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# *N*-(2-Methoxyphenyl)benzene-sulfonamide

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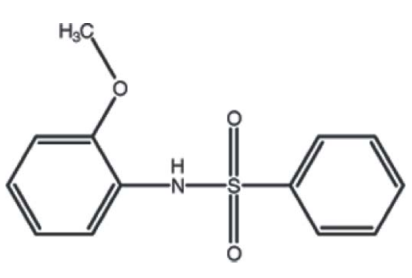
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.047; $wR$ factor = 0.113; data-to-parameter ratio = 19.0.

The asymmetric unit of the title compound, $C_{13}H_{13}NO_3S$, contains two crystallographically independent molecules in which the dihedral angles between the phenyl and benzene rings are 88.16 (12) and 44.50 (12)°. One of the molecules features an intramolecular N—H···O hydrogen bond. In the crystal, the molecules are linked into dimers by pairs of N—H···O hydrogen bonds. The dimers are further connected by C—H···O and C—H···$\pi$ interactions, forming a three-dimensional network.

## Related literature

For the biological activity of sulfonamides, see: Arshad *et al.* (2008); Gennarti *et al.* (1994); Kayser *et al.* (2004); Rough *et al.* (1998).




## Experimental

### Crystal data

$C_{13}H_{13}NO_3S$
$M_r$ = 263.31
Monoclinic, $P2_1/n$
$a$ = 8.7705 (2) Å
$b$ = 28.1684 (7) Å
$c$ = 10.7256 (3) Å
$\beta$ = 105.968 (1)°
$V$ = 2547.53 (11) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.25 mm$^{-1}$
$T$ = 296 K
0.25 × 0.17 × 0.07 mm

### Data collection

Bruker APEXII CCD diffractometer
24823 measured reflections
6318 independent reflections
4145 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.043

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.113
$S$ = 1.02
6318 reflections
333 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

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

*Cg*4 is the centroid of the C7′–C12′ phenyl ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1′—H1*N*′···O2 | 0.828 (18) | 2.310 (17) | 3.074 (2) | 153.6 (17) |
| N1—H1*N*···O1′ | 0.843 (17) | 2.129 (17) | 2.961 (2) | 168.7 (17) |
| N1—H1*N*···O3 | 0.843 (17) | 2.258 (18) | 2.592 (2) | 103.8 (14) |
| C4—H4···O2′$^{i}$ | 0.93 | 2.47 | 3.377 (3) | 167 |
| C4′—H4′···*Cg*4$^{ii}$ | 0.93 | 2.85 | 3.601 (2) | 138 |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

The authors are grateful to the Higher Education Commission of Pakistan for financial support to purchase the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5501).

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## supplementary materials

*Acta Cryst.* (2010). E**66**, o1769 [ doi:10.1107/S1600536810023871 ]

## *N*-(2-Methoxyphenyl)benzenesulfonamide

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### Comment

Sulfonamides are well known for their enormous potential as biologically active molecules (Rough *et al.*, 1998) in areas such as anti-microbial (Kayser *et al.*, 2004), anti-convulsant (Arshad *et al.*, 2008), anti-cancer agents and for the treatment of inflammatory rheumatic and non-rheumatic processes including onsets and traumatologic lesions (Gennarti *et al.*, 1994). In the present paper, the structure of *N*-(2-methoxyphenyl)benzene sulfonamide has been determined as part of a research program involving the synthesis and biological evaluation of sulfur containing compounds.

In the crystal structure of the title compound (I), (Fig. 1), there exist two independent molecules, A (with S1) and B (with S1'). Both independent molecules are bent at their *S* atoms with the C—S—N(H)—C torsion angles of 67.25 (15)° in molecule A and -81.17 (16)° in molecule B. The dihedral angles between the phenyl and benzene rings is 88.16 (12)° in molecule A and 44.50 (12)° in molecule B.

Molecular packing of (I) is stabilized by N–H···O, C—H···O interactions and C—H···π interactions, forming a three dimensional network (Table 1). Fig. 2 shows N—H···O hydrogen bonds between the molecules A and B in the asymmetric unit.

### Experimental

A mixture benzenesulfonyl chloride (10.0 mmol; 1.45 ml), *ortho*-methoxy aniline (*o*-anisidine) (10.0 mmol; 1.12 ml), aqueous sodium carbonate (10%; 15.0 ml) and water (25 ml) was stirred for one hour at room temperature. The crude mixture was washed with water and dried. The product was dissolved in methanol and recrystallized by slow evaporation of the solvent, to generate colourless blocks of (I) in 74% yield.

### Refinement

The H atoms of the NH groups were located in a difference Fourier map and refined with the N—H distance restrained to 0.86 (2) %A. The other H atoms were positioned geometrically using a riding model with C–H = 0.93 and 0.96 Å. All H atoms were refined with isotropic displacement parameters with $U_{iso}$(H) = 1.2$U_{eq}$(aromatic, NH) and $U_{iso}$(H) = 1.5$U_{eq}$(methyl).

### Figures

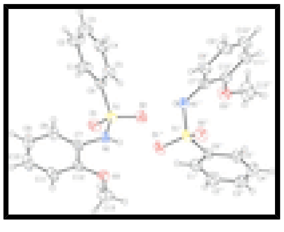

Fig. 1. View of the two independent molecules in the asymmetric unit of (I0 with displacement ellipsoids drawn at the 30% probability level.

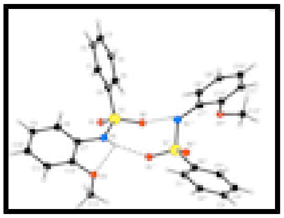

Fig. 2. View of N—H···O hydrogen bonds shown as dashed lines between the two independent molecules in the asymmetric unit.

### *N*-(2-Methoxyphenyl)benzenesulfonamide

*Crystal data*

| | |
|---|---|
| $C_{13}H_{13}NO_3S$ | $F(000) = 1104$ |
| $M_r = 263.31$ | $D_x = 1.373$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2yn | Cell parameters from 5117 reflections |
| $a = 8.7705$ (2) Å | $\theta = 2.5–23.9°$ |
| $b = 28.1684$ (7) Å | $\mu = 0.25$ mm$^{-1}$ |
| $c = 10.7256$ (3) Å | $T = 296$ K |
| $\beta = 105.968$ (1)° | Block, colourless |
| $V = 2547.53$ (11) Å$^3$ | 0.25 × 0.17 × 0.07 mm |
| $Z = 8$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 4145 reflections with $I > 2\sigma(I)$ |
| Radiation source: sealed tube | $R_{int} = 0.043$ |
| graphite | $\theta_{max} = 28.3°$, $\theta_{min} = 3.3°$ |
| φ and ω scans | $h = -11 \rightarrow 11$ |
| 24823 measured reflections | $k = -37 \rightarrow 37$ |
| 6318 independent reflections | $l = -14 \rightarrow 14$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.047$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.113$ | H atoms treated by a mixture of independent and constrained refinement |
| $S = 1.02$ | $w = 1/[\sigma^2(F_o^2) + (0.0488P)^2 + 0.3381P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 6318 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 333 parameters | $\Delta\rho_{max} = 0.29$ e Å$^{-3}$ |
| 2 restraints | $\Delta\rho_{min} = -0.29$ e Å$^{-3}$ |

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement on $F^2$ for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.33115 (5) | 0.81887 (2) | 0.56961 (5) | 0.0412 (2) |
| O1 | 0.29814 (16) | 0.77142 (5) | 0.59898 (15) | 0.0561 (5) |
| O2 | 0.21225 (14) | 0.84480 (5) | 0.47617 (14) | 0.0518 (5) |
| O3 | 0.68975 (15) | 0.82034 (5) | 0.38159 (14) | 0.0507 (5) |
| N1 | 0.48440 (18) | 0.81979 (6) | 0.51516 (16) | 0.0430 (5) |
| C1 | 0.3503 (3) | 0.83266 (9) | 0.8243 (2) | 0.0681 (9) |
| C2 | 0.3878 (4) | 0.85873 (11) | 0.9379 (3) | 0.0865 (11) |
| C3 | 0.4523 (3) | 0.90282 (11) | 0.9397 (3) | 0.0764 (10) |
| C4 | 0.4848 (3) | 0.92123 (8) | 0.8326 (3) | 0.0663 (9) |
| C5 | 0.4496 (2) | 0.89536 (7) | 0.7189 (2) | 0.0511 (7) |
| C6 | 0.3823 (2) | 0.85108 (7) | 0.71581 (19) | 0.0424 (6) |
| C7 | 0.6322 (2) | 0.79744 (6) | 0.57144 (18) | 0.0388 (6) |
| C8 | 0.6717 (3) | 0.77602 (7) | 0.6914 (2) | 0.0536 (7) |
| C9 | 0.8209 (3) | 0.75621 (9) | 0.7392 (3) | 0.0681 (9) |
| C10 | 0.9276 (3) | 0.75748 (9) | 0.6684 (3) | 0.0728 (9) |
| C11 | 0.8897 (2) | 0.77854 (8) | 0.5478 (3) | 0.0596 (8) |
| C12 | 0.7411 (2) | 0.79839 (6) | 0.4983 (2) | 0.0417 (6) |
| C13 | 0.7966 (3) | 0.82674 (9) | 0.3050 (2) | 0.0653 (9) |
| S1' | 0.31232 (5) | 0.92918 (2) | 0.25688 (5) | 0.0434 (2) |
| O1' | 0.41671 (16) | 0.89021 (5) | 0.30204 (16) | 0.0599 (5) |
| O2' | 0.37153 (17) | 0.97058 (5) | 0.21000 (15) | 0.0587 (5) |
| O3' | −0.07087 (16) | 0.95549 (5) | 0.29180 (16) | 0.0619 (5) |
| N1' | 0.24881 (18) | 0.94574 (6) | 0.37937 (16) | 0.0432 (6) |
| C1' | 0.1023 (3) | 0.86096 (7) | 0.1393 (2) | 0.0540 (7) |
| C2' | −0.0250 (3) | 0.84437 (9) | 0.0434 (3) | 0.0675 (9) |
| C3' | −0.1041 (3) | 0.87391 (10) | −0.0551 (2) | 0.0720 (10) |
| C4' | −0.0567 (3) | 0.92019 (9) | −0.0586 (2) | 0.0687 (9) |
| C5' | 0.0710 (3) | 0.93721 (8) | 0.0355 (2) | 0.0542 (7) |
| C6' | 0.1504 (2) | 0.90740 (7) | 0.13445 (18) | 0.0412 (6) |
| C7' | 0.1746 (2) | 0.99118 (7) | 0.37841 (18) | 0.0415 (6) |
| C8' | 0.2668 (3) | 1.02998 (7) | 0.4245 (2) | 0.0570 (8) |
| C9' | 0.1992 (3) | 1.07399 (8) | 0.4279 (3) | 0.0711 (10) |

| | | | | |
|---|---|---|---|---|
| C10' | 0.0390 (3) | 1.07863 (9) | 0.3853 (3) | 0.0694 (10) |
| C11' | −0.0561 (3) | 1.04027 (8) | 0.3392 (2) | 0.0593 (8) |
| C12' | 0.0103 (2) | 0.99586 (7) | 0.33485 (19) | 0.0453 (7) |
| C13' | −0.2368 (3) | 0.95970 (11) | 0.2309 (3) | 0.0931 (13) |
| H1 | 0.30370 | 0.80290 | 0.82150 | 0.0820* |
| H1N | 0.476 (2) | 0.8381 (6) | 0.4514 (17) | 0.0520* |
| H2 | 0.36910 | 0.84620 | 1.01260 | 0.1040* |
| H3 | 0.47460 | 0.92060 | 1.01560 | 0.0910* |
| H4 | 0.53060 | 0.95110 | 0.83600 | 0.0800* |
| H5 | 0.47120 | 0.90770 | 0.64510 | 0.0610* |
| H8 | 0.59870 | 0.77490 | 0.74000 | 0.0640* |
| H9 | 0.84830 | 0.74190 | 0.82050 | 0.0820* |
| H10 | 1.02730 | 0.74400 | 0.70170 | 0.0870* |
| H11 | 0.96360 | 0.77940 | 0.50010 | 0.0710* |
| H13A | 0.88270 | 0.84670 | 0.35050 | 0.0980* |
| H13B | 0.74210 | 0.84140 | 0.22420 | 0.0980* |
| H13C | 0.83730 | 0.79650 | 0.28840 | 0.0980* |
| H1' | 0.15550 | 0.84110 | 0.20650 | 0.0650* |
| H1N' | 0.210 (2) | 0.9225 (6) | 0.4068 (19) | 0.0520* |
| H2' | −0.05770 | 0.81300 | 0.04530 | 0.0810* |
| H3' | −0.19020 | 0.86250 | −0.11970 | 0.0860* |
| H4' | −0.11130 | 0.94010 | −0.12520 | 0.0820* |
| H5' | 0.10370 | 0.96850 | 0.03280 | 0.0650* |
| H8' | 0.37640 | 1.02660 | 0.45380 | 0.0680* |
| H9' | 0.26260 | 1.10020 | 0.45910 | 0.0850* |
| H10' | −0.00680 | 1.10830 | 0.38740 | 0.0830* |
| H11' | −0.16560 | 1.04410 | 0.31080 | 0.0710* |
| H13D | −0.28950 | 0.97050 | 0.29310 | 0.1400* |
| H13E | −0.27860 | 0.92930 | 0.19770 | 0.1400* |
| H13F | −0.25390 | 0.98210 | 0.16090 | 0.1400* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0350 (2) | 0.0431 (3) | 0.0485 (3) | 0.0004 (2) | 0.0165 (2) | −0.0006 (2) |
| O1 | 0.0577 (9) | 0.0437 (8) | 0.0721 (11) | −0.0080 (7) | 0.0265 (8) | −0.0027 (7) |
| O2 | 0.0329 (7) | 0.0658 (9) | 0.0574 (9) | 0.0070 (6) | 0.0137 (6) | 0.0053 (7) |
| O3 | 0.0403 (7) | 0.0654 (9) | 0.0508 (8) | 0.0048 (7) | 0.0200 (6) | 0.0008 (7) |
| N1 | 0.0351 (8) | 0.0546 (10) | 0.0419 (9) | 0.0105 (7) | 0.0148 (7) | 0.0079 (7) |
| C1 | 0.0940 (18) | 0.0595 (15) | 0.0663 (16) | −0.0063 (13) | 0.0479 (14) | −0.0035 (12) |
| C2 | 0.114 (2) | 0.098 (2) | 0.0639 (18) | 0.0013 (19) | 0.0522 (17) | −0.0102 (16) |
| C3 | 0.0722 (17) | 0.093 (2) | 0.0642 (17) | 0.0062 (15) | 0.0193 (14) | −0.0275 (15) |
| C4 | 0.0516 (13) | 0.0576 (15) | 0.0858 (19) | −0.0042 (11) | 0.0126 (13) | −0.0189 (13) |
| C5 | 0.0466 (11) | 0.0494 (12) | 0.0588 (14) | −0.0019 (10) | 0.0169 (10) | 0.0001 (10) |
| C6 | 0.0410 (10) | 0.0436 (11) | 0.0469 (11) | 0.0050 (8) | 0.0195 (9) | 0.0004 (9) |
| C7 | 0.0333 (9) | 0.0354 (10) | 0.0463 (11) | 0.0035 (8) | 0.0084 (8) | −0.0031 (8) |
| C8 | 0.0521 (12) | 0.0505 (13) | 0.0560 (13) | 0.0049 (10) | 0.0114 (10) | 0.0089 (10) |
| C9 | 0.0635 (15) | 0.0601 (15) | 0.0686 (16) | 0.0082 (12) | −0.0022 (13) | 0.0190 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10 | 0.0448 (12) | 0.0618 (16) | 0.101 (2) | 0.0167 (11) | 0.0017 (13) | 0.0162 (14) |
| C11 | 0.0365 (11) | 0.0537 (13) | 0.0886 (18) | 0.0076 (10) | 0.0174 (11) | −0.0007 (12) |
| C12 | 0.0328 (9) | 0.0362 (10) | 0.0543 (12) | 0.0000 (8) | 0.0091 (8) | −0.0062 (9) |
| C13 | 0.0596 (13) | 0.0753 (16) | 0.0730 (16) | −0.0073 (12) | 0.0383 (13) | −0.0062 (13) |
| S1' | 0.0351 (2) | 0.0419 (3) | 0.0543 (3) | 0.0050 (2) | 0.0143 (2) | 0.0066 (2) |
| O1' | 0.0452 (8) | 0.0579 (9) | 0.0768 (11) | 0.0199 (7) | 0.0172 (7) | 0.0121 (8) |
| O2' | 0.0542 (8) | 0.0521 (9) | 0.0770 (11) | −0.0079 (7) | 0.0304 (8) | 0.0062 (8) |
| O3' | 0.0368 (7) | 0.0664 (10) | 0.0780 (11) | −0.0051 (7) | 0.0085 (7) | −0.0066 (8) |
| N1' | 0.0405 (9) | 0.0425 (10) | 0.0463 (10) | 0.0013 (7) | 0.0113 (7) | 0.0067 (7) |
| C1' | 0.0641 (13) | 0.0433 (12) | 0.0555 (13) | 0.0007 (10) | 0.0178 (11) | 0.0076 (10) |
| C2' | 0.0769 (16) | 0.0555 (15) | 0.0686 (16) | −0.0142 (12) | 0.0174 (14) | −0.0068 (12) |
| C3' | 0.0709 (16) | 0.0831 (19) | 0.0549 (15) | −0.0082 (14) | 0.0053 (12) | −0.0136 (13) |
| C4' | 0.0729 (16) | 0.0741 (17) | 0.0503 (14) | 0.0100 (13) | 0.0023 (12) | 0.0064 (12) |
| C5' | 0.0635 (13) | 0.0466 (12) | 0.0515 (13) | 0.0081 (10) | 0.0141 (11) | 0.0089 (10) |
| C6' | 0.0431 (10) | 0.0406 (11) | 0.0429 (11) | 0.0061 (8) | 0.0168 (9) | 0.0027 (8) |
| C7' | 0.0403 (10) | 0.0456 (11) | 0.0391 (10) | 0.0035 (8) | 0.0120 (8) | 0.0001 (8) |
| C8' | 0.0460 (11) | 0.0542 (13) | 0.0696 (15) | −0.0039 (10) | 0.0141 (11) | −0.0114 (11) |
| C9' | 0.0695 (16) | 0.0507 (14) | 0.094 (2) | −0.0067 (12) | 0.0242 (14) | −0.0202 (13) |
| C10' | 0.0766 (17) | 0.0563 (15) | 0.0807 (18) | 0.0155 (13) | 0.0306 (14) | −0.0106 (13) |
| C11' | 0.0474 (12) | 0.0714 (16) | 0.0611 (15) | 0.0170 (11) | 0.0183 (11) | −0.0006 (12) |
| C12' | 0.0389 (10) | 0.0543 (13) | 0.0433 (11) | 0.0013 (9) | 0.0122 (9) | −0.0005 (9) |
| C13' | 0.0414 (13) | 0.098 (2) | 0.123 (3) | −0.0113 (13) | −0.0060 (14) | −0.0054 (18) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S1—O1 | 1.4212 (15) | C5—H5 | 0.9300 |
| S1—O2 | 1.4319 (15) | C8—H8 | 0.9300 |
| S1—N1 | 1.6063 (17) | C9—H9 | 0.9300 |
| S1—C6 | 1.760 (2) | C10—H10 | 0.9300 |
| S1'—C6' | 1.7582 (19) | C11—H11 | 0.9300 |
| S1'—N1' | 1.6299 (17) | C13—H13A | 0.9600 |
| S1'—O1' | 1.4260 (15) | C13—H13C | 0.9600 |
| S1'—O2' | 1.4235 (15) | C13—H13B | 0.9600 |
| O3—C12 | 1.357 (2) | C1'—C2' | 1.375 (4) |
| O3—C13 | 1.417 (3) | C1'—C6' | 1.380 (3) |
| O3'—C12' | 1.354 (2) | C2'—C3' | 1.374 (4) |
| O3'—C13' | 1.427 (3) | C3'—C4' | 1.372 (4) |
| N1—C7 | 1.418 (2) | C4'—C5' | 1.372 (3) |
| N1—H1N | 0.843 (17) | C5'—C6' | 1.382 (3) |
| N1'—C7' | 1.435 (3) | C7'—C12' | 1.394 (3) |
| N1'—H1N' | 0.828 (18) | C7'—C8' | 1.369 (3) |
| C1—C2 | 1.383 (4) | C8'—C9' | 1.379 (3) |
| C1—C6 | 1.372 (3) | C9'—C10' | 1.359 (4) |
| C2—C3 | 1.363 (4) | C10'—C11' | 1.371 (4) |
| C3—C4 | 1.360 (4) | C11'—C12' | 1.386 (3) |
| C4—C5 | 1.381 (4) | C1'—H1' | 0.9300 |
| C5—C6 | 1.376 (3) | C2'—H2' | 0.9300 |
| C7—C12 | 1.393 (3) | C3'—H3' | 0.9300 |
| C7—C8 | 1.376 (3) | C4'—H4' | 0.9300 |

| | | | |
|---|---|---|---|
| C8—C9 | 1.385 (4) | C5'—H5' | 0.9300 |
| C9—C10 | 1.358 (4) | C8'—H8' | 0.9300 |
| C10—C11 | 1.378 (4) | C9'—H9' | 0.9300 |
| C11—C12 | 1.383 (3) | C10'—H10' | 0.9300 |
| C1—H1 | 0.9300 | C11'—H11' | 0.9300 |
| C2—H2 | 0.9300 | C13'—H13D | 0.9600 |
| C3—H3 | 0.9300 | C13'—H13E | 0.9600 |
| C4—H4 | 0.9300 | C13'—H13F | 0.9600 |

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|---|---|---|---|
| O1—S1—O2 | 118.77 (9) | C9—C10—H10 | 120.00 |
| O1—S1—N1 | 109.73 (9) | C11—C10—H10 | 120.00 |
| O1—S1—C6 | 107.75 (9) | C10—C11—H11 | 120.00 |
| O2—S1—N1 | 104.98 (9) | C12—C11—H11 | 120.00 |
| O2—S1—C6 | 108.59 (9) | O3—C13—H13A | 109.00 |
| N1—S1—C6 | 106.38 (9) | H13A—C13—H13C | 109.00 |
| O1'—S1'—O2' | 119.21 (9) | H13B—C13—H13C | 109.00 |
| O1'—S1'—N1' | 106.05 (9) | H13A—C13—H13B | 109.00 |
| O1'—S1'—C6' | 107.24 (9) | O3—C13—H13B | 109.00 |
| O2'—S1'—N1' | 106.80 (9) | O3—C13—H13C | 110.00 |
| O2'—S1'—C6' | 108.68 (9) | C2'—C1'—C6' | 119.2 (2) |
| N1'—S1'—C6' | 108.48 (9) | C1'—C2'—C3' | 120.3 (2) |
| C12—O3—C13 | 119.21 (16) | C2'—C3'—C4' | 120.3 (2) |
| C12'—O3'—C13' | 117.44 (18) | C3'—C4'—C5' | 120.3 (2) |
| S1—N1—C7 | 126.62 (14) | C4'—C5'—C6' | 119.3 (2) |
| C7—N1—H1N | 118.8 (12) | S1'—C6'—C5' | 119.63 (16) |
| S1—N1—H1N | 114.2 (12) | C1'—C6'—C5' | 120.68 (19) |
| S1'—N1'—C7' | 120.30 (13) | S1'—C6'—C1' | 119.68 (15) |
| C7'—N1'—H1N' | 118.5 (13) | C8'—C7'—C12' | 119.96 (19) |
| S1'—N1'—H1N' | 109.0 (13) | N1'—C7'—C8' | 119.22 (18) |
| C2—C1—C6 | 119.5 (2) | N1'—C7'—C12' | 120.80 (17) |
| C1—C2—C3 | 119.6 (3) | C7'—C8'—C9' | 120.8 (2) |
| C2—C3—C4 | 121.2 (3) | C8'—C9'—C10' | 119.3 (2) |
| C3—C4—C5 | 119.8 (2) | C9'—C10'—C11' | 121.0 (2) |
| C4—C5—C6 | 119.3 (2) | C10'—C11'—C12' | 120.3 (2) |
| C1—C6—C5 | 120.58 (19) | C7'—C12'—C11' | 118.65 (19) |
| S1—C6—C1 | 119.96 (16) | O3'—C12'—C7' | 115.67 (17) |
| S1—C6—C5 | 119.42 (15) | O3'—C12'—C11' | 125.68 (18) |
| C8—C7—C12 | 119.97 (19) | C2'—C1'—H1' | 120.00 |
| N1—C7—C8 | 123.93 (19) | C6'—C1'—H1' | 120.00 |
| N1—C7—C12 | 116.10 (16) | C1'—C2'—H2' | 120.00 |
| C7—C8—C9 | 119.5 (2) | C3'—C2'—H2' | 120.00 |
| C8—C9—C10 | 120.6 (3) | C2'—C3'—H3' | 120.00 |
| C9—C10—C11 | 120.7 (3) | C4'—C3'—H3' | 120.00 |
| C10—C11—C12 | 119.5 (2) | C3'—C4'—H4' | 120.00 |
| C7—C12—C11 | 119.7 (2) | C5'—C4'—H4' | 120.00 |
| O3—C12—C7 | 115.04 (16) | C4'—C5'—H5' | 120.00 |
| O3—C12—C11 | 125.23 (19) | C6'—C5'—H5' | 120.00 |
| C6—C1—H1 | 120.00 | C7'—C8'—H8' | 120.00 |
| C2—C1—H1 | 120.00 | C9'—C8'—H8' | 120.00 |
| C3—C2—H2 | 120.00 | C8'—C9'—H9' | 120.00 |

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|---|---|---|---|
| C1—C2—H2 | 120.00 | C10'—C9'—H9' | 120.00 |
| C4—C3—H3 | 119.00 | C9'—C10'—H10' | 119.00 |
| C2—C3—H3 | 119.00 | C11'—C10'—H10' | 120.00 |
| C5—C4—H4 | 120.00 | C10'—C11'—H11' | 120.00 |
| C3—C4—H4 | 120.00 | C12'—C11'—H11' | 120.00 |
| C4—C5—H5 | 120.00 | O3'—C13'—H13D | 109.00 |
| C6—C5—H5 | 120.00 | O3'—C13'—H13E | 109.00 |
| C7—C8—H8 | 120.00 | O3'—C13'—H13F | 109.00 |
| C9—C8—H8 | 120.00 | H13D—C13'—H13E | 109.00 |
| C10—C9—H9 | 120.00 | H13D—C13'—H13F | 109.00 |
| C8—C9—H9 | 120.00 | H13E—C13'—H13F | 110.00 |

| | | | |
|---|---|---|---|
| O1—S1—N1—C7 | −49.05 (18) | C4—C5—C6—S1 | 177.86 (17) |
| O2—S1—N1—C7 | −177.75 (15) | C4—C5—C6—C1 | 0.0 (3) |
| C6—S1—N1—C7 | 67.25 (18) | C12—C7—C8—C9 | 1.0 (3) |
| O1—S1—C6—C1 | −14.8 (2) | N1—C7—C12—O3 | −0.7 (2) |
| O1—S1—C6—C5 | 167.32 (15) | N1—C7—C8—C9 | −178.4 (2) |
| O2—S1—C6—C1 | 115.07 (18) | C8—C7—C12—O3 | 179.93 (17) |
| O2—S1—C6—C5 | −62.83 (17) | C8—C7—C12—C11 | −1.2 (3) |
| N1—S1—C6—C1 | −132.41 (18) | N1—C7—C12—C11 | 178.21 (18) |
| N1—S1—C6—C5 | 49.70 (18) | C7—C8—C9—C10 | −0.5 (4) |
| N1'—S1'—C6'—C5' | 95.33 (18) | C8—C9—C10—C11 | 0.1 (4) |
| O1'—S1'—N1'—C7' | 163.92 (14) | C9—C10—C11—C12 | −0.3 (4) |
| O2'—S1'—N1'—C7' | 35.80 (17) | C10—C11—C12—C7 | 0.8 (3) |
| C6'—S1'—N1'—C7' | −81.17 (16) | C10—C11—C12—O3 | 179.6 (2) |
| O1'—S1'—C6'—C1' | 30.5 (2) | C6'—C1'—C2'—C3' | −0.7 (4) |
| O1'—S1'—C6'—C5' | −150.54 (17) | C2'—C1'—C6'—S1' | 179.66 (19) |
| O2'—S1'—C6'—C1' | 160.64 (17) | C2'—C1'—C6'—C5' | 0.7 (3) |
| O2'—S1'—C6'—C5' | −20.4 (2) | C1'—C2'—C3'—C4' | 0.0 (4) |
| N1'—S1'—C6'—C1' | −83.61 (19) | C2'—C3'—C4'—C5' | 0.7 (4) |
| C13—O3—C12—C7 | 174.60 (17) | C3'—C4'—C5'—C6' | −0.6 (4) |
| C13—O3—C12—C11 | −4.2 (3) | C4'—C5'—C6'—S1' | −179.01 (18) |
| C13'—O3'—C12'—C7' | −172.1 (2) | C4'—C5'—C6'—C1' | −0.1 (3) |
| C13'—O3'—C12'—C11' | 8.2 (3) | N1'—C7'—C8'—C9' | −178.5 (2) |
| S1—N1—C7—C8 | −8.1 (3) | C12'—C7'—C8'—C9' | −0.3 (3) |
| S1—N1—C7—C12 | 172.47 (14) | N1'—C7'—C12'—O3' | −1.5 (3) |
| S1'—N1'—C7'—C8' | −88.1 (2) | N1'—C7'—C12'—C11' | 178.22 (18) |
| S1'—N1'—C7'—C12' | 93.8 (2) | C8'—C7'—C12'—O3' | −179.62 (18) |
| C2—C1—C6—C5 | −0.7 (4) | C8'—C7'—C12'—C11' | 0.1 (3) |
| C6—C1—C2—C3 | 1.6 (4) | C7'—C8'—C9'—C10' | 0.3 (4) |
| C2—C1—C6—S1 | −178.6 (2) | C8'—C9'—C10'—C11' | 0.1 (4) |
| C1—C2—C3—C4 | −1.9 (5) | C9'—C10'—C11'—C12' | −0.3 (4) |
| C2—C3—C4—C5 | 1.2 (4) | C10'—C11'—C12'—O3' | 179.9 (2) |
| C3—C4—C5—C6 | −0.2 (4) | C10'—C11'—C12'—C7' | 0.2 (3) |

*Hydrogen-bond geometry (Å, °)*

Cg4 is the centroid of the C7'–C12' phenyl ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1'—H1N'···O2 | 0.828 (18) | 2.310 (17) | 3.074 (2) | 153.6 (17) |

| | | | | |
|---|---|---|---|---|
| N1—H1N···O1' | 0.843 (17) | 2.129 (17) | 2.961 (2) | 168.7 (17) |
| N1—H1N···O3 | 0.843 (17) | 2.258 (18) | 2.592 (2) | 103.8 (14) |
| C4—H4···O2'$^{i}$ | 0.93 | 2.47 | 3.377 (3) | 167 |
| C4'—H4'···Cg4$^{ii}$ | 0.93 | 2.85 | 3.601 (2) | 138 |

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

**Fig. 1**

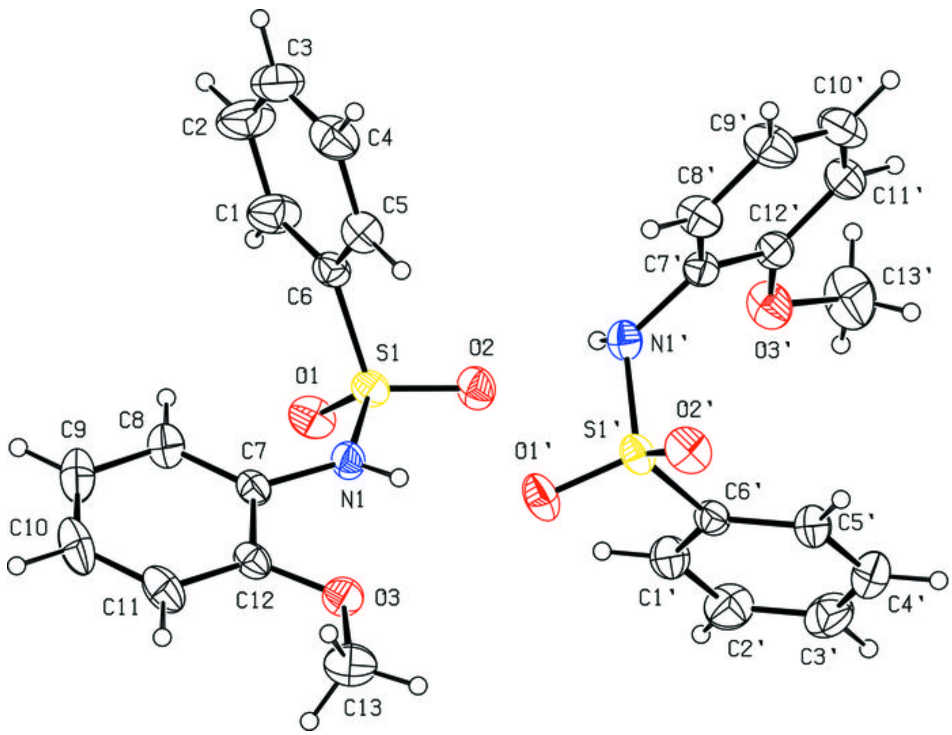
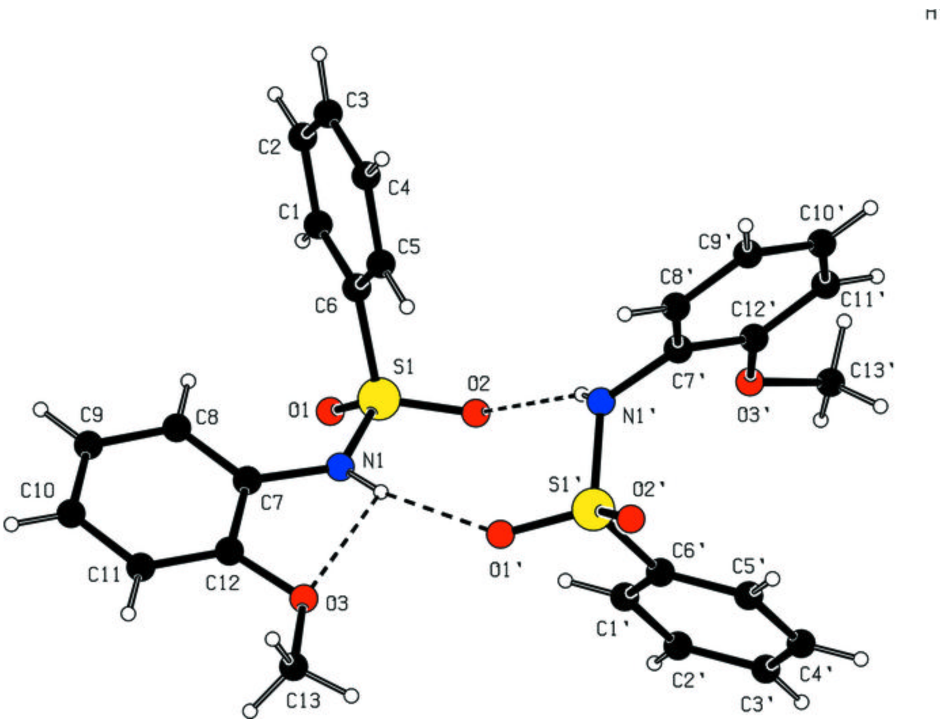

C3
C2
C4
C1
C5
C6
S1
O2
O1
C9
C8
C7
N1
C10
C11
C12
O3
C13
C10'
C9'
C8'
C11'
C12'
C7'
C13'
N1'
O3'
O2'
S1'
O1'
C6'
C5'
C1'
C4'
C2'
C3'

Fig. 2


H1
C3
C2
C4
C1
C5
C6
S1
O2
O1
C9
C8
N1
C7
C10
C11
C12
O3
C13
C10'
C9'
C8'
C12'
C11'
C7'
C13'
O3'
N1'
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C6'
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C4'