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N-(2,4-Dimethylphenyl)-2-nitrobenzenesulfonamide

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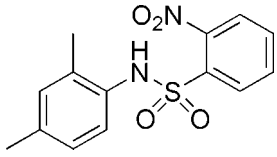
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.102; data-to-parameter ratio = 14.8.

The molecular conformation of the title compound, $C_{14}H_{14}N_2O_4S$, is stabilized by an N—H···O hydrogen bond. The packing is influenced by π–π stacking interactions between nitrophenyl rings [centroid-to-centroid separation 3.744 (13) Å].

Related literature

For *N*-arylbenzenesulfonamides, see: Shi (2007); Chang *et al.* (2007); Yu *et al.* (2007); Xing *et al.* (2006); Yu (2006); Xing & Zeng (2005).



Experimental

Crystal data

$C_{14}H_{14}N_2O_4S$
M_r = 306.33
Monoclinic, $C2/c$
a = 25.663 (4) Å
b = 8.2546 (11) Å
c = 14.894 (2) Å
β = 115.779 (2)°
V = 2841.1 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 294 (2) K
0.30 × 0.28 × 0.20 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.918, T_{max} = 0.953
7858 measured reflections
2908 independent reflections
2245 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.102
S = 1.02
2908 reflections
197 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3	0.78 (2)	2.50 (2)	3.017 (2)	125 (2)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2524).

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supplementary materials

Acta Cryst. (2007). E**63**, o4372 [**doi:10.1107/S1600536807050489**]

N-(2,4-Dimethylphenyl)-2-nitrobenzenesulfonamide

F.-E. Shi

Comment

The molecular conformation of the title compound is stabilized by a N—H···O hydrogen bond. The dihedral angle between the xylene and nitrobenzen ring is 62.61 (10) °. The nitro group has an angle of 50.50 (12) ° with its connected benzene ring.

In the crystal of (I), aromatic π-π interaction [centroid separation = 3.744 (13) Å] between nitrobenzene rings (symmetry operator for the second ring 1/2-*X*, 3/2-Y, –*Z*) makes a great contribution to the packing. No significant intermolecular H-bonds were observed as reported in other *N*-arylbenzenesulfonamides.

Experimental

The title compound was prepared according to the modified method of Shi (2007). Yellow blocks of the title compound were grown by evaporation of a MeOH-CH_2Cl_2 solution.

Refinement

The N-bound H atoms were refined freely while the other H atoms were positioned geometrically (C—H = 0.93 and 0.96 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The N—H distance was restrained to 0.86 (3) Å.

Figures

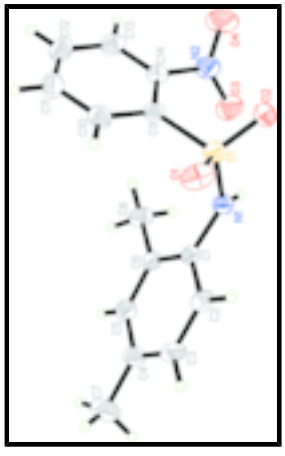

Fig. 1. The molecular structure of the title compound, with the atom-numbering scheme and 30% probability displacement ellipsoids for the non-hydrogen atoms.

2-nitro-*N*-(2,4-dimethylphenyl)benzenesulfonamide

Crystal data

$C_{14}H_{14}N_2O_4S$ F_{000} = 1280

M_r = 306.33	D_x = 1.432 Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 3333 reflections
a = 25.663 (4) Å	θ = 2.6–26.3º
b = 8.2546 (11) Å	μ = 0.25 mm^{-1}
c = 14.894 (2) Å	T = 294 (2) K
β = 115.779 (2)º	Block, yellow
V = 2841.1 (7) Å^3	0.30 × 0.28 × 0.20 mm
Z = 8	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	2908 independent reflections
Radiation source: fine-focus sealed tube	2245 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 294(2) K	θ_{max} = 26.4º
ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −32→31
T_{min} = 0.918, T_{max} = 0.953	k = −10→6
7858 measured reflections	l = −17→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.036	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.102	$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 1.9478P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.002
2908 reflections	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
197 parameters	$\Delta\rho_{min}$ = −0.39 e Å^{-3}
1 restraint	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0133 (7)

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.

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 $F^2 > 2\text{sigma}(F^2)$ 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}
S1	0.386258 (19)	0.71442 (6)	0.03736 (4)	0.04352 (17)
O1	0.41070 (6)	0.71700 (19)	0.14319 (11)	0.0610 (4)
O2	0.37524 (6)	0.86075 (17)	−0.01820 (13)	0.0647 (4)
O3	0.32493 (7)	0.6616 (2)	−0.19350 (12)	0.0742 (5)
O4	0.24466 (9)	0.7872 (3)	−0.23360 (15)	0.1012 (7)
N1	0.42726 (6)	0.60625 (19)	0.00522 (12)	0.0416 (4)
H1	0.4219 (9)	0.621 (3)	−0.0499 (14)	0.054 (7)*
N2	0.28263 (8)	0.6957 (2)	−0.18045 (13)	0.0582 (5)
C1	0.45760 (7)	0.4646 (2)	0.05671 (12)	0.0359 (4)
C2	0.50813 (7)	0.4835 (2)	0.14326 (13)	0.0423 (4)
H2	0.5203	0.5864	0.1693	0.051*
C3	0.54036 (8)	0.3492 (3)	0.19081 (14)	0.0491 (5)
H3	0.5742	0.3627	0.2492	0.059*
C4	0.52342 (8)	0.1959 (3)	0.15347 (15)	0.0492 (5)
C5	0.47274 (8)	0.1794 (2)	0.06744 (15)	0.0494 (5)
H5	0.4608	0.0761	0.0418	0.059*
C6	0.43880 (7)	0.3109 (2)	0.01757 (14)	0.0404 (4)
C7	0.55902 (12)	0.0497 (3)	0.2044 (2)	0.0782 (8)
H7A	0.5383	−0.0468	0.1728	0.117*
H7B	0.5664	0.0496	0.2733	0.117*
H7C	0.5951	0.0530	0.1995	0.117*
C8	0.38413 (9)	0.2852 (3)	−0.07680 (17)	0.0579 (6)
H8A	0.3894	0.3264	−0.1326	0.087*
H8B	0.3527	0.3413	−0.0719	0.087*
H8C	0.3755	0.1715	−0.0860	0.087*
C9	0.31865 (7)	0.6138 (2)	−0.00189 (13)	0.0378 (4)
C10	0.30726 (9)	0.5333 (2)	0.06886 (15)	0.0480 (5)
H10	0.3353	0.5304	0.1347	0.058*
C11	0.25484 (10)	0.4573 (3)	0.04321 (18)	0.0592 (6)
H11	0.2482	0.4012	0.0914	0.071*
C12	0.21268 (10)	0.4638 (3)	−0.05224 (19)	0.0609 (6)
H12	0.1773	0.4129	−0.0688	0.073*
C13	0.22224 (8)	0.5449 (3)	−0.12369 (16)	0.0549 (5)
H13	0.1933	0.5509	−0.1886	0.066*
C14	0.27490 (8)	0.6177 (2)	−0.09893 (13)	0.0422 (4)

Atomic displacement parameters (Å^2)

U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

S1	0.0382 (3)	0.0363 (3)	0.0528 (3)	−0.00032 (19)	0.0167 (2)	−0.0073 (2)
O1	0.0486 (8)	0.0741 (10)	0.0519 (8)	0.0006 (7)	0.0142 (7)	−0.0265 (7)
O2	0.0541 (8)	0.0360 (8)	0.1018 (12)	0.0017 (6)	0.0319 (8)	0.0053 (8)
O3	0.0621 (10)	0.1056 (14)	0.0635 (10)	0.0115 (9)	0.0354 (8)	0.0187 (9)
O4	0.0744 (12)	0.1410 (19)	0.0808 (13)	0.0417 (12)	0.0269 (10)	0.0620 (13)
N1	0.0402 (8)	0.0432 (9)	0.0430 (9)	0.0043 (7)	0.0197 (7)	0.0038 (7)
N2	0.0474 (10)	0.0746 (13)	0.0445 (9)	0.0060 (9)	0.0124 (8)	0.0118 (9)
C1	0.0314 (8)	0.0403 (9)	0.0387 (9)	0.0020 (7)	0.0178 (7)	0.0017 (7)
C2	0.0360 (9)	0.0511 (11)	0.0418 (10)	−0.0039 (8)	0.0190 (8)	−0.0076 (8)
C3	0.0355 (9)	0.0720 (14)	0.0366 (10)	0.0076 (9)	0.0127 (8)	0.0012 (9)
C4	0.0444 (10)	0.0575 (13)	0.0496 (11)	0.0124 (9)	0.0242 (9)	0.0103 (9)
C5	0.0490 (11)	0.0408 (11)	0.0616 (13)	0.0006 (8)	0.0270 (10)	0.0007 (9)
C6	0.0332 (8)	0.0424 (10)	0.0446 (10)	−0.0016 (7)	0.0160 (8)	−0.0014 (8)
C7	0.0756 (16)	0.0785 (18)	0.0764 (16)	0.0342 (14)	0.0291 (13)	0.0232 (14)
C8	0.0440 (11)	0.0509 (12)	0.0633 (13)	−0.0035 (9)	0.0089 (10)	−0.0113 (10)
C9	0.0370 (8)	0.0331 (9)	0.0442 (10)	0.0054 (7)	0.0184 (8)	−0.0025 (7)
C10	0.0537 (11)	0.0463 (11)	0.0460 (11)	0.0073 (9)	0.0236 (9)	0.0017 (9)
C11	0.0675 (14)	0.0487 (12)	0.0772 (15)	−0.0004 (10)	0.0460 (13)	0.0051 (11)
C12	0.0501 (12)	0.0517 (13)	0.0879 (17)	−0.0101 (10)	0.0365 (12)	−0.0113 (12)
C13	0.0407 (10)	0.0580 (12)	0.0581 (12)	−0.0007 (9)	0.0141 (9)	−0.0091 (10)
C14	0.0391 (9)	0.0424 (10)	0.0432 (10)	0.0050 (8)	0.0162 (8)	0.0009 (8)

Geometric parameters (Å, °)

S1—O1	1.4207 (15)	C5—H5	0.9300
S1—O2	1.4213 (16)	C6—C8	1.508 (3)
S1—N1	1.6037 (16)	C7—H7A	0.9600
S1—C9	1.7777 (18)	C7—H7B	0.9600
O3—N2	1.216 (2)	C7—H7C	0.9600
O4—N2	1.215 (2)	C8—H8A	0.9600
N1—C1	1.429 (2)	C8—H8B	0.9600
N1—H1	0.781 (18)	C8—H8C	0.9600
N2—C14	1.462 (3)	C9—C10	1.380 (3)
C1—C2	1.383 (2)	C9—C14	1.393 (2)
C1—C6	1.392 (2)	C10—C11	1.379 (3)
C2—C3	1.380 (3)	C10—H10	0.9300
C2—H2	0.9300	C11—C12	1.363 (3)
C3—C4	1.375 (3)	C11—H11	0.9300
C3—H3	0.9300	C12—C13	1.367 (3)
C4—C5	1.379 (3)	C12—H12	0.9300
C4—C7	1.504 (3)	C13—C14	1.375 (3)
C5—C6	1.388 (3)	C13—H13	0.9300
O1—S1—O2	120.87 (10)	C4—C7—H7A	109.5
O1—S1—N1	108.01 (9)	C4—C7—H7B	109.5
O2—S1—N1	106.84 (9)	H7A—C7—H7B	109.5
O1—S1—C9	105.58 (9)	C4—C7—H7C	109.5
O2—S1—C9	106.69 (9)	H7A—C7—H7C	109.5
N1—S1—C9	108.35 (8)	H7B—C7—H7C	109.5
C1—N1—S1	124.79 (13)	C6—C8—H8A	109.5

C1—N1—H1	120.1 (17)	C6—C8—H8B	109.5
S1—N1—H1	112.7 (16)	H8A—C8—H8B	109.5
O4—N2—O3	123.94 (19)	C6—C8—H8C	109.5
O4—N2—C14	117.07 (19)	H8A—C8—H8C	109.5
O3—N2—C14	118.93 (17)	H8B—C8—H8C	109.5
C2—C1—C6	120.47 (16)	C10—C9—C14	117.44 (17)
C2—C1—N1	118.61 (16)	C10—C9—S1	118.32 (14)
C6—C1—N1	120.81 (15)	C14—C9—S1	124.15 (14)
C3—C2—C1	119.81 (18)	C11—C10—C9	120.82 (19)
C3—C2—H2	120.1	C11—C10—H10	119.6
C1—C2—H2	120.1	C9—C10—H10	119.6
C4—C3—C2	121.23 (17)	C12—C11—C10	120.5 (2)
C4—C3—H3	119.4	C12—C11—H11	119.8
C2—C3—H3	119.4	C10—C11—H11	119.8
C3—C4—C5	118.10 (18)	C11—C12—C13	120.1 (2)
C3—C4—C7	121.3 (2)	C11—C12—H12	119.9
C5—C4—C7	120.6 (2)	C13—C12—H12	119.9
C4—C5—C6	122.60 (19)	C12—C13—C14	119.6 (2)
C4—C5—H5	118.7	C12—C13—H13	120.2
C6—C5—H5	118.7	C14—C13—H13	120.2
C5—C6—C1	117.78 (16)	C13—C14—C9	121.53 (18)
C5—C6—C8	120.11 (17)	C13—C14—N2	116.24 (17)
C1—C6—C8	122.10 (17)	C9—C14—N2	122.21 (16)
O1—S1—N1—C1	35.73 (17)	N1—S1—C9—C10	103.50 (15)
O2—S1—N1—C1	167.19 (14)	O1—S1—C9—C14	164.47 (15)
C9—S1—N1—C1	−78.19 (16)	O2—S1—C9—C14	34.70 (18)
S1—N1—C1—C2	−78.53 (19)	N1—S1—C9—C14	−80.02 (17)
S1—N1—C1—C6	105.39 (18)	C14—C9—C10—C11	1.3 (3)
C6—C1—C2—C3	0.4 (3)	S1—C9—C10—C11	178.03 (15)
N1—C1—C2—C3	−175.64 (16)	C9—C10—C11—C12	−1.7 (3)
C1—C2—C3—C4	0.4 (3)	C10—C11—C12—C13	0.5 (3)
C2—C3—C4—C5	−0.8 (3)	C11—C12—C13—C14	1.0 (3)
C2—C3—C4—C7	179.02 (19)	C12—C13—C14—C9	−1.4 (3)
C3—C4—C5—C6	0.3 (3)	C12—C13—C14—N2	177.30 (19)
C7—C4—C5—C6	−179.5 (2)	C10—C9—C14—C13	0.2 (3)
C4—C5—C6—C1	0.5 (3)	S1—C9—C14—C13	−176.31 (15)
C4—C5—C6—C8	179.36 (19)	C10—C9—C14—N2	−178.38 (17)
C2—C1—C6—C5	−0.9 (3)	S1—C9—C14—N2	5.1 (3)
N1—C1—C6—C5	175.14 (16)	O4—N2—C14—C13	49.3 (3)
C2—C1—C6—C8	−179.73 (18)	O3—N2—C14—C13	−128.1 (2)
N1—C1—C6—C8	−3.7 (3)	O4—N2—C14—C9	−132.0 (2)
O1—S1—C9—C10	−12.01 (17)	O3—N2—C14—C9	50.6 (3)
O2—S1—C9—C10	−141.79 (15)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3	0.78 (2)	2.50 (2)	3.017 (2)	125 (2)

Fig. 1