# organic compounds

# N,N'-Diethyl-N,N'-[1,3-phenylene-bis(methylene)]dibenzenesulfonamide

Ejaz,[a] Islam Ullah Khan,[a]* Hira Ahmad,[a] William T. A. Harrison[b] and Tahir Ali Sheikh[c]

[a]Materials Chemistry Laboratry, Department of Chemistry, GC University, Lahore 54000, Pakistan, [b]Department of Chemistry, University of Aberdeen, Meston Walk, Aberdeen AB24 3UE, Scotland, and [c]Materials Chemistry Laboratry, Department of Chemistry, GC University, Lahore-54000, Pakistan
Correspondence e-mail: iuklodhi@yahoo.com

In the title compound, $C_{24}H_{28}N_2O_4S_2$, the dihedral angles between the central benzene ring and the pendant rings are 77.44 (11) and 79.23 (10)°, and the dihedral angle between the pendant rings is 23.31 (12)°. Both sulfonamide groups project to the same side of the central benzene ring and the molecule has approximate non-crystallographic mirror symmetry. One of the ethyl side chains is disordered over two sets of sites in a 0.526 (14):0.474 (14) ratio. In the crystal, inversion dimers linked by pairs of weak C—H···O interactions occur, generating $R_2^2(28)$ loops.

## Related literature

For a related structure, see: Khan *et al.* (2011).
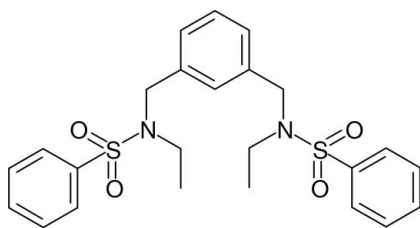
## Experimental

### Crystal data

| | |
|---|---|
| $C_{24}H_{28}N_2O_4S_2$ | $V$ = 2421.02 (15) Å$^3$ |
| $M_r$ = 472.60 | $Z$ = 4 |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation |
| $a$ = 9.1865 (3) Å | $\mu$ = 0.25 mm$^{-1}$ |
| $b$ = 19.0679 (7) Å | $T$ = 296 K |
| $c$ = 14.3870 (5) Å | $0.13 \times 0.10 \times 0.09$ mm |
| $\beta$ = 106.122 (1)° | |

### Data collection

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 6013 independent reflections |
| | 4188 reflections with $I > 2\sigma(I)$ |
| 23272 measured reflections | $R_{int}$ = 0.025 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.045 | 290 parameters |
| $wR(F^2)$ = 0.132 | H-atom parameters constrained |
| $S$ = 1.01 | $\Delta\rho_{max}$ = 0.29 e Å$^{-3}$ |
| 6013 reflections | $\Delta\rho_{min}$ = −0.38 e Å$^{-3}$ |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C17—H17···O1$^i$ | 0.93 | 2.57 | 3.409 (3) | 151 |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); 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: *SHELXL97* (Sheldrick, 2008).

## References

Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Khan, I. U., Sheikh, T. A., Ejaz & Harrison, W. T. A. (2011). *Acta Cryst.* E**67**, o2371.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

**supplementary materials**

# *N,N'*-Diethyl-*N,N'*-[1,3-phenylenebis(methylene)]dibenzenesulfonamide

## Ejaz, I. U. Khan, H. Ahmad, W. T. A. Harrison and T. A. Sheikh

### Comment

As part of our ongoing structural studies of sulfonamides (Khan *et al.*, 2011), the synthesis and structure of the title compound, (I), (Fig. 1), are now described.

The dihedral angles between the central benzene ring and the pendant rings are almost equal at 77.44 (11) and 79.23 (10)° and the dihedral angle between the pendant rings is 23.31 (12)°. Both sulfonamode groups project to the same side of the central ring and the molecule has approximate non-crystallographic mirror symmetry. The C8—S1—N1—C7 and C15—S2—N2—C14 torsion angles are -66.87 (15) and 70.98 (15)°, respectively. The S1—N1—C7—C6 and S2—N2—C14—C2 trsion angles are -148.14 (14) and 144.01 (14)°, respectively. One of the terminal methyl groups is disordered over two sets of sites in a 0.526 (14):0.474 (14) ratio.

In the crystal, inversion dimers linked by pairs of weak C—H···O interactions occur (Fig. 2, Table 1).

### Experimental

A mixture of *N,N'*-diethyl-(benzene-1,3-diyldimethanediyl)dibenzenesulfonamide (0.2 g, 0.43 mmol), sodium hydride (0.21 g; 0.88 mmol) and N, *N*-dimethylformamide (10.0 ml) was stirred in a 100-ml RB flask at room temperature for half an hour followed by the addition of ethyl iodide (0.134 g; 0.86 mmol). The reaction mixture was further stirred for five hours, and its completion was monitored by TLC. After completion, the contents were poured over crushed ice. The precipitated product was isolated, washed and crystallized from methanol to yield colourless blocks of (I).

### Refinement

The N-bound H atom was located in a difference Fourier map and its position was freely refined with the constraint $U_{iso}(H) = 1.2U_{eq}(N)$. The C-bound hydrogen atoms were placed in calculated positions (C—H = 0.93–0.97 Å) and refined as riding atoms with $U_{iso}(H) = 1.2U_{eq}(C)$. One of the ethyl side chains is disordered over two sets of sites in a 0.526 (14):0.474 (14) ratio for atoms C22A:C22B, which were refined isotropically.
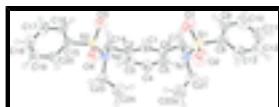
### Figures



Fig. 1. The molecular structure of the title molecule, showing the numbering scheme and 50% displacement ellipsoids. Only one orientation of the disordered atom C22 and its attached H atoms is shown.
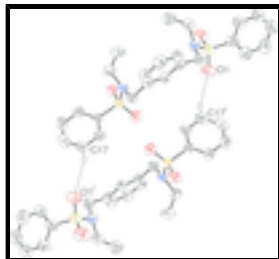
# supplementary materials



Fig. 2. A view of the inversion dimer in the crystal structure of the title compound. All H atoms except H17 have been omitted for clarity, and the C—H⋯O interactions are shown as dashed lines [Symmetry code: (i) 1–x, –y, 1–z].

## *N,N'*-Diethyl-*N,N'*-[1,3- phenylenebis(methylene)]dibenzenesulfonamide

*Crystal data*

| | |
|---|---|
| $C_{24}H_{28}N_2O_4S_2$ | $F(000) = 1000$ |
| $M_r = 472.60$ | $D_x = 1.297$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2yn | Cell parameters from 6013 reflections |
| $a = 9.1865$ (3) Å | $\theta = 2.6–28.3°$ |
| $b = 19.0679$ (7) Å | $\mu = 0.25$ mm$^{-1}$ |
| $c = 14.3870$ (5) Å | $T = 296$ K |
| $\beta = 106.122$ (1)° | Block, colourless |
| $V = 2421.02$ (15) Å$^3$ | $0.13 \times 0.10 \times 0.09$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 4188 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int} = 0.025$ |
| graphite | $\theta_{max} = 28.3°$, $\theta_{min} = 2.6°$ |
| ω scans | $h = -12{\rightarrow}8$ |
| 23272 measured reflections | $k = -24{\rightarrow}25$ |
| 6013 independent reflections | $l = -17{\rightarrow}19$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.045$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.132$ | H-atom parameters constrained |
| $S = 1.01$ | $w = 1/[\sigma^2(F_o^2) + (0.060P)^2 + 0.7693P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 6013 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 290 parameters | $\Delta\rho_{max} = 0.29$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.38$ e Å$^{-3}$ |

*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 $F^2 > \sigma(F^2)$ 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 ($Å^2$)*

|      | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ | Occ. (<1) |
|------|------|------|------|------|------|
| C1 | 0.78689 (19) | 0.13374 (9) | 0.68904 (13) | 0.0448 (4) | |
| H1 | 0.7268 | 0.1480 | 0.6288 | 0.054* | |
| C2 | 0.73697 (19) | 0.08014 (9) | 0.73745 (14) | 0.0449 (4) | |
| C3 | 0.8266 (2) | 0.05935 (11) | 0.82682 (15) | 0.0554 (5) | |
| H3 | 0.7942 | 0.0233 | 0.8598 | 0.066* | |
| C4 | 0.9639 (2) | 0.09163 (13) | 0.86768 (15) | 0.0614 (5) | |
| H4 | 1.0237 | 0.0775 | 0.9281 | 0.074* | |
| C5 | 1.0123 (2) | 0.14489 (11) | 0.81882 (15) | 0.0545 (5) | |
| H5 | 1.1049 | 0.1666 | 0.8466 | 0.065* | |
| C6 | 0.92480 (19) | 0.16639 (9) | 0.72889 (14) | 0.0452 (4) | |
| C7 | 0.9798 (2) | 0.22228 (10) | 0.67292 (17) | 0.0557 (5) | |
| H7A | 1.0849 | 0.2329 | 0.7054 | 0.067* | |
| H7B | 0.9751 | 0.2045 | 0.6090 | 0.067* | |
| C8 | 1.0539 (3) | 0.36406 (11) | 0.56934 (15) | 0.0582 (5) | |
| C9 | 1.1599 (3) | 0.32027 (13) | 0.54866 (18) | 0.0702 (6) | |
| H9 | 1.1345 | 0.2745 | 0.5280 | 0.084* | |
| C10 | 1.3050 (3) | 0.34546 (17) | 0.5591 (2) | 0.0881 (8) | |
| H10 | 1.3785 | 0.3162 | 0.5467 | 0.106* | |
| C11 | 1.3404 (4) | 0.41342 (19) | 0.5877 (2) | 0.0957 (10) | |
| H11 | 1.4381 | 0.4299 | 0.5947 | 0.115* | |
| C12 | 1.2346 (4) | 0.45677 (18) | 0.6058 (2) | 0.1002 (10) | |
| H12 | 1.2595 | 0.5030 | 0.6238 | 0.120* | |
| C13 | 1.0910 (3) | 0.43270 (13) | 0.5975 (2) | 0.0796 (7) | |
| H13 | 1.0188 | 0.4623 | 0.6107 | 0.096* | |
| C14 | 0.5875 (2) | 0.04462 (10) | 0.69110 (16) | 0.0517 (5) | |
| H14A | 0.5908 | 0.0235 | 0.6304 | 0.062* | |
| H14B | 0.5708 | 0.0076 | 0.7332 | 0.062* | |
| C15 | 0.22235 (19) | 0.00993 (9) | 0.59280 (13) | 0.0437 (4) | |
| C16 | 0.2729 (2) | −0.05564 (10) | 0.57526 (16) | 0.0553 (5) | |
| H16 | 0.3584 | −0.0602 | 0.5531 | 0.066* | |
| C17 | 0.1955 (3) | −0.11417 (11) | 0.59097 (18) | 0.0676 (6) | |
| H17 | 0.2282 | −0.1586 | 0.5790 | 0.081* | |
| C18 | 0.0694 (3) | −0.10715 (13) | 0.62447 (19) | 0.0728 (7) | |

| | | | | | |
|---|---|---|---|---|---|
| H18 | 0.0180 | −0.1469 | 0.6356 | 0.087* | |
| C19 | 0.0198 (3) | −0.04250 (14) | 0.64141 (18) | 0.0697 (6) | |
| H19 | −0.0661 | −0.0383 | 0.6633 | 0.084* | |
| C20 | 0.0957 (2) | 0.01662 (11) | 0.62643 (16) | 0.0558 (5) | |
| H20 | 0.0623 | 0.0608 | 0.6388 | 0.067* | |
| C21 | 0.9119 (3) | 0.32830 (13) | 0.75365 (18) | 0.0700 (6) | |
| H21A | 0.9693 | 0.3704 | 0.7501 | 0.084* | |
| H21B | 0.9692 | 0.3008 | 0.8083 | 0.084* | |
| C22A | 0.7607 (7) | 0.3480 (4) | 0.7682 (5) | 0.079 (2)* | 0.526 (14) |
| H22A | 0.7765 | 0.3746 | 0.8269 | 0.119* | 0.526 (14) |
| H22B | 0.7046 | 0.3063 | 0.7725 | 0.119* | 0.526 (14) |
| H22C | 0.7048 | 0.3759 | 0.7145 | 0.119* | 0.526 (14) |
| C22B | 0.7963 (9) | 0.3175 (6) | 0.8056 (7) | 0.095 (3)* | 0.474 (14) |
| H22D | 0.8201 | 0.3458 | 0.8630 | 0.143* | 0.474 (14) |
| H22E | 0.7947 | 0.2690 | 0.8231 | 0.143* | 0.474 (14) |
| H22F | 0.6987 | 0.3306 | 0.7645 | 0.143* | 0.474 (14) |
| C23 | 0.4252 (2) | 0.12225 (12) | 0.76072 (16) | 0.0597 (5) | |
| H23A | 0.3194 | 0.1129 | 0.7553 | 0.072* | |
| H23B | 0.4857 | 0.0974 | 0.8171 | 0.072* | |
| C24 | 0.4538 (4) | 0.19853 (14) | 0.7750 (2) | 0.0879 (8) | |
| H24A | 0.5597 | 0.2078 | 0.7849 | 0.132* | |
| H24B | 0.4240 | 0.2138 | 0.8307 | 0.132* | |
| H24C | 0.3961 | 0.2234 | 0.7189 | 0.132* | |
| S1 | 0.87268 (6) | 0.33183 (3) | 0.56484 (4) | 0.05927 (16) | |
| S2 | 0.32295 (5) | 0.08483 (2) | 0.57589 (4) | 0.04724 (14) | |
| N1 | 0.88989 (17) | 0.28716 (8) | 0.66325 (12) | 0.0512 (4) | |
| N2 | 0.46183 (16) | 0.09500 (8) | 0.67317 (12) | 0.0484 (4) | |
| O1 | 0.82899 (19) | 0.28392 (9) | 0.48611 (12) | 0.0765 (5) | |
| O2 | 0.77734 (19) | 0.39036 (9) | 0.56817 (15) | 0.0850 (5) | |
| O3 | 0.38878 (17) | 0.07049 (8) | 0.49896 (11) | 0.0615 (4) | |
| O4 | 0.22630 (16) | 0.14401 (7) | 0.57007 (12) | 0.0634 (4) | |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0399 (8) | 0.0470 (10) | 0.0441 (10) | 0.0051 (7) | 0.0063 (7) | −0.0007 (8) |
| C2 | 0.0399 (8) | 0.0434 (10) | 0.0506 (10) | 0.0043 (7) | 0.0113 (8) | −0.0030 (8) |
| C3 | 0.0532 (11) | 0.0572 (12) | 0.0570 (12) | 0.0080 (9) | 0.0173 (9) | 0.0120 (9) |
| C4 | 0.0490 (10) | 0.0816 (15) | 0.0479 (11) | 0.0100 (10) | 0.0041 (9) | 0.0077 (10) |
| C5 | 0.0358 (8) | 0.0674 (13) | 0.0560 (12) | 0.0034 (8) | 0.0057 (8) | −0.0092 (10) |
| C6 | 0.0385 (8) | 0.0441 (10) | 0.0540 (10) | 0.0041 (7) | 0.0145 (8) | −0.0031 (8) |
| C7 | 0.0427 (9) | 0.0502 (11) | 0.0763 (14) | 0.0030 (8) | 0.0200 (9) | 0.0027 (10) |
| C8 | 0.0683 (12) | 0.0491 (11) | 0.0539 (12) | −0.0051 (9) | 0.0117 (10) | 0.0015 (9) |
| C9 | 0.0817 (16) | 0.0574 (13) | 0.0753 (15) | −0.0027 (11) | 0.0281 (13) | 0.0091 (11) |
| C10 | 0.0849 (18) | 0.096 (2) | 0.094 (2) | 0.0008 (16) | 0.0428 (16) | 0.0184 (16) |
| C11 | 0.091 (2) | 0.110 (3) | 0.089 (2) | −0.0403 (19) | 0.0303 (17) | 0.0000 (18) |
| C12 | 0.119 (2) | 0.087 (2) | 0.106 (2) | −0.0455 (19) | 0.049 (2) | −0.0221 (17) |
| C13 | 0.0994 (19) | 0.0578 (14) | 0.0856 (18) | −0.0164 (13) | 0.0322 (15) | −0.0105 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C14 | 0.0459 (9) | 0.0407 (10) | 0.0667 (12) | 0.0010 (8) | 0.0123 (9) | −0.0021 (9) |
| C15 | 0.0380 (8) | 0.0434 (9) | 0.0468 (10) | −0.0011 (7) | 0.0072 (7) | −0.0072 (8) |
| C16 | 0.0461 (10) | 0.0473 (11) | 0.0698 (13) | 0.0003 (8) | 0.0116 (9) | −0.0116 (9) |
| C17 | 0.0636 (13) | 0.0445 (11) | 0.0858 (17) | −0.0032 (10) | 0.0061 (12) | −0.0072 (11) |
| C18 | 0.0654 (14) | 0.0633 (14) | 0.0829 (17) | −0.0207 (11) | 0.0091 (12) | 0.0073 (12) |
| C19 | 0.0542 (12) | 0.0799 (17) | 0.0783 (16) | −0.0141 (11) | 0.0240 (11) | −0.0028 (13) |
| C20 | 0.0475 (10) | 0.0573 (12) | 0.0639 (13) | −0.0006 (9) | 0.0174 (9) | −0.0110 (10) |
| C21 | 0.0774 (15) | 0.0623 (14) | 0.0712 (15) | −0.0154 (11) | 0.0223 (12) | −0.0171 (11) |
| C23 | 0.0568 (11) | 0.0632 (13) | 0.0605 (13) | −0.0029 (10) | 0.0187 (10) | −0.0101 (10) |
| C24 | 0.107 (2) | 0.0684 (16) | 0.0941 (19) | −0.0111 (15) | 0.0384 (17) | −0.0337 (15) |
| S1 | 0.0548 (3) | 0.0474 (3) | 0.0663 (3) | 0.0028 (2) | 0.0013 (2) | −0.0028 (2) |
| S2 | 0.0431 (2) | 0.0417 (2) | 0.0565 (3) | 0.00114 (18) | 0.0131 (2) | −0.0028 (2) |
| N1 | 0.0474 (8) | 0.0412 (8) | 0.0643 (10) | −0.0011 (6) | 0.0140 (7) | −0.0090 (7) |
| N2 | 0.0399 (7) | 0.0448 (8) | 0.0598 (10) | −0.0005 (6) | 0.0127 (7) | −0.0110 (7) |
| O1 | 0.0781 (10) | 0.0737 (11) | 0.0641 (10) | −0.0086 (8) | −0.0031 (8) | −0.0132 (8) |
| O2 | 0.0706 (10) | 0.0608 (10) | 0.1129 (15) | 0.0211 (8) | 0.0075 (10) | 0.0060 (10) |
| O3 | 0.0645 (9) | 0.0673 (9) | 0.0570 (8) | −0.0022 (7) | 0.0239 (7) | −0.0007 (7) |
| O4 | 0.0549 (8) | 0.0441 (8) | 0.0862 (11) | 0.0089 (6) | 0.0111 (7) | −0.0004 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.385 (3) | C16—C17 | 1.376 (3) |
| C1—C6 | 1.385 (2) | C16—H16 | 0.9300 |
| C1—H1 | 0.9300 | C17—C18 | 1.379 (3) |
| C2—C3 | 1.378 (3) | C17—H17 | 0.9300 |
| C2—C14 | 1.510 (3) | C18—C19 | 1.360 (4) |
| C3—C4 | 1.380 (3) | C18—H18 | 0.9300 |
| C3—H3 | 0.9300 | C19—C20 | 1.374 (3) |
| C4—C5 | 1.377 (3) | C19—H19 | 0.9300 |
| C4—H4 | 0.9300 | C20—H20 | 0.9300 |
| C5—C6 | 1.382 (3) | C21—C22B | 1.473 (7) |
| C5—H5 | 0.9300 | C21—N1 | 1.484 (3) |
| C6—C7 | 1.505 (3) | C21—C22A | 1.509 (6) |
| C7—N1 | 1.473 (2) | C21—H21A | 0.9700 |
| C7—H7A | 0.9700 | C21—H21B | 0.9700 |
| C7—H7B | 0.9700 | C22A—H22A | 0.9600 |
| C8—C9 | 1.377 (3) | C22A—H22B | 0.9600 |
| C8—C13 | 1.384 (3) | C22A—H22C | 0.9600 |
| C8—S1 | 1.759 (2) | C22B—H22D | 0.9600 |
| C9—C10 | 1.385 (4) | C22B—H22E | 0.9600 |
| C9—H9 | 0.9300 | C22B—H22F | 0.9600 |
| C10—C11 | 1.371 (4) | C23—C24 | 1.482 (3) |
| C10—H10 | 0.9300 | C23—N2 | 1.485 (3) |
| C11—C12 | 1.355 (4) | C23—H23A | 0.9700 |
| C11—H11 | 0.9300 | C23—H23B | 0.9700 |
| C12—C13 | 1.370 (4) | C24—H24A | 0.9600 |
| C12—H12 | 0.9300 | C24—H24B | 0.9600 |
| C13—H13 | 0.9300 | C24—H24C | 0.9600 |
| C14—N2 | 1.469 (2) | S1—O1 | 1.4235 (16) |

| | | | |
|---|---|---|---|
| C14—H14A | 0.9700 | S1—O2 | 1.4276 (16) |
| C14—H14B | 0.9700 | S1—N1 | 1.6220 (18) |
| C15—C16 | 1.381 (3) | S2—O4 | 1.4239 (14) |
| C15—C20 | 1.385 (3) | S2—O3 | 1.4274 (15) |
| C15—S2 | 1.7543 (18) | S2—N2 | 1.6224 (16) |
| C2—C1—C6 | 121.08 (17) | C17—C18—H18 | 119.8 |
| C2—C1—H1 | 119.5 | C18—C19—C20 | 120.4 (2) |
| C6—C1—H1 | 119.5 | C18—C19—H19 | 119.8 |
| C3—C2—C1 | 119.08 (17) | C20—C19—H19 | 119.8 |
| C3—C2—C14 | 121.14 (18) | C19—C20—C15 | 119.5 (2) |
| C1—C2—C14 | 119.76 (17) | C19—C20—H20 | 120.3 |
| C2—C3—C4 | 120.50 (19) | C15—C20—H20 | 120.3 |
| C2—C3—H3 | 119.7 | C22B—C21—N1 | 115.4 (3) |
| C4—C3—H3 | 119.7 | C22B—C21—C22A | 31.0 (3) |
| C5—C4—C3 | 119.87 (19) | N1—C21—C22A | 110.3 (3) |
| C5—C4—H4 | 120.1 | C22B—C21—H21A | 128.4 |
| C3—C4—H4 | 120.1 | N1—C21—H21A | 109.6 |
| C4—C5—C6 | 120.67 (18) | C22A—C21—H21A | 109.6 |
| C4—C5—H5 | 119.7 | C22B—C21—H21B | 79.5 |
| C6—C5—H5 | 119.7 | N1—C21—H21B | 109.6 |
| C5—C6—C1 | 118.79 (18) | C22A—C21—H21B | 109.6 |
| C5—C6—C7 | 121.08 (17) | H21A—C21—H21B | 108.1 |
| C1—C6—C7 | 120.09 (17) | C21—C22A—H22A | 109.5 |
| N1—C7—C6 | 112.47 (15) | C21—C22A—H22B | 109.5 |
| N1—C7—H7A | 109.1 | H22A—C22A—H22B | 109.5 |
| C6—C7—H7A | 109.1 | C21—C22A—H22C | 109.5 |
| N1—C7—H7B | 109.1 | H22A—C22A—H22C | 109.5 |
| C6—C7—H7B | 109.1 | H22B—C22A—H22C | 109.5 |
| H7A—C7—H7B | 107.8 | C21—C22B—H22D | 109.5 |
| C9—C8—C13 | 120.4 (2) | C21—C22B—H22E | 109.5 |
| C9—C8—S1 | 119.95 (17) | H22D—C22B—H22E | 109.5 |
| C13—C8—S1 | 119.6 (2) | C21—C22B—H22F | 109.5 |
| C8—C9—C10 | 118.9 (2) | H22D—C22B—H22F | 109.5 |
| C8—C9—H9 | 120.5 | H22E—C22B—H22F | 109.5 |
| C10—C9—H9 | 120.5 | C24—C23—N2 | 112.85 (19) |
| C11—C10—C9 | 120.1 (3) | C24—C23—H23A | 109.0 |
| C11—C10—H10 | 120.0 | N2—C23—H23A | 109.0 |
| C9—C10—H10 | 120.0 | C24—C23—H23B | 109.0 |
| C12—C11—C10 | 120.7 (3) | N2—C23—H23B | 109.0 |
| C12—C11—H11 | 119.6 | H23A—C23—H23B | 107.8 |
| C10—C11—H11 | 119.6 | C23—C24—H24A | 109.5 |
| C11—C12—C13 | 120.2 (3) | C23—C24—H24B | 109.5 |
| C11—C12—H12 | 119.9 | H24A—C24—H24B | 109.5 |
| C13—C12—H12 | 119.9 | C23—C24—H24C | 109.5 |
| C12—C13—C8 | 119.7 (3) | H24A—C24—H24C | 109.5 |
| C12—C13—H13 | 120.2 | H24B—C24—H24C | 109.5 |
| C8—C13—H13 | 120.2 | O1—S1—O2 | 119.23 (11) |
| N2—C14—C2 | 111.00 (15) | O1—S1—N1 | 107.17 (10) |
| N2—C14—H14A | 109.4 | O2—S1—N1 | 107.05 (10) |

| | | | |
|---|---|---|---|
| C2—C14—H14A | 109.4 | O1—S1—C8 | 107.96 (11) |
| N2—C14—H14B | 109.4 | O2—S1—C8 | 107.99 (11) |
| C2—C14—H14B | 109.4 | N1—S1—C8 | 106.83 (9) |
| H14A—C14—H14B | 108.0 | O4—S2—O3 | 119.85 (10) |
| C16—C15—C20 | 120.34 (18) | O4—S2—N2 | 106.51 (9) |
| C16—C15—S2 | 119.65 (14) | O3—S2—N2 | 106.90 (9) |
| C20—C15—S2 | 119.98 (14) | O4—S2—C15 | 108.02 (8) |
| C17—C16—C15 | 119.26 (19) | O3—S2—C15 | 107.73 (9) |
| C17—C16—H16 | 120.4 | N2—S2—C15 | 107.22 (8) |
| C15—C16—H16 | 120.4 | C7—N1—C21 | 115.15 (17) |
| C16—C17—C18 | 120.1 (2) | C7—N1—S1 | 116.09 (13) |
| C16—C17—H17 | 119.9 | C21—N1—S1 | 116.36 (14) |
| C18—C17—H17 | 119.9 | C14—N2—C23 | 115.60 (17) |
| C19—C18—C17 | 120.4 (2) | C14—N2—S2 | 117.71 (13) |
| C19—C18—H18 | 119.8 | C23—N2—S2 | 117.68 (13) |
| | | | |
| C6—C1—C2—C3 | 0.1 (3) | C9—C8—S1—O2 | −167.52 (19) |
| C6—C1—C2—C14 | −178.75 (16) | C13—C8—S1—O2 | 15.1 (2) |
| C1—C2—C3—C4 | 0.2 (3) | C9—C8—S1—N1 | 77.6 (2) |
| C14—C2—C3—C4 | 179.06 (18) | C13—C8—S1—N1 | −99.8 (2) |
| C2—C3—C4—C5 | −0.2 (3) | C16—C15—S2—O4 | 162.80 (16) |
| C3—C4—C5—C6 | −0.1 (3) | C20—C15—S2—O4 | −19.20 (19) |
| C4—C5—C6—C1 | 0.5 (3) | C16—C15—S2—O3 | 31.99 (18) |
| C4—C5—C6—C7 | −177.20 (18) | C20—C15—S2—O3 | −150.01 (16) |
| C2—C1—C6—C5 | −0.5 (3) | C16—C15—S2—N2 | −82.76 (17) |
| C2—C1—C6—C7 | 177.22 (16) | C20—C15—S2—N2 | 95.24 (17) |
| C5—C6—C7—N1 | −112.7 (2) | C6—C7—N1—C21 | 71.0 (2) |
| C1—C6—C7—N1 | 69.7 (2) | C6—C7—N1—S1 | −148.14 (14) |
| C13—C8—C9—C10 | 1.8 (4) | C22B—C21—N1—C7 | −98.2 (6) |
| S1—C8—C9—C10 | −175.61 (19) | C22A—C21—N1—C7 | −131.5 (4) |
| C8—C9—C10—C11 | −1.3 (4) | C22B—C21—N1—S1 | 121.0 (6) |
| C9—C10—C11—C12 | −0.2 (5) | C22A—C21—N1—S1 | 87.7 (4) |
| C10—C11—C12—C13 | 1.3 (5) | O1—S1—N1—C7 | 48.65 (16) |
| C11—C12—C13—C8 | −0.8 (5) | O2—S1—N1—C7 | 177.65 (14) |
| C9—C8—C13—C12 | −0.7 (4) | C8—S1—N1—C7 | −66.87 (15) |
| S1—C8—C13—C12 | 176.7 (2) | O1—S1—N1—C21 | −170.94 (15) |
| C3—C2—C14—N2 | 120.3 (2) | O2—S1—N1—C21 | −41.94 (17) |
| C1—C2—C14—N2 | −60.8 (2) | C8—S1—N1—C21 | 73.54 (16) |
| C20—C15—C16—C17 | 0.4 (3) | C2—C14—N2—C23 | −69.5 (2) |
| S2—C15—C16—C17 | 178.43 (17) | C2—C14—N2—S2 | 144.01 (14) |
| C15—C16—C17—C18 | −0.4 (3) | C24—C23—N2—C14 | 114.9 (2) |
| C16—C17—C18—C19 | 0.6 (4) | C24—C23—N2—S2 | −98.7 (2) |
| C17—C18—C19—C20 | −0.8 (4) | O4—S2—N2—C14 | −173.57 (14) |
| C18—C19—C20—C15 | 0.8 (3) | O3—S2—N2—C14 | −44.33 (16) |
| C16—C15—C20—C19 | −0.6 (3) | C15—S2—N2—C14 | 70.98 (15) |
| S2—C15—C20—C19 | −178.58 (17) | O4—S2—N2—C23 | 40.68 (17) |
| C9—C8—S1—O1 | −37.4 (2) | O3—S2—N2—C23 | 169.93 (15) |
| C13—C8—S1—O1 | 145.2 (2) | C15—S2—N2—C23 | −74.77 (16) |

*Hydrogen-bond geometry (Å, °)*

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C17—H17···O1[i] | 0.93 | 2.57 | 3.409 (3) | 151 |

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

**Fig. 1**

**Fig. 2**