—C11—H11	120.0
C3—C4—C5	122.8 (3)	C7—C12—C11	119.2 (4)
C3—C4—N2	119.0 (4)	C7—C12—H12	120.4
C5—C4—N2	118.1 (4)	C11—C12—H12	120.4
C6—C5—C4	118.0 (4)	C7—N1—S2	118.4 (3)
C6—C5—H5	121.0	C7—N1—H1N	114 (3)
C4—C5—H5	121.0	S2—N1—H1N	108 (3)
C5—C6—C1	119.8 (3)	O4—N2—O3	123.7 (4)
C5—C6—H6	120.1	O4—N2—C4	118.1 (4)
C1—C6—H6	120.1	O3—N2—C4	118.1 (4)
C8—C7—C12	120.4 (4)	O1—S2—O2	120.20 (16)
C8—C7—N1	120.7 (4)	O1—S2—N1	107.82 (18)
C12—C7—N1	118.9 (4)	O2—S2—N1	106.00 (18)
C7—C8—C9	120.2 (5)	O1—S2—C1	107.61 (16)
C7—C8—H8	119.9	O2—S2—C1	108.63 (17)
C9—C8—H8	119.9	N1—S2—C1	105.71 (18)

C6—C1—C2—C3	−0.3 (7)	C10—C11—C12—C7	−1.0 (8)
S2—C1—C2—C3	173.8 (3)	C8—C7—N1—S2	−98.6 (4)
C1—C2—C3—C4	−0.3 (7)	C12—C7—N1—S2	82.0 (5)
C2—C3—C4—C5	0.6 (7)	C3—C4—N2—O4	172.7 (5)
C2—C3—C4—N2	−178.4 (4)	C5—C4—N2—O4	−6.3 (6)
C3—C4—C5—C6	−0.3 (7)	C3—C4—N2—O3	−6.2 (6)
N2—C4—C5—C6	178.7 (4)	C5—C4—N2—O3	174.8 (5)
C4—C5—C6—C1	−0.3 (7)	C7—N1—S2—O1	−53.0 (3)
C2—C1—C6—C5	0.6 (7)	C7—N1—S2—O2	177.1 (3)
S2—C1—C6—C5	−173.5 (4)	C7—N1—S2—C1	61.9 (3)
C12—C7—C8—C9	−1.0 (8)	C2—C1—S2—O1	29.2 (4)

N1—C7—C8—C9	179.5 (4)	C6—C1—S2—O1	−156.6 (3)
C7—C8—C9—C10	−0.8 (8)	C2—C1—S2—O2	160.8 (4)
C8—C9—C10—C11	1.7 (9)	C6—C1—S2—O2	−25.0 (4)
C9—C10—C11—C12	−0.8 (9)	C2—C1—S2—N1	−85.9 (4)
C8—C7—C12—C11	1.9 (7)	C6—C1—S2—N1	88.4 (4)
N1—C7—C12—C11	−178.6 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O1^{i}	0.85 (2)	2.28 (2)	3.094 (4)	162 (4)

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