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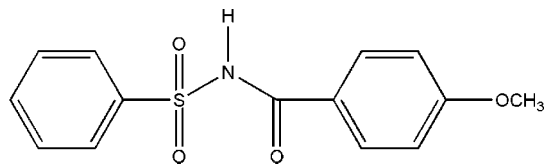
N-(4-Methoxybenzoyl)benzenesulfonamideS. Sreenivasa,^a M. S. Nanjundaswamy,^b S. Madankumar,^c
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.068; wR factor = 0.158; data-to-parameter ratio = 11.7.

In the title compound, $\text{C}_{14}\text{H}_{13}\text{NO}_4\text{S}$, the dihedral angle between the aromatic rings is $69.81(1)^\circ$; the dihedral angle between the planes defined by the $\text{S}-\text{N}-\text{C}=\text{O}$ segment of the central chain and the sulfonyl benzene ring is $74.91(1)^\circ$. In the crystal, the molecules are linked by weak $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds into $C(4)$ chains running along $[100]$. The molecules in adjacent chains are linked by weak $\text{C}-\text{H}\cdots\text{O}$ interactions, generating $R_2^2(16)$ dimeric pairs. Weak $\text{C}-\text{H}\cdots\pi$ interactions connect the double chains into (001) sheets.

Related literature

For similar structures, see: Gowda *et al.* (2009); Suchetan *et al.* (2009, 2010); Sreenivasa *et al.* (2013).

Experimental

Crystal data

 $\text{C}_{14}\text{H}_{13}\text{NO}_4\text{S}$
 $M_r = 291.31$
Triclinic, $P\bar{1}$
 $a = 5.3059(5)$ Å $b = 10.6343(10)$ Å
 $c = 11.9139(11)$ Å
 $\alpha = 89.792(3)^\circ$
 $\beta = 87.392(3)^\circ$ $\gamma = 83.944(3)^\circ$
 $V = 667.79(11)$ Å³
 $Z = 2$
Cu $K\alpha$ radiation $\mu = 2.28$ mm⁻¹
 $T = 293$ K
 $0.37 \times 0.26 \times 0.20$ mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan
(*SADABS*; Bruker, 2009)
 $T_{\text{min}} = 0.515$, $T_{\text{max}} = 0.633$ 8561 measured reflections
2168 independent reflections
2076 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.049$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.068$
 $wR(F^2) = 0.158$
 $S = 1.13$
2168 reflections
186 parameters
1 restraintH atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.33$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.84$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

 C_g is the centroid of the methoxybenzene ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H}\text{N1}\cdots\text{O1}^{\text{i}}$	0.83 (3)	2.41 (3)	3.1662 (3)	153
$\text{C12}-\text{H12}\cdots\text{O2}^{\text{ii}}$	0.93	2.58	3.286 (3)	133
$\text{C4}-\text{H4}\cdots\text{C}_g^{\text{iii}}$	0.93	2.90	3.7396	150

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *APEX2* and *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge the IOE X-ray diffractometer facility, University of Mysore, Mysore, for the data collection.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7187).

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supplementary materials

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N-(4-Methoxybenzoyl)benzenesulfonamide

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1. Introduction

As a part of our continued efforts to study the crystal structures of N-(aroyl)-arylsulfonamides (Suchetan *et al.*, 2009, 2010; Sreenivasa *et al.*, 2013; Gowda *et al.*, 2009), we report here the crystal structure of the title compound (I) (Fig 1).

2. Experimental

2.1. Synthesis and crystallization

The title compound (I) was prepared by refluxing a mixture of 4-methoxybenzoic acid, benzenesulfonamide and phosphorous oxychloride (POCl₃) for 2 h on a water bath. The resultant mixture was cooled and poured into ice cold water. The solid obtained was filtered and washed thoroughly with water and then dissolved in sodium bicarbonate solution. The compound was later reprecipitated by acidifying the filtered solution with dilute HCl. The compound obtained was filtered and later dried (Melting point: 399 K).

Colorless prisms of (I) were obtained from a slow evaporation of its aqueous methanolic solution at room temperature.

2.2. Refinement

The H atom of the NH group was located in a difference map and later restrained to N—H = 0.86 (4) Å. The other H atoms were positioned with idealized geometry using a riding model with C—H = 0.93-0.96 Å. All H atoms were refined with isotropic displacement parameters (set to 1.2-1.5 times of the U eq of the parent atom).

3. Results and discussion

In (I), the dihedral angle between the aromatic rings is 69.81 (1)°. Compared to this, the dihedral angle is 80.3 (1)° in N-(benzoyl)-benzenesulfonamide (II) (Gowda *et al.*, 2009), 68.6 (1)° in N-(4-chlorobenzoyl)-benzenesulfonamide (III) (Suchetan *et al.*, 2009), 71.9 (1)° in N-(4-methylbenzoyl)-benzenesulfonamide (IV) (Suchetan *et al.*, 2010) and 78.62 (16)° in N-(4-methoxybenzoyl)-4-methylbenzenesulfonamide (V) (Sreenivasa *et al.*, 2013). This shows that introducing a substituent into the *para* position of the benzoyl ring correlates with a decrease of the dihedral angle between the aromatic rings. Further, the molecule is twisted at the S atom, the dihedral angle between the planes defined by the S—N—C=O segment in the central chain and the sulfonyl benzene ring being 74.91 (1)°.

In the crystal, both strong classical N—H···O hydrogen bonds and weaker C—H···O and C—H···Cg interactions are observed. The molecules are linked to one another through strong N1—HN1···O1 hydrogen bonds into C(4) chains running along [100]. The molecules in the adjacent chains are linked through weak C12—H12···O2 interactions, generating R₂² (16) dimeric pairs. Combination of the N1—HN1···O1 linked chains and C12—H12···O2 linked dimers form columns along a *axis* (Figure 2 & 3). The molecules are further connected into C(10) chains running along [010] through C4—H4···Cg interactions (Figure 4) resulting in a two dimensional architecture.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *APEX2* and *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

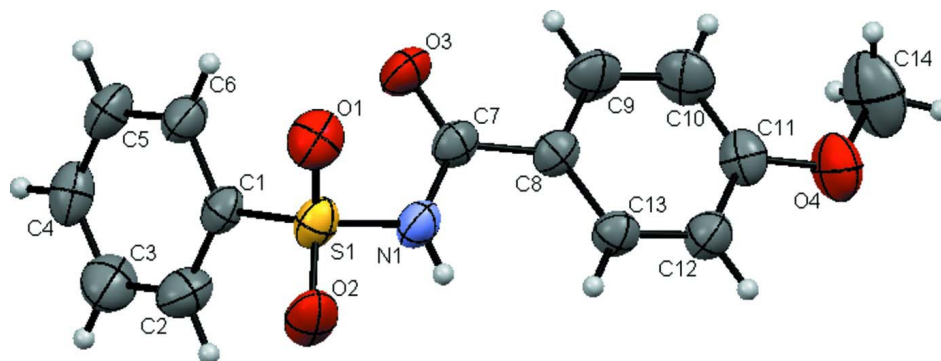


Figure 1

Molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level.

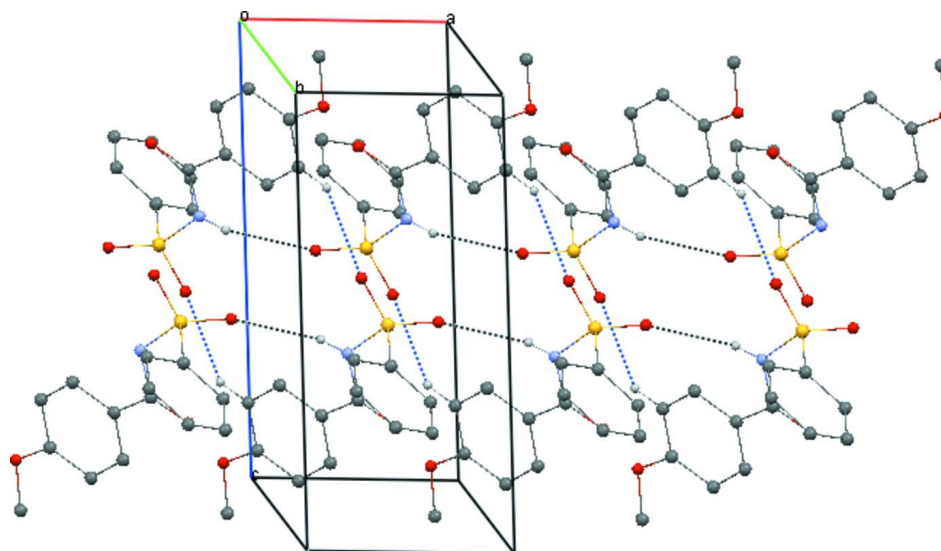


Figure 2

Columns generated from the combination of N1—HN1...O1 linked chains and C12—H12...O2 linked dimers in (I) when viewed along the *a*-axis. H-atoms not involved in H-bonds are omitted for clarity purpose.

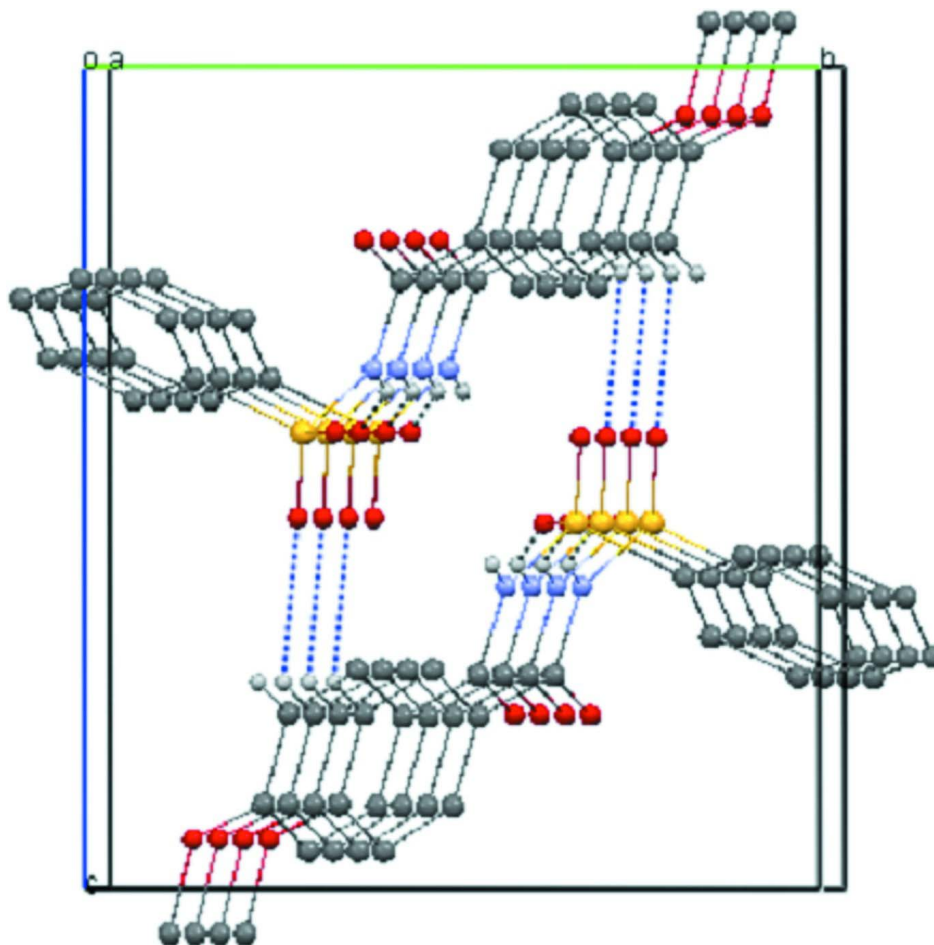


Figure 3

Columns generated from the combination of N1—HN1...O1 linked chains and C12—H12...O2 linked dimers in (I) when viewed down a *axis*. H-atoms not involved in H-bonds are omitted for clarity purpose.

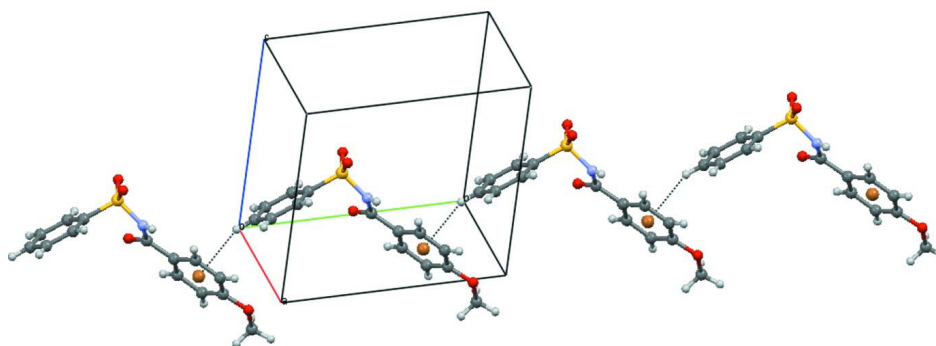


Figure 4

C4—H4...C_g interaction observed in the structure of (I). C_g is the centroid of the methoxyphenyl ring.

***N*-(4-Methoxybenzoyl)benzenesulfonamide**

Crystal data

$C_{14}H_{13}NO_4S$	$F(000) = 304$
$M_r = 291.31$	Prism
Triclinic, $P\bar{1}$	$D_x = 1.449 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Melting point: 399 K
$a = 5.3059 (5) \text{ \AA}$	Cu $K\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$
$b = 10.6343 (10) \text{ \AA}$	Cell parameters from 25 reflections
$c = 11.9139 (11) \text{ \AA}$	$\theta = 3.7\text{--}64.8^\circ$
$\alpha = 89.792 (3)^\circ$	$\mu = 2.28 \text{ mm}^{-1}$
$\beta = 87.392 (3)^\circ$	$T = 293 \text{ K}$
$\gamma = 83.944 (3)^\circ$	Prism, colourless
$V = 667.79 (11) \text{ \AA}^3$	$0.37 \times 0.26 \times 0.20 \text{ mm}$
$Z = 2$	

Data collection

Bruker APEXII diffractometer	2168 independent reflections
Radiation source: fine-focus sealed tube	2076 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\text{int}} = 0.049$
phi and φ scans	$\theta_{\text{max}} = 64.8^\circ$, $\theta_{\text{min}} = 3.7^\circ$
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2009)	$h = -6 \rightarrow 6$
$T_{\text{min}} = 0.515$, $T_{\text{max}} = 0.633$	$k = -12 \rightarrow 12$
8561 measured reflections	$l = -13 \rightarrow 13$
	3 standard reflections every 120 min
	intensity decay: 1%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.068$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.158$	$w = 1/[\sigma^2(F_o^2) + (0.1013P)^2 + 0.1754P]$
$S = 1.13$	where $P = (F_o^2 + 2F_c^2)/3$
2168 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
186 parameters	$\Delta\rho_{\text{max}} = 0.33 \text{ e \AA}^{-3}$
1 restraint	$\Delta\rho_{\text{min}} = -0.84 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.2427 (3)	0.36646 (17)	0.44504 (16)	0.0596 (5)

N1	0.6766 (4)	0.40318 (19)	0.36803 (17)	0.0478 (5)
O3	0.4534 (3)	0.39943 (16)	0.21164 (15)	0.0559 (5)
O4	1.1816 (4)	0.81223 (19)	0.06023 (17)	0.0695 (6)
C13	0.9563 (4)	0.5966 (2)	0.26610 (18)	0.0421 (5)
H13	0.9898	0.5737	0.3398	0.051*
C7	0.6197 (4)	0.4435 (2)	0.25993 (19)	0.0424 (5)
O2	0.6259 (4)	0.30297 (18)	0.54898 (15)	0.0624 (5)
C9	0.7269 (6)	0.5777 (3)	0.1010 (2)	0.0609 (7)
H9	0.6030	0.5417	0.0631	0.073*
C1	0.5310 (4)	0.1655 (2)	0.37956 (18)	0.0405 (5)
C12	1.0878 (4)	0.6857 (2)	0.2130 (2)	0.0475 (6)
H12	1.2101	0.7227	0.2512	0.057*
C8	0.7732 (4)	0.5405 (2)	0.21008 (18)	0.0402 (5)
C11	1.0410 (5)	0.7213 (2)	0.1032 (2)	0.0472 (6)
C5	0.3772 (5)	0.0164 (2)	0.2584 (2)	0.0564 (6)
H5	0.2579	-0.0048	0.2089	0.068*
C3	0.7531 (5)	-0.0405 (3)	0.3552 (3)	0.0649 (8)
H3	0.8890	-0.0996	0.3709	0.078*
C4	0.5776 (5)	-0.0707 (2)	0.2829 (2)	0.0547 (6)
H4	0.5930	-0.1504	0.2500	0.066*
C2	0.7307 (5)	0.0778 (3)	0.4055 (2)	0.0574 (6)
H2	0.8487	0.0979	0.4562	0.069*
C14	1.1590 (10)	0.8451 (4)	-0.0546 (3)	0.0986 (13)
H14A	1.2092	0.7720	-0.1005	0.148*
H14B	1.2665	0.9100	-0.0734	0.148*
H14C	0.9860	0.8757	-0.0676	0.148*
C6	0.3516 (4)	0.1360 (2)	0.3071 (2)	0.0498 (6)
H6	0.2157	0.1948	0.2910	0.060*
C10	0.8596 (6)	0.6669 (3)	0.0467 (2)	0.0635 (7)
H10	0.8267	0.6899	-0.0270	0.076*
S1	0.50162 (10)	0.31426 (5)	0.44550 (4)	0.0452 (3)
HN1	0.808 (6)	0.419 (4)	0.397 (3)	0.091 (12)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0540 (10)	0.0592 (10)	0.0642 (11)	-0.0033 (8)	0.0092 (8)	-0.0138 (8)
N1	0.0543 (12)	0.0501 (11)	0.0432 (11)	-0.0222 (9)	-0.0093 (9)	0.0000 (8)
O3	0.0563 (10)	0.0581 (10)	0.0573 (10)	-0.0197 (8)	-0.0149 (8)	-0.0071 (8)
O4	0.0829 (14)	0.0677 (12)	0.0582 (12)	-0.0183 (10)	0.0158 (10)	0.0140 (9)
C13	0.0460 (12)	0.0463 (11)	0.0348 (11)	-0.0079 (9)	-0.0035 (9)	-0.0026 (9)
C7	0.0460 (12)	0.0400 (11)	0.0419 (12)	-0.0065 (9)	-0.0039 (9)	-0.0105 (9)
O2	0.0851 (13)	0.0689 (11)	0.0385 (9)	-0.0294 (10)	-0.0111 (9)	-0.0024 (8)
C9	0.0753 (18)	0.0729 (17)	0.0393 (13)	-0.0241 (13)	-0.0155 (12)	-0.0048 (11)
C1	0.0383 (11)	0.0445 (11)	0.0403 (11)	-0.0142 (8)	0.0036 (8)	-0.0022 (8)
C12	0.0477 (12)	0.0519 (13)	0.0445 (12)	-0.0126 (10)	-0.0019 (9)	-0.0006 (10)
C8	0.0427 (11)	0.0417 (11)	0.0361 (11)	-0.0047 (9)	0.0001 (9)	-0.0081 (8)
C11	0.0523 (13)	0.0460 (12)	0.0418 (12)	-0.0035 (10)	0.0118 (10)	-0.0010 (9)
C5	0.0568 (14)	0.0537 (14)	0.0624 (16)	-0.0215 (11)	-0.0058 (11)	-0.0110 (11)
C3	0.0542 (15)	0.0558 (15)	0.083 (2)	0.0029 (12)	-0.0004 (14)	-0.0073 (13)

C4	0.0572 (14)	0.0445 (12)	0.0628 (16)	-0.0153 (10)	0.0159 (12)	-0.0095 (10)
C2	0.0450 (13)	0.0652 (15)	0.0628 (15)	-0.0071 (11)	-0.0084 (11)	-0.0083 (12)
C14	0.147 (4)	0.091 (2)	0.0561 (19)	-0.018 (2)	0.032 (2)	0.0156 (17)
C6	0.0449 (12)	0.0469 (12)	0.0598 (14)	-0.0128 (9)	-0.0081 (10)	-0.0050 (10)
C10	0.084 (2)	0.0740 (17)	0.0338 (12)	-0.0134 (14)	-0.0043 (12)	0.0032 (11)
S1	0.0516 (4)	0.0468 (4)	0.0393 (4)	-0.0156 (3)	0.0011 (3)	-0.0074 (2)

Geometric parameters (Å, °)

O1—S1	1.4264 (19)	C1—S1	1.758 (2)
N1—C7	1.392 (3)	C12—C11	1.387 (3)
N1—S1	1.646 (2)	C12—H12	0.9300
N1—HN1	0.82 (3)	C11—C10	1.376 (4)
O3—C7	1.211 (3)	C5—C4	1.376 (4)
O4—C11	1.367 (3)	C5—C6	1.390 (4)
O4—C14	1.418 (4)	C5—H5	0.9300
C13—C12	1.371 (3)	C3—C4	1.360 (4)
C13—C8	1.389 (3)	C3—C2	1.388 (4)
C13—H13	0.9300	C3—H3	0.9300
C7—C8	1.486 (3)	C4—H4	0.9300
O2—S1	1.4232 (19)	C2—H2	0.9300
C9—C10	1.381 (4)	C14—H14A	0.9600
C9—C8	1.382 (3)	C14—H14B	0.9600
C9—H9	0.9300	C14—H14C	0.9600
C1—C6	1.375 (3)	C6—H6	0.9300
C1—C2	1.381 (4)	C10—H10	0.9300
C7—N1—S1	123.91 (17)	C4—C3—C2	120.4 (2)
C7—N1—HN1	122 (3)	C4—C3—H3	119.8
S1—N1—HN1	114 (3)	C2—C3—H3	119.8
C11—O4—C14	118.2 (3)	C3—C4—C5	120.2 (2)
C12—C13—C8	120.1 (2)	C3—C4—H4	119.9
C12—C13—H13	119.9	C5—C4—H4	119.9
C8—C13—H13	119.9	C1—C2—C3	119.2 (2)
O3—C7—N1	120.0 (2)	C1—C2—H2	120.4
O3—C7—C8	123.6 (2)	C3—C2—H2	120.4
N1—C7—C8	116.42 (19)	O4—C14—H14A	109.5
C10—C9—C8	121.9 (2)	O4—C14—H14B	109.5
C10—C9—H9	119.1	H14A—C14—H14B	109.5
C8—C9—H9	119.1	O4—C14—H14C	109.5
C6—C1—C2	121.0 (2)	H14A—C14—H14C	109.5
C6—C1—S1	120.16 (18)	H14B—C14—H14C	109.5
C2—C1—S1	118.81 (18)	C1—C6—C5	118.7 (2)
C13—C12—C11	120.9 (2)	C1—C6—H6	120.6
C13—C12—H12	119.5	C5—C6—H6	120.6
C11—C12—H12	119.5	C11—C10—C9	119.1 (2)
C9—C8—C13	118.3 (2)	C11—C10—H10	120.4
C9—C8—C7	117.3 (2)	C9—C10—H10	120.4
C13—C8—C7	124.4 (2)	O2—S1—O1	119.44 (12)
O4—C11—C10	125.0 (2)	O2—S1—N1	103.74 (11)

O4—C11—C12	115.3 (2)	O1—S1—N1	109.21 (11)
C10—C11—C12	119.6 (2)	O2—S1—C1	108.88 (11)
C4—C5—C6	120.5 (2)	O1—S1—C1	108.65 (10)
C4—C5—H5	119.7	N1—S1—C1	106.11 (10)
C6—C5—H5	119.7		
S1—N1—C7—O3	-10.3 (3)	S1—C1—C2—C3	179.0 (2)
S1—N1—C7—C8	169.94 (15)	C4—C3—C2—C1	-1.4 (4)
C8—C13—C12—C11	0.0 (3)	C2—C1—C6—C5	-1.2 (4)
C10—C9—C8—C13	1.0 (4)	S1—C1—C6—C5	-178.49 (18)
C10—C9—C8—C7	-179.8 (2)	C4—C5—C6—C1	0.4 (4)
C12—C13—C8—C9	-0.6 (3)	O4—C11—C10—C9	-178.6 (2)
C12—C13—C8—C7	-179.8 (2)	C12—C11—C10—C9	0.1 (4)
O3—C7—C8—C9	-2.4 (3)	C8—C9—C10—C11	-0.7 (4)
N1—C7—C8—C9	177.3 (2)	C7—N1—S1—O2	-177.30 (19)
O3—C7—C8—C13	176.8 (2)	C7—N1—S1—O1	-48.9 (2)
N1—C7—C8—C13	-3.5 (3)	C7—N1—S1—C1	68.0 (2)
C14—O4—C11—C10	-6.6 (4)	C6—C1—S1—O2	153.0 (2)
C14—O4—C11—C12	174.7 (3)	C2—C1—S1—O2	-24.3 (2)
C13—C12—C11—O4	179.0 (2)	C6—C1—S1—O1	21.4 (2)
C13—C12—C11—C10	0.2 (4)	C2—C1—S1—O1	-155.9 (2)
C2—C3—C4—C5	0.6 (4)	C6—C1—S1—N1	-95.9 (2)
C6—C5—C4—C3	-0.1 (4)	C2—C1—S1—N1	86.8 (2)
C6—C1—C2—C3	1.7 (4)		

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

Cg is the centroid of the methoxybenzene ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—HM1 \cdots O1 ⁱ	0.83 (3)	2.41 (3)	3.1662 (3)	153
C12—H12 \cdots O2 ⁱⁱ	0.93	2.58	3.286 (3)	133
C4—H4 \cdots Cg ⁱⁱⁱ	0.93	2.90	3.7396	150

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