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2,5-Dimethoxy-*N*-phenylbenzenesulfonamide

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‡ These authors contributed equally

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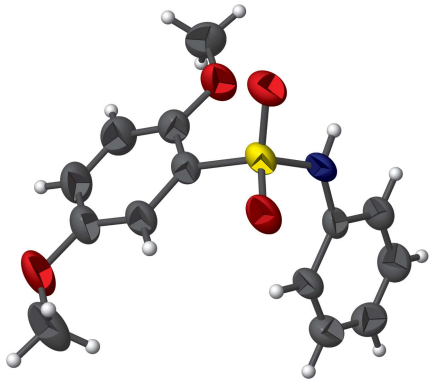
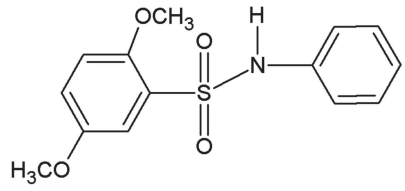
Structural data: full structural data are available from iucrdata.iucr.org

The molecule of the title compound, $C_{14}H_{15}NO_4S$, is L-shaped, with the central C—S—N—C segment having a torsion angle of −62.9 (2)°. The dihedral angle between the benzene rings is 89.17 (9)°. The C atoms of the methoxy groups are close to coplanar with their attached benzene ring [deviations = 0.084 (4) and −0.192 (5) Å]. An intramolecular C—H···O hydrogen bond occurs. In the crystal, inversion dimers linked by pairs of N—H···O(S) hydrogen bonds generate $R_2^2(8)$ loops.

3D view



Chemical scheme



Structure description

In recent years, extensive research has been carried out on the synthesis and evaluation of the pharmacological activities of molecules containing the sulfonamide moiety (Mohan *et al.*, 2013). As part of our ongoing studies on sulfonamides (Suchetan *et al.*, 2016), we report herein the crystal structure of the title compound.

The molecule of the title compound (Fig. 1) is L-shaped with the central C1—S1—N1—C7 segment having a torsion angle of −62.9 (2)° and the dihedral angle between the benzene rings being 89.17 (9)°. The two methoxy groups are close to coplanar with their attached benzene ring, the values of the torsion angles of the segment C1—C2—O3—C13 and C6—C5—O4—C14, respectively, being −175.2 (3) and −6.0 (5)°. The molecular conformation is consolidated by an intramolecular C12—H12···O1 hydrogen bond (Table 1) forming a closed $S(6)$ motif.

The crystal structure features inversion-related $R_2^2(8)$ dimers linked by pairs of N1—H1···O2^{i} (Table 1 and Fig. 2) hydrogen bonds.

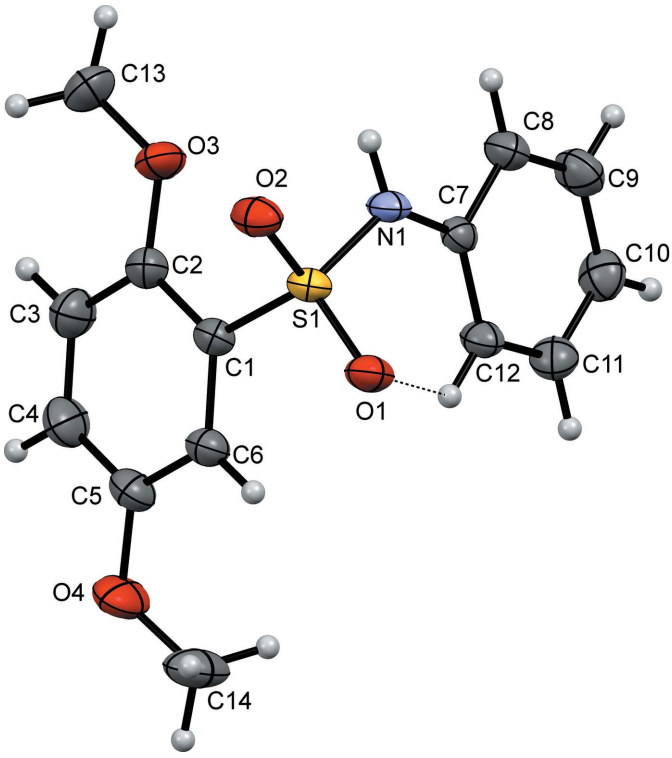


Figure 1
A view of the molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level. The intramolecular hydrogen bond is indicated by a dashed line.

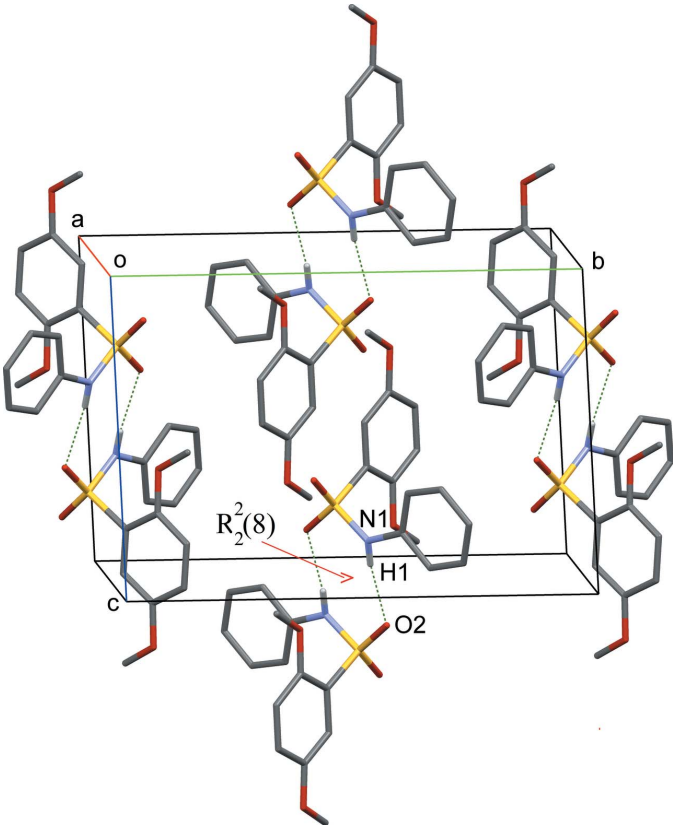


Figure 2
A view of the $R_2^2(8)$ loops displayed in the crystal structure of the title compound due to N—H···O hydrogen bonds (dashed lines, see Table 1).

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O1	0.93	2.52	3.1128	121
N1—H1···O2^{i}	0.85	2.17	3.0116 (10)	170

Symmetry code: (i) $-x+1, -y+2, -z+1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{15}NO_4S$
M_r	293.33
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	10.4328 (12), 14.3157 (15), 10.4869 (12)
β (°)	117.064 (6)
V (Å^3)	1394.7 (3)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.19
Crystal size (mm)	0.28 × 0.22 × 0.17
Data collection	
Diffractometer	Bruker APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.589, 0.689
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10083, 2305, 1943
R_{int}	0.065
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.586
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.067, 0.186, 1.04
No. of reflections	2305
No. of parameters	188
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.33

Computer programs: *APEX2*, *SAINT-Plus* and *XPREP* (Bruker, 2009), *SHELXT2016* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*) and *Mercury* (Macrae *et al.*, 2008).

Synthesis and crystallization

The title compound was prepared according to a literature method (Vinola *et al.*, 2015). The purity of the compound was checked by determining its melting point. Prismatic single crystals suitable for X-ray diffraction study were obtained by slow evaporation of an ethanolic solution of the compound at room temperature.

Refinement

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

Acknowledgements

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the single-crystal X-ray diffraction data. KS is thankful to the University Grants Commission (UGC), New Delhi for the financial assistance under its MRP scheme.

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full crystallographic data

IUCrData (2017). **2**, x170311 [https://doi.org/10.1107/S2414314617003111X]

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Crystal data

$C_{14}H_{15}NO_4S$
M_r = 293.33
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 10.4328 (12) Å
b = 14.3157 (15) Å
c = 10.4869 (12) Å
β = 117.064 (6)°
V = 1394.7 (3) Å^3
Z = 4
$F(000)$ = 616
Prism
D_x = 1.397 Mg m^{-3}
Melting point: 439 K
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 143 reflections
θ = 7.8–64.5°
μ = 2.19 mm^{-1}
T = 296 K
Prism, colourless
0.28 × 0.22 × 0.17 mm

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.589, T_{max} = 0.689
10083 measured reflections
2305 independent reflections
1943 reflections with $I > 2\sigma(I)$
R_{int} = 0.065
θ_{max} = 64.5°, θ_{min} = 7.8°
h = −12→11
k = −16→16
l = −12→11
1 standard reflections every 1 reflections
intensity decay: 0.1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.186
S = 1.04
2305 reflections
188 parameters
1 restraint
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1364P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Extinction correction: SHELXL2016 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0106 (19)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3763 (3)	0.95415 (17)	0.1449 (3)	0.0446 (6)
C2	0.4926 (3)	0.8928 (2)	0.2056 (3)	0.0554 (7)
C3	0.5215 (4)	0.8363 (2)	0.1138 (4)	0.0729 (9)
H3	0.598056	0.794521	0.151637	0.087*
C4	0.4387 (4)	0.8413 (3)	−0.0311 (4)	0.0770 (10)
H4	0.460099	0.803009	−0.090500	0.092*
C5	0.3243 (3)	0.9021 (2)	−0.0908 (3)	0.0629 (8)
C6	0.2922 (3)	0.95933 (18)	−0.0021 (3)	0.0517 (7)
H6	0.215095	1.000645	−0.040936	0.062*
C7	0.1886 (3)	0.89741 (16)	0.3259 (3)	0.0408 (6)
C8	0.1959 (3)	0.8411 (2)	0.4360 (3)	0.0560 (7)
H8	0.272972	0.846112	0.527111	0.067*
C9	0.0868 (4)	0.7771 (2)	0.4089 (4)	0.0691 (9)
H9	0.090240	0.739609	0.482882	0.083*
C10	−0.0254 (3)	0.7683 (2)	0.2754 (3)	0.0642 (8)
H10	−0.097532	0.724621	0.258041	0.077*
C11	−0.0312 (3)	0.8241 (2)	0.1673 (3)	0.0592 (7)
H11	−0.108127	0.818391	0.076232	0.071*
C12	0.0749 (3)	0.88843 (18)	0.1910 (3)	0.0490 (7)
H12	0.070090	0.925756	0.116314	0.059*
C13	0.6919 (3)	0.8361 (3)	0.4161 (4)	0.0818 (10)
H13A	0.666377	0.771490	0.394795	0.123*
H13B	0.736012	0.845323	0.517872	0.123*
H13C	0.758229	0.853612	0.380173	0.123*
C14	0.1182 (5)	0.9532 (3)	−0.3002 (4)	0.0897 (12)
H14A	0.056384	0.935813	−0.258691	0.135*
H14B	0.070058	0.941372	−0.401306	0.135*
H14C	0.140914	1.018497	−0.283666	0.135*
N1	0.3015 (3)	0.96370 (15)	0.3628 (2)	0.0477 (6)
O1	0.2068 (2)	1.07776 (12)	0.16321 (19)	0.0545 (6)
O2	0.4588 (2)	1.08222 (13)	0.3458 (2)	0.0583 (6)
O3	0.5672 (2)	0.89154 (16)	0.3507 (2)	0.0716 (7)
O4	0.2466 (3)	0.90022 (19)	−0.2364 (2)	0.0871 (8)
S1	0.33445 (6)	1.02855 (4)	0.25483 (6)	0.0437 (3)
H1	0.375 (2)	0.9564 (18)	0.443 (2)	0.050 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0469 (15)	0.0512 (13)	0.0360 (14)	0.0014 (11)	0.0191 (12)	0.0032 (10)
C2	0.0495 (15)	0.0704 (17)	0.0467 (16)	0.0083 (13)	0.0223 (13)	0.0076 (13)
C3	0.0640 (19)	0.087 (2)	0.068 (2)	0.0248 (17)	0.0306 (17)	0.0030 (16)
C4	0.077 (2)	0.100 (2)	0.062 (2)	0.0176 (19)	0.0388 (18)	−0.0133 (17)
C5	0.070 (2)	0.0805 (19)	0.0414 (17)	0.0047 (16)	0.0285 (15)	−0.0040 (13)
C6	0.0559 (17)	0.0604 (15)	0.0372 (15)	0.0038 (12)	0.0199 (13)	0.0033 (11)
C7	0.0440 (13)	0.0473 (13)	0.0334 (13)	0.0067 (10)	0.0196 (10)	−0.0005 (10)
C8	0.0577 (16)	0.0681 (17)	0.0401 (15)	0.0002 (13)	0.0204 (13)	0.0067 (12)
C9	0.080 (2)	0.0732 (19)	0.0603 (19)	−0.0054 (16)	0.0372 (17)	0.0132 (15)
C10	0.0610 (18)	0.0627 (17)	0.071 (2)	−0.0115 (14)	0.0316 (16)	−0.0060 (14)
C11	0.0561 (16)	0.0654 (17)	0.0498 (17)	−0.0063 (13)	0.0186 (13)	−0.0098 (13)
C12	0.0509 (15)	0.0578 (15)	0.0345 (14)	−0.0051 (12)	0.0161 (11)	−0.0023 (11)
C13	0.0550 (19)	0.107 (3)	0.072 (2)	0.0266 (18)	0.0196 (16)	0.0222 (19)
C14	0.110 (3)	0.102 (3)	0.0386 (18)	0.032 (2)	0.018 (2)	0.0003 (18)
N1	0.0444 (13)	0.0642 (14)	0.0255 (12)	−0.0043 (10)	0.0079 (10)	0.0028 (9)
O1	0.0630 (12)	0.0582 (11)	0.0360 (10)	0.0137 (9)	0.0170 (9)	0.0046 (7)
O2	0.0625 (12)	0.0601 (11)	0.0430 (11)	−0.0144 (9)	0.0160 (9)	−0.0012 (8)
O3	0.0617 (13)	0.0988 (16)	0.0441 (12)	0.0310 (11)	0.0151 (10)	0.0137 (10)
O4	0.0956 (18)	0.122 (2)	0.0404 (12)	0.0229 (15)	0.0278 (12)	−0.0134 (12)
S1	0.0481 (5)	0.0484 (5)	0.0295 (5)	0.0005 (2)	0.0130 (3)	0.0020 (2)

Geometric parameters (Å, º)

C1—C6	1.386 (4)	C9—H9	0.9300
C1—C2	1.395 (4)	C10—C11	1.366 (4)
C1—S1	1.764 (3)	C10—H10	0.9300
C2—O3	1.359 (3)	C11—C12	1.373 (4)
C2—C3	1.391 (4)	C11—H11	0.9300
C3—C4	1.366 (5)	C12—H12	0.9300
C3—H3	0.9300	C13—O3	1.407 (4)
C4—C5	1.376 (4)	C13—H13A	0.9600
C4—H4	0.9300	C13—H13B	0.9600
C5—O4	1.365 (4)	C13—H13C	0.9600
C5—C6	1.390 (4)	C14—O4	1.416 (4)
C6—H6	0.9300	C14—H14A	0.9600
C7—C12	1.378 (4)	C14—H14B	0.9600
C7—C8	1.382 (4)	C14—H14C	0.9600
C7—N1	1.422 (3)	N1—S1	1.618 (2)
C8—C9	1.387 (4)	N1—H1	0.849 (18)
C8—H8	0.9300	O1—S1	1.4240 (19)
C9—C10	1.362 (4)	O2—S1	1.4345 (19)
C6—C1—C2	121.3 (2)	C10—C11—C12	121.0 (3)
C6—C1—S1	118.3 (2)	C10—C11—H11	119.5
C2—C1—S1	120.3 (2)	C12—C11—H11	119.5

O3—C2—C3	125.0 (3)	C11—C12—C7	119.7 (2)
O3—C2—C1	117.1 (2)	C11—C12—H12	120.2
C3—C2—C1	117.9 (3)	C7—C12—H12	120.2
C4—C3—C2	120.8 (3)	O3—C13—H13A	109.5
C4—C3—H3	119.6	O3—C13—H13B	109.5
C2—C3—H3	119.6	H13A—C13—H13B	109.5
C3—C4—C5	121.2 (3)	O3—C13—H13C	109.5
C3—C4—H4	119.4	H13A—C13—H13C	109.5
C5—C4—H4	119.4	H13B—C13—H13C	109.5
O4—C5—C4	116.5 (3)	O4—C14—H14A	109.5
O4—C5—C6	124.0 (3)	O4—C14—H14B	109.5
C4—C5—C6	119.4 (3)	H14A—C14—H14B	109.5
C1—C6—C5	119.3 (3)	O4—C14—H14C	109.5
C1—C6—H6	120.3	H14A—C14—H14C	109.5
C5—C6—H6	120.3	H14B—C14—H14C	109.5
C12—C7—C8	119.9 (2)	C7—N1—S1	127.30 (18)
C12—C7—N1	124.1 (2)	C7—N1—H1	116.7 (19)
C8—C7—N1	116.0 (2)	S1—N1—H1	113 (2)
C7—C8—C9	119.1 (3)	C2—O3—C13	119.0 (2)
C7—C8—H8	120.4	C5—O4—C14	118.0 (2)
C9—C8—H8	120.4	O1—S1—O2	117.96 (12)
C10—C9—C8	120.9 (3)	O1—S1—N1	108.95 (12)
C10—C9—H9	119.6	O2—S1—N1	104.93 (11)
C8—C9—H9	119.6	O1—S1—C1	106.93 (11)
C9—C10—C11	119.5 (3)	O2—S1—C1	109.90 (12)
C9—C10—H10	120.3	N1—S1—C1	107.79 (13)
C11—C10—H10	120.3		

C6—C1—C2—O3	−178.9 (3)	C10—C11—C12—C7	−0.4 (4)
S1—C1—C2—O3	2.0 (3)	C8—C7—C12—C11	0.6 (4)
C6—C1—C2—C3	−0.4 (4)	N1—C7—C12—C11	−177.9 (2)
S1—C1—C2—C3	−179.5 (2)	C12—C7—N1—S1	−10.5 (4)
O3—C2—C3—C4	178.8 (3)	C8—C7—N1—S1	170.9 (2)
C1—C2—C3—C4	0.4 (5)	C3—C2—O3—C13	6.4 (5)
C2—C3—C4—C5	−0.2 (6)	C1—C2—O3—C13	−175.2 (3)
C3—C4—C5—O4	−178.6 (3)	C4—C5—O4—C14	172.4 (3)
C3—C4—C5—C6	−0.1 (5)	C6—C5—O4—C14	−6.0 (5)
C2—C1—C6—C5	0.1 (4)	C7—N1—S1—O1	52.9 (2)
S1—C1—C6—C5	179.2 (2)	C7—N1—S1—O2	−179.9 (2)
O4—C5—C6—C1	178.5 (3)	C7—N1—S1—C1	−62.9 (2)
C4—C5—C6—C1	0.1 (4)	C6—C1—S1—O1	4.3 (2)
C12—C7—C8—C9	−0.9 (4)	C2—C1—S1—O1	−176.6 (2)
N1—C7—C8—C9	177.8 (2)	C6—C1—S1—O2	−124.9 (2)
C7—C8—C9—C10	1.0 (5)	C2—C1—S1—O2	54.3 (2)
C8—C9—C10—C11	−0.7 (5)	C6—C1—S1—N1	121.3 (2)
C9—C10—C11—C12	0.4 (5)	C2—C1—S1—N1	−59.5 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O1	0.93	2.52	3.1128	121
N1—H1···O2^{i}	0.85	2.17	3.0116 (10)	170

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