Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# *N*-Acetyl-4-(benzenesulfonamido)-benzenesulfonamide

**Muhammad Ashfaq,[a] M. Nawaz Tahir,[b]* Islam Ullah Khan,[a] Muhammad Nadeem Arshad[a] and Syed Saeed-ul-Hassan[c]**

[a]Department of Chemistry, Government College University, Lahore, Pakistan, [b]Department of Physics, University of Sargodha, Sagrodha, Pakistan, and [c]University College of Pharmacy, University of the Punjab, Lahore, Pakistan
Correspondence e-mail: dmntahir_uos@yahoo.com

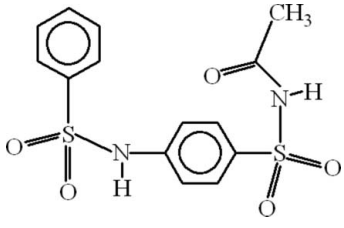
Received 26 April 2009; accepted 28 April 2009

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.049; $wR$ factor = 0.128; data-to-parameter ratio = 19.3.

In the molecule of the title compound, $C_{14}H_{14}N_2O_5S_2$, the dihedral angle between the aromatic rings is 77.75 (9)°. The acetamide group is planar [maximum deviation = 0.002 (3) Å] and oriented at dihedral angles of 13.49 (21) and 73.94 (10)° with respect to the aromatic rings. An intramolecular C—H···O interaction results in the formation of a six-membered ring. In the crystal structure, intermolecular N—H···O and C—H···O interactions link the molecules into a three-dimensional network, forming $R_2^2(20)$ ring motifs.

## Related literature

For related structures, see: Chohan *et al.* (2008, 2009); Deng & Mani (2006); Ellingboe *et al.* (1992); Shad *et al.* (2009); Tahir *et al.* (2008). For ring-motifs, see: Bernstein *et al.* (1995).



## Experimental

### *Crystal data*

$C_{14}H_{14}N_2O_5S_2$
$M_r$ = 354.39
Monoclinic, $P2_1/n$
$a$ = 9.9316 (9) Å
$b$ = 9.4828 (8) Å
$c$ = 17.6490 (17) Å
$\beta$ = 103.169 (5)°
$V$ = 1618.5 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.36 mm$^{-1}$
$T$ = 296 K
0.28 × 0.22 × 0.18 mm

### *Data collection*

Bruker Kappa APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.909, $T_{max}$ = 0.940
17674 measured reflections
4034 independent reflections
2423 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.060

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.128
$S$ = 1.02
4034 reflections
209 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.36 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*N*···O5$^{i}$ | 0.86 | 2.25 | 2.839 (3) | 126 |
| N2—H2*N*···O1$^{ii}$ | 0.86 | 2.14 | 2.922 (3) | 151 |
| C8—H8···O2 | 0.93 | 2.49 | 3.116 (3) | 125 |
| C9—H9···O4$^{iii}$ | 0.93 | 2.60 | 3.237 (3) | 126 |
| C14—H14*A*···O2$^{iv}$ | 0.96 | 2.56 | 3.401 (4) | 147 |

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iv) $x-1, y, z$.

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 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

MA greatfully acknowledges the Higher Education Commission, Islamabad, Pakistan, for providing him with a Scholaship under the Indigenous PhD Program (PIN 042-120556-PS2-275).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2676).

## References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chohan, Z. H., Shad, H. A. & Tahir, M. N. (2009). *Acta Cryst.* E**65**, o57.
Chohan, Z. H., Tahir, M. N., Shad, H. A. & Khan, I. U. (2008). *Acta Cryst.* E**64**, o648.
Deng, X. & Mani, N. S. (2006). *Green Chem.* **8**, 835–838.
Ellingboe, J. W., Spinelli, W., Winkley, M. W., Nguyen, T. T., Parsons, R. W., Moubarak, I. F., Kitzen, J. M., Engen, D. V. & Bagli, J. F. (1992). *J. Med. Chem.*, **35**, 705–716.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Shad, H. A., Tahir, M. N. & Chohan, Z. H. (2009). *Acta Cryst.* E**65**, o98–o99.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Tahir, M. N., Chohan, Z. H., Shad, H. A. & Khan, I. U. (2008). *Acta Cryst.* E**64**, o720.

# supplementary materials

*Acta Cryst.* (2009). E**65**, o1180 [ **doi:10.1107/S1600536809015876** ]

# *N*-Acetyl-4-(benzenesulfonamido)benzenesulfonamide

**M. Ashfaq, M. N. Tahir, I. U. Khan, M. N. Arshad and S. Saeed-ul-Hassan**

## Comment

Sulfonamides have attracted much attention, due to their extensive use in medicine. We have reported the syntheses and crystal structures of sulfonamides, which have the central portion of title compound as common (Chohan *et al.*, 2008, 2009; Shad *et al.*, 2009; Tahir *et al.*, 2008). Similarly, the crystal structure of *N*-Methyl-*N*-(2-(methyl(1-methyl-1*H*-benzimidazol-2-yl)amino)- ethyl)-4-((methylsulfonyl)amino)-benzenesulfonamide (Ellingboe *et al.*, 1992) has been reported, which also has a central portion as in the title compound.

In the molecule of the title compound (Fig 1), rings A (C1-C6) and B (C7-C12) are, of course, planar. The acetamide moiety C (N2/O5/C13/C14) is also planar with a maximum deviation of 0.002 (3) Å for atom C13. The diheadral angles between them are A/B = 77.75 (9), A/C = 13.49 (21) and B/C = 73.94 (10) °. The $SO_2$ groups are oriented at a dihedral angle of 71.02 (15)°. Intramolecular C-H···O interaction (Table 1) results in the formation of a six-membered ring D (S1/O2/N1/C7/C8/H8) having twisted conformation.

In the crystal structure, intermolecular N-H···O and C-H···O interactions (Table 1) link the molecules into a three-dimensional network forming $R_2^2(20)$ ring motifs (Bernstein *et al.*, 1995), in which they may be effective in the stabilization of the structure.

## Experimental

The title compound was synthesized according to a literature method (Deng & Mani, 2006). For the preparation of the title compound, phenylglycine (2 g, 5.3 mmol) was dissolved in distilled water, and then benzene sulfonyl chloride (0.93 g, 5.3 mmol) was added. It was stirred at room temperature. During the reaction pH was maintained at 8-9, strictly using $Na_2CO_3$ (1 M), since HCl was produced as a byproduct, which lowers the pH. The completion of reaction was observed by the consumption of the oily drops of benzene sulfonyl chloride. On completion, pH was adjusted to 2-3 using HCl (2 N). The precipitate formed was filtered, washed with distilled water and recrystalyzed from methanol.

## Refinement

H atoms were positioned geometrically, with N-H = 0.86 Å (for NH) and C-H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C,N)$, where x = 1.5 for methyl H and x = 1.2 for all other H atoms.

## Figures

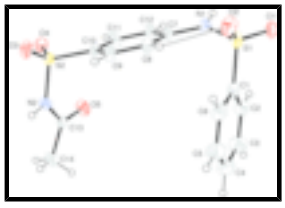


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bond is shown as dashed line.

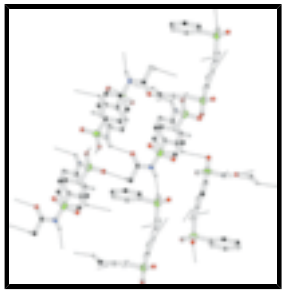


Fig. 2. A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

## *N*-Acetyl-4-(benzenesulfonamido)benzenesulfonamide

*Crystal data*

| | |
|---|---|
| $C_{14}H_{14}N_2O_5S_2$ | $F_{000}$ = 736 |
| $M_r$ = 354.39 | $D_x$ = 1.454 Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2yn | Cell parameters from 4034 reflections |
| $a$ = 9.9316 (9) Å | θ = 2.4–28.3º |
| $b$ = 9.4828 (8) Å | μ = 0.36 mm$^{-1}$ |
| $c$ = 17.6490 (17) Å | $T$ = 296 K |
| β = 103.169 (5)º | Prism, colorless |
| $V$ = 1618.5 (3) Å$^3$ | 0.28 × 0.22 × 0.18 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker Kappa APEXII CCD area-detector diffractometer | 4034 independent reflections |
| Radiation source: fine-focus sealed tube | 2423 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.060 |
| Detector resolution: 7.40 pixels mm$^{-1}$ | $\theta_{max}$ = 28.3º |
| $T$ = 296 K | $\theta_{min}$ = 2.4º |
| ω scans | $h$ = −13→13 |
| Absorption correction: multi-scan (SADABS; Bruker, 2005) | $k$ = −11→12 |
| $T_{min}$ = 0.909, $T_{max}$ = 0.940 | $l$ = −22→23 |
| 17674 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.049$ | H-atom parameters constrained |
| $wR(F^2) = 0.128$ | $w = 1/[\sigma^2(F_o^2) + (0.052P)^2 + 0.3831P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.02$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 4034 reflections | $\Delta\rho_{max} = 0.31$ e Å$^{-3}$ |
| 209 parameters | $\Delta\rho_{min} = -0.36$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | |

*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 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.90183 (7) | 0.28463 (8) | −0.04571 (4) | 0.0407 (3) |
| S2 | 0.58491 (7) | 0.45284 (7) | 0.26062 (4) | 0.0374 (2) |
| O1 | 0.9231 (2) | 0.3308 (2) | −0.11946 (11) | 0.0530 (7) |
| O2 | 1.01569 (19) | 0.2335 (2) | 0.01166 (11) | 0.0546 (7) |
| O3 | 0.68083 (19) | 0.4029 (2) | 0.32790 (10) | 0.0564 (7) |
| O4 | 0.5257 (2) | 0.58953 (19) | 0.26098 (11) | 0.0510 (7) |
| O5 | 0.3371 (2) | 0.4255 (2) | 0.13539 (11) | 0.0560 (7) |
| N1 | 0.8361 (2) | 0.4215 (2) | −0.01260 (12) | 0.0384 (7) |
| N2 | 0.4595 (2) | 0.3347 (2) | 0.24701 (12) | 0.0387 (7) |
| C1 | 0.7705 (3) | 0.1563 (3) | −0.06104 (15) | 0.0396 (9) |
| C2 | 0.6519 (3) | 0.1794 (3) | −0.11844 (17) | 0.0518 (11) |
| C3 | 0.5482 (3) | 0.0815 (4) | −0.1295 (2) | 0.0703 (14) |
| C4 | 0.5621 (4) | −0.0385 (4) | −0.0833 (3) | 0.0759 (17) |
| C5 | 0.6797 (4) | −0.0586 (3) | −0.0265 (2) | 0.0729 (16) |
| C6 | 0.7849 (3) | 0.0381 (3) | −0.01472 (18) | 0.0545 (11) |
| C7 | 0.7799 (2) | 0.4241 (3) | 0.05379 (14) | 0.0315 (8) |
| C8 | 0.8129 (3) | 0.3261 (3) | 0.11352 (15) | 0.0417 (9) |
| C9 | 0.7502 (3) | 0.3347 (3) | 0.17563 (14) | 0.0389 (9) |
| C10 | 0.6584 (3) | 0.4411 (3) | 0.17997 (14) | 0.0321 (8) |

| | | | | |
|---|---|---|---|---|
| C11 | 0.6272 (3) | 0.5403 (3) | 0.12140 (17) | 0.0472 (10) |
| C12 | 0.6873 (3) | 0.5305 (3) | 0.05858 (16) | 0.0446 (10) |
| C13 | 0.3439 (3) | 0.3407 (3) | 0.18721 (15) | 0.0393 (9) |
| C14 | 0.2314 (3) | 0.2385 (4) | 0.19149 (18) | 0.0655 (13) |
| H1N | 0.83546 | 0.49926 | −0.03774 | 0.0461* |
| H2 | 0.64289 | 0.26019 | −0.14902 | 0.0622* |
| H2N | 0.46714 | 0.26548 | 0.27920 | 0.0464* |
| H3 | 0.46813 | 0.09538 | −0.16798 | 0.0843* |
| H4 | 0.49166 | −0.10523 | −0.09098 | 0.0910* |
| H5 | 0.68825 | −0.13877 | 0.00460 | 0.0874* |
| H6 | 0.86471 | 0.02409 | 0.02393 | 0.0655* |
| H8 | 0.87684 | 0.25522 | 0.11176 | 0.0501* |
| H9 | 0.77038 | 0.26763 | 0.21503 | 0.0467* |
| H11 | 0.56602 | 0.61331 | 0.12432 | 0.0566* |
| H12 | 0.66522 | 0.59658 | 0.01874 | 0.0536* |
| H14A | 0.19294 | 0.20141 | 0.14056 | 0.0984* |
| H14B | 0.16038 | 0.28576 | 0.21067 | 0.0984* |
| H14C | 0.26868 | 0.16277 | 0.22601 | 0.0984* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0359 (4) | 0.0556 (5) | 0.0317 (4) | 0.0099 (3) | 0.0102 (3) | −0.0074 (3) |
| S2 | 0.0349 (4) | 0.0507 (4) | 0.0281 (3) | −0.0047 (3) | 0.0104 (3) | −0.0067 (3) |
| O1 | 0.0571 (13) | 0.0707 (14) | 0.0371 (11) | 0.0023 (11) | 0.0232 (10) | −0.0102 (10) |
| O2 | 0.0387 (11) | 0.0718 (14) | 0.0482 (12) | 0.0218 (10) | −0.0006 (10) | −0.0091 (10) |
| O3 | 0.0407 (11) | 0.0984 (16) | 0.0271 (10) | −0.0047 (11) | 0.0013 (9) | −0.0017 (10) |
| O4 | 0.0557 (12) | 0.0467 (11) | 0.0586 (13) | −0.0019 (10) | 0.0294 (10) | −0.0167 (10) |
| O5 | 0.0474 (12) | 0.0781 (15) | 0.0391 (11) | −0.0021 (11) | 0.0025 (10) | 0.0205 (11) |
| N1 | 0.0451 (13) | 0.0396 (12) | 0.0341 (12) | 0.0070 (10) | 0.0163 (10) | 0.0013 (10) |
| N2 | 0.0379 (12) | 0.0473 (13) | 0.0291 (12) | −0.0050 (10) | 0.0042 (10) | 0.0113 (10) |
| C1 | 0.0409 (15) | 0.0424 (15) | 0.0356 (15) | 0.0128 (13) | 0.0089 (12) | −0.0048 (12) |
| C2 | 0.0467 (18) | 0.0586 (19) | 0.0480 (18) | 0.0087 (15) | 0.0062 (15) | 0.0005 (15) |
| C3 | 0.046 (2) | 0.085 (3) | 0.074 (2) | 0.000 (2) | 0.0015 (18) | −0.008 (2) |
| C4 | 0.072 (3) | 0.066 (3) | 0.095 (3) | −0.016 (2) | 0.030 (2) | −0.021 (2) |
| C5 | 0.093 (3) | 0.046 (2) | 0.082 (3) | 0.002 (2) | 0.025 (2) | 0.0040 (18) |
| C6 | 0.063 (2) | 0.0479 (18) | 0.0515 (19) | 0.0132 (16) | 0.0109 (16) | −0.0028 (15) |
| C7 | 0.0290 (13) | 0.0378 (14) | 0.0279 (13) | −0.0014 (11) | 0.0067 (10) | −0.0040 (11) |
| C8 | 0.0456 (16) | 0.0467 (16) | 0.0347 (15) | 0.0180 (13) | 0.0130 (13) | 0.0028 (12) |
| C9 | 0.0460 (16) | 0.0421 (15) | 0.0291 (14) | 0.0109 (13) | 0.0095 (12) | 0.0051 (12) |
| C10 | 0.0313 (13) | 0.0358 (14) | 0.0306 (13) | 0.0013 (11) | 0.0098 (11) | −0.0013 (11) |
| C11 | 0.0574 (18) | 0.0407 (16) | 0.0517 (18) | 0.0180 (14) | 0.0298 (15) | 0.0084 (13) |
| C12 | 0.0578 (18) | 0.0403 (16) | 0.0420 (16) | 0.0159 (14) | 0.0242 (14) | 0.0124 (12) |
| C13 | 0.0376 (15) | 0.0549 (17) | 0.0272 (14) | −0.0049 (13) | 0.0109 (12) | 0.0006 (12) |
| C14 | 0.0526 (19) | 0.100 (3) | 0.0427 (18) | −0.0311 (19) | 0.0083 (15) | 0.0000 (17) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S1—O1 | 1.434 (2) | C7—C12 | 1.381 (4) |

| | | | |
|---|---|---|---|
| S1—O2 | 1.420 (2) | C7—C8 | 1.387 (4) |
| S1—N1 | 1.621 (2) | C8—C9 | 1.381 (4) |
| S1—C1 | 1.759 (3) | C9—C10 | 1.374 (4) |
| S2—O3 | 1.4235 (19) | C10—C11 | 1.380 (4) |
| S2—O4 | 1.424 (2) | C11—C12 | 1.377 (4) |
| S2—N2 | 1.652 (2) | C13—C14 | 1.494 (5) |
| S2—C10 | 1.745 (3) | C2—H2 | 0.9300 |
| O5—C13 | 1.208 (3) | C3—H3 | 0.9300 |
| N1—C7 | 1.408 (3) | C4—H4 | 0.9300 |
| N2—C13 | 1.372 (3) | C5—H5 | 0.9300 |
| N1—H1N | 0.8600 | C6—H6 | 0.9300 |
| N2—H2N | 0.8600 | C8—H8 | 0.9300 |
| C1—C6 | 1.375 (4) | C9—H9 | 0.9300 |
| C1—C2 | 1.385 (4) | C11—H11 | 0.9300 |
| C2—C3 | 1.367 (5) | C12—H12 | 0.9300 |
| C3—C4 | 1.388 (6) | C14—H14A | 0.9600 |
| C4—C5 | 1.368 (6) | C14—H14B | 0.9600 |
| C5—C6 | 1.370 (5) | C14—H14C | 0.9600 |
| S1···H8 | 2.8600 | C8···C6 | 3.517 (4) |
| O1···N2$^{i}$ | 2.922 (3) | C9···O4$^{xi}$ | 3.237 (3) |
| O2···C6$^{ii}$ | 3.242 (4) | C10···O5 | 3.111 (4) |
| O2···C5$^{ii}$ | 3.407 (4) | C11···O5 | 3.142 (4) |
| O2···C8 | 3.116 (3) | C12···O5$^{vi}$ | 3.402 (3) |
| O2···C14$^{iii}$ | 3.401 (4) | C14···O4$^{xii}$ | 3.193 (4) |
| O4···O5 | 2.992 (3) | C14···O2$^{xiii}$ | 3.401 (4) |
| O4···C8$^{iv}$ | 3.300 (3) | C2···H14B$^{i}$ | 3.0500 |
| O4···C9$^{iv}$ | 3.237 (3) | C2···H11$^{vi}$ | 2.9100 |
| O4···C14$^{v}$ | 3.193 (4) | C5···H14A$^{x}$ | 2.9400 |
| O5···C11 | 3.142 (4) | C6···H8 | 3.0200 |
| O5···N1$^{vi}$ | 2.839 (3) | H1N···H12 | 2.3400 |
| O5···O4 | 2.992 (3) | H1N···O2$^{vii}$ | 2.9200 |
| O5···C12$^{vi}$ | 3.402 (3) | H1N···O5$^{vi}$ | 2.2500 |
| O5···C10 | 3.111 (4) | H2···O1 | 2.7900 |
| O1···H14C$^{i}$ | 2.8100 | H2···O4$^{vi}$ | 2.6900 |
| O1···H2 | 2.7900 | H2···H11$^{vi}$ | 2.5200 |
| O1···H2N$^{i}$ | 2.1400 | H2···H14B$^{i}$ | 2.5600 |
| O2···H8 | 2.4900 | H2N···H14C | 2.2100 |
| O2···H6$^{ii}$ | 2.8500 | H2N···O1$^{ix}$ | 2.1400 |
| O2···H6 | 2.5300 | H3···O3$^{xiv}$ | 2.8400 |
| O2···H1N$^{vii}$ | 2.9200 | H5···H12$^{xv}$ | 2.5400 |
| O2···H14A$^{iii}$ | 2.5600 | H6···O2 | 2.5300 |
| O3···H3$^{viii}$ | 2.8400 | H6···O2$^{ii}$ | 2.8500 |
| O3···H9 | 2.6900 | H8···S1 | 2.8600 |
| O4···H11 | 2.5400 | H8···O2 | 2.4900 |

| | | | |
|---|---|---|---|
| O4···H14B$^{v}$ | 2.7500 | H8···C6 | 3.0200 |
| O4···H2$^{vi}$ | 2.6900 | H8···O4$^{xi}$ | 2.7300 |
| O4···H8$^{iv}$ | 2.7300 | H9···O3 | 2.6900 |
| O4···H9$^{iv}$ | 2.6000 | H9···O4$^{xi}$ | 2.6000 |
| O5···H1N$^{vi}$ | 2.2500 | H11···O4 | 2.5400 |
| O5···H12$^{vi}$ | 2.7200 | H11···C2$^{vi}$ | 2.9100 |
| N1···O5$^{vi}$ | 2.839 (3) | H11···H2$^{vi}$ | 2.5200 |
| N2···O1$^{ix}$ | 2.922 (3) | H12···H1N | 2.3400 |
| C1···C8 | 3.416 (4) | H12···H5$^{xvi}$ | 2.5400 |
| C4···C5$^{x}$ | 3.534 (6) | H12···O5$^{vi}$ | 2.7200 |
| C4···C4$^{x}$ | 3.515 (7) | H14A···O2$^{xiii}$ | 2.5600 |
| C5···O2$^{ii}$ | 3.407 (4) | H14A···C5$^{x}$ | 2.9400 |
| C5···C4$^{x}$ | 3.534 (6) | H14B···O4$^{xii}$ | 2.7500 |
| C6···C8 | 3.517 (4) | H14B···C2$^{ix}$ | 3.0500 |
| C6···O2$^{ii}$ | 3.242 (4) | H14B···H2$^{ix}$ | 2.5600 |
| C8···O2 | 3.116 (3) | H14C···H2N | 2.2100 |
| C8···C1 | 3.416 (4) | H14C···O1$^{ix}$ | 2.8100 |
| C8···O4$^{xi}$ | 3.300 (3) | | |
| O1—S1—O2 | 119.56 (12) | S2—C10—C11 | 120.2 (2) |
| O1—S1—N1 | 103.74 (11) | C9—C10—C11 | 119.9 (3) |
| O1—S1—C1 | 109.21 (12) | C10—C11—C12 | 119.5 (3) |
| O2—S1—N1 | 109.70 (11) | C7—C12—C11 | 121.0 (3) |
| O2—S1—C1 | 108.39 (13) | O5—C13—C14 | 123.8 (3) |
| N1—S1—C1 | 105.31 (12) | N2—C13—C14 | 116.0 (2) |
| O3—S2—O4 | 119.85 (12) | O5—C13—N2 | 120.2 (3) |
| O3—S2—N2 | 103.58 (11) | C1—C2—H2 | 121.00 |
| O3—S2—C10 | 109.54 (13) | C3—C2—H2 | 120.00 |
| O4—S2—N2 | 108.64 (11) | C2—C3—H3 | 120.00 |
| O4—S2—C10 | 108.16 (13) | C4—C3—H3 | 120.00 |
| N2—S2—C10 | 106.25 (12) | C3—C4—H4 | 120.00 |
| S1—N1—C7 | 125.64 (18) | C5—C4—H4 | 120.00 |
| S2—N2—C13 | 123.70 (18) | C4—C5—H5 | 120.00 |
| C7—N1—H1N | 117.00 | C6—C5—H5 | 120.00 |
| S1—N1—H1N | 117.00 | C1—C6—H6 | 121.00 |
| S2—N2—H2N | 118.00 | C5—C6—H6 | 121.00 |
| C13—N2—H2N | 118.00 | C7—C8—H8 | 120.00 |
| S1—C1—C2 | 118.7 (2) | C9—C8—H8 | 120.00 |
| S1—C1—C6 | 120.0 (2) | C8—C9—H9 | 120.00 |
| C2—C1—C6 | 121.3 (3) | C10—C9—H9 | 120.00 |
| C1—C2—C3 | 119.0 (3) | C10—C11—H11 | 120.00 |
| C2—C3—C4 | 120.1 (3) | C12—C11—H11 | 120.00 |
| C3—C4—C5 | 119.9 (3) | C7—C12—H12 | 119.00 |
| C4—C5—C6 | 120.8 (3) | C11—C12—H12 | 120.00 |
| C1—C6—C5 | 118.9 (3) | C13—C14—H14A | 109.00 |
| C8—C7—C12 | 119.2 (2) | C13—C14—H14B | 109.00 |

| | | | |
|---|---|---|---|
| N1—C7—C8 | 123.4 (2) | C13—C14—H14C | 109.00 |
| N1—C7—C12 | 117.4 (2) | H14A—C14—H14B | 109.00 |
| C7—C8—C9 | 119.5 (3) | H14A—C14—H14C | 110.00 |
| C8—C9—C10 | 120.8 (2) | H14B—C14—H14C | 109.00 |
| S2—C10—C9 | 119.9 (2) | | |
| O1—S1—N1—C7 | 171.1 (2) | S2—N2—C13—O5 | 9.3 (4) |
| O2—S1—N1—C7 | −60.1 (2) | S2—N2—C13—C14 | −170.4 (2) |
| C1—S1—N1—C7 | 56.4 (2) | S1—C1—C2—C3 | −178.6 (2) |
| O1—S1—C1—C2 | −44.2 (3) | C6—C1—C2—C3 | −0.8 (4) |
| O1—S1—C1—C6 | 137.9 (2) | S1—C1—C6—C5 | 178.4 (2) |
| O2—S1—C1—C2 | −176.0 (2) | C2—C1—C6—C5 | 0.5 (5) |
| O2—S1—C1—C6 | 6.1 (3) | C1—C2—C3—C4 | 0.4 (5) |
| N1—S1—C1—C2 | 66.7 (3) | C2—C3—C4—C5 | 0.1 (6) |
| N1—S1—C1—C6 | −111.2 (2) | C3—C4—C5—C6 | −0.4 (6) |
| O3—S2—N2—C13 | −179.6 (2) | C4—C5—C6—C1 | 0.0 (5) |
| O4—S2—N2—C13 | 52.0 (2) | N1—C7—C8—C9 | −178.4 (2) |
| C10—S2—N2—C13 | −64.2 (2) | C12—C7—C8—C9 | 1.5 (4) |
| O3—S2—C10—C9 | 32.2 (3) | N1—C7—C12—C11 | 179.7 (3) |
| O3—S2—C10—C11 | −146.2 (2) | C8—C7—C12—C11 | −0.2 (4) |
| O4—S2—C10—C9 | 164.5 (2) | C7—C8—C9—C10 | −1.7 (4) |
| O4—S2—C10—C11 | −14.0 (3) | C8—C9—C10—S2 | −177.9 (2) |
| N2—S2—C10—C9 | −79.1 (3) | C8—C9—C10—C11 | 0.5 (4) |
| N2—S2—C10—C11 | 102.5 (2) | S2—C10—C11—C12 | 179.2 (2) |
| S1—N1—C7—C8 | 22.2 (3) | C9—C10—C11—C12 | 0.8 (4) |
| S1—N1—C7—C12 | −157.8 (2) | C10—C11—C12—C7 | −1.0 (4) |

Symmetry codes: (i) *x*+1/2, −*y*+1/2, *z*−1/2; (ii) −*x*+2, −*y*, −*z*; (iii) *x*+1, *y*, *z*; (iv) −*x*+3/2, *y*+1/2, −*z*+1/2; (v) −*x*+1/2, *y*+1/2, −*z*+1/2; (vi) −*x*+1, −*y*+1, −*z*; (vii) −*x*+2, −*y*+1, −*z*; (viii) *x*+1/2, −*y*+1/2, *z*+1/2; (ix) *x*−1/2, −*y*+1/2, *z*+1/2; (x) −*x*+1, −*y*, −*z*; (xi) −*x*+3/2, *y*−1/2, −*z*+1/2; (xii) −*x*+1/2, *y*−1/2, −*z*+1/2; (xiii) *x*−1, *y*, *z*; (xiv) *x*−1/2, −*y*+1/2, *z*−1/2; (xv) *x*, *y*−1, *z*; (xvi) *x*, *y*+1, *z*.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1N···O5$^{vi}$ | 0.86 | 2.25 | 2.839 (3) | 126 |
| N2—H2N···O1$^{ix}$ | 0.86 | 2.14 | 2.922 (3) | 151 |
| C8—H8···O2 | 0.93 | 2.49 | 3.116 (3) | 125 |
| C9—H9···O4$^{xi}$ | 0.93 | 2.60 | 3.237 (3) | 126 |
| C14—H14A···O2$^{xiii}$ | 0.96 | 2.56 | 3.401 (4) | 147 |

Symmetry codes: (vi) −*x*+1, −*y*+1, −*z*; (ix) *x*−1/2, −*y*+1/2, *z*+1/2; (xi) −*x*+3/2, *y*−1/2, −*z*+1/2; (xiii) *x*−1, *y*, *z*.

**Fig. 1**

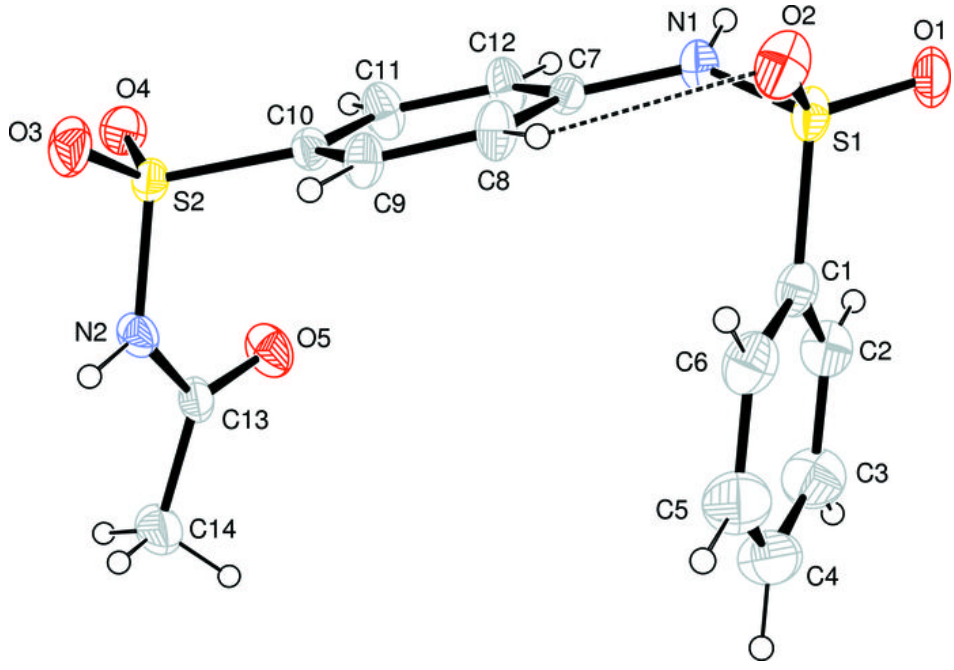

N1
O2
O1
C12
C7
C11
O4
O3
C10
S1
S2
C8
C9
C1
N2
O5
C6
C2
C13
C3
C5
C14
C4

**Fig. 2**