Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-Nitro-*N*,*N*-bis(*p*-tolylsulfonyl)aniline

Ke-Jian Zhao,[a] Xiang-Xiang Wu,[b] Guoping Wang[c] and Mao-Lin Hu[a]*

[a]College of Chemistry and Materials Engineering, Wenzhou University, Zhejiang, Wenzhou 325027, People's Republic of China, [b]College of Pharmacy, Henan University of Traditional Chinese Medicine, Henan, Zhengzhou 450008, People's Republic of China, and [c]Department of Chemistry, College of Science, Zhejiang University, Zhejiang, Hangzhou 310027, People's Republic of China
Correspondence e-mail: hu403cn@yahoo.com.cn

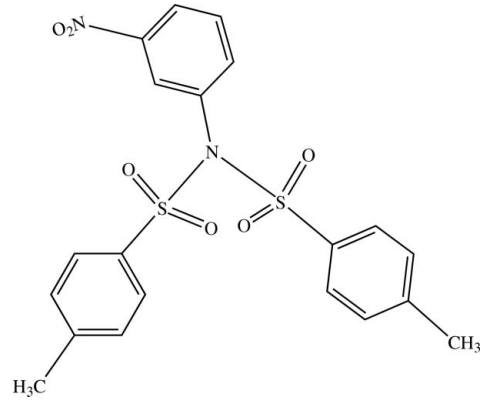
Received 20 October 2007; accepted 25 October 2007

Key indicators: single-crystal X-ray study; T = 278 K; mean σ(C–C) = 0.004 Å; R factor = 0.054; wR factor = 0.135; data-to-parameter ratio = 13.2.

In the title compound, $C_{20}H_{18}N_2O_6S_2$, all bond lengths and angles are within normal ranges. The configuration around central N atom is almost planar; the r.m.s. deviation for the fitted atoms is 0.0218 Å. The electron-withdrawing effect of the S atom is observed in this structure, *i.e.* the *ortho–meta–para* C—C—C angles in the attached rings are greater than 120°.

Related literature

For related literature, see: Allen *et al.* (1987); Krishnaiah *et al.* (1995); Patani & Lavoie (1996); Yan *et al.* (2007); Creaser *et al.* (2001); Kazak *et al.* (2000); Yu (2006).



Experimental

Crystal data

$C_{20}H_{18}N_2O_6S_2$
M_r = 446.48
Monoclinic, $C2/c$
a = 25.7789 (9) Å
b = 9.7238 (7) Å
c = 16.4653 (8) Å
β = 99.507 (1)°
V = 4070.7 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 278 (2) K
0.41 × 0.29 × 0.26 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.886, T_{max} = 0.926
10446 measured reflections
3607 independent reflections
3249 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.135
S = 1.15
3607 reflections
273 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

We acknowledge financial support by the Medical Science Research Foundation of Zhejiang Province, China (No. 2005 A071) and the National Natural Science Foundation of China (No. 20571057).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2445).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2002). *SADABS* (Version 2.03), *SAINT* (Version 6.02), *SMART* (Version 5.62) and *SHELXTL* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Creaser, S. P., Pyke, S. M. & Tiekink, E. R. T. (2001). *Z. Kristallogr. New Cryst. Struct.* **216**, 1267–640.
Kazak, C., Aygün, M., Turgut, G., Odabaşoğlu, M., Özbey, S. & Büyükgüngör, O. (2000). *Acta Cryst.* C**56**, 1044–1045.
Krishnaiah, M., Narayana Raju, K. V., Lu, I.-L., Chen, Y.-S. & Narasinga Rao, S. (1995). *Acta Cryst.* C**51**, 2429–2430.
Patani, G. A. & Lavoie, E. J. (1996). *Chem. Rev.* **96**, 3147–3176.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Yan, X.-W., Hu, M.-L. & Xiong, J. (2007). *Acta Cryst.* E**63**, o678–o679.
Yu, Y.-Y. (2006). *Acta Cryst.* E**62**, o2308–o2309.

  doi:10.1107/S160053680705307X

supplementary materials

Acta Cryst. (2007). E**63**, o4472 [**doi:10.1107/S160053680705307X**]

3-Nitro-*N*,*N*-bis(*p*-tolylsulfonyl)aniline

K.-J. Zhao, X.-X. Wu, G. Wang and M.-L. Hu

Comment

The sulfonamide group is present in many bioactive compounds and be used as protecting group (Krishnaiah *et al.*, 1995; Patani & Lavoie, 1996). Some crystal structures involving sulfonamide groups have been published, including a recent report from our labratory (Yan, *et al.*, 2007). As an extension of this research, we report the synthesis and the crystal structure of $C_{20}H_{18}N_2O_6S_2$ (I), namely *N*,*N*-bis(toluene-4-sulfonylamino)-3-nitroaniline.

In (I) (Fig. 1), all bond lengths and angles show normal values (Allen *et al.*, 1987) and are unremarkable when compared with those found in our previous report (Yan, *et al.*, 2007). The three independent benzene rings C2—C7 (P_1), C9—C14 (P_2) and C15—C20 (P_3) are essentially planar with r.m.s. deviation of 0.0029 Å, 0.0091 Å and 0.0041 Å, respectively. The dihedral angles P1/P2, P1/P3 and P2/P3 are 41.74 (14), 31.82 (14) and 19.50 (14)°, respectively. The bond angles of C4—C3—C2 and C6—C7—C2 should be more than 120°. The experimental results are 121.1 (3)° and 121.6 (3)°, respectively. It shows that the S atoms introduce electron-withdrawing effect (Kazak *et al.*, 2000).

Experimental

Aqueous NaOH (20 ml, 10%) was added dropwise to a mixture of 4-methylbenzene-1-sulfonyl chloride (10 mmol, 1.905 g) and 3-nitroaniline (5 mmol, 1.38 g) with constant stirring for 4 h. After column chromatography separation with the silica stationary phase and the eluent of petroleum ether and acetic ester with relative proportions (*v*/*v*, 5/1), the purified product was dissolved in ethanol and allowed to stand for approximately 8 d until single crystals formed.

Refinement

The all H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of Csp^2—H = 0.93 Å with U_{iso} = 1.2U_{eq}(parent atom), Csp^3—H = 0.96 Å with U_{iso} = 1.5U_{eq}(parent atom).

Figures

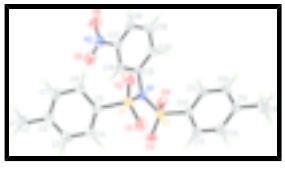


Fig. 1. The molecular structure of (I) showing 30% probability displacement ellipsoids and the atomic numbering.

3-Nitro-*N*,*N*-bis(*p*-tolylsulfonyl)aniline

Crystal data

$C_{20}H_{18}N_2O_6S_2$	F_{000} = 1856
M_r = 446.48	D_x = 1.457 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 3381 reflections
a = 25.7789 (9) Å	θ = 2.5–25.0º
b = 9.7238 (7) Å	μ = 0.30 mm^{-1}
c = 16.4653 (8) Å	*T* = 278 (2) K
β = 99.5070 (10)º	Blcok, colourless
V = 4070.7 (4) Å^3	0.41 × 0.29 × 0.26 mm
Z = 8	

Data collection

Bruker APEX area-detector diffractometer	3607 independent reflections
Radiation source: fine-focus sealed tube	3249 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.025
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Bruker, 2002)	*h* = −30→28
T_{min} = 0.886, T_{max} = 0.926	*k* = −11→11
10446 measured reflections	*l* = −13→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.055	H-atom parameters constrained
$wR(F^2)$ = 0.135	$w = 1/[\sigma^2(F_o^2) + (0.057P)^2 + 4.9858P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.15	$(\Delta/\sigma)_{max}$ = 0.001
3607 reflections	$\Delta\rho_{max}$ = 0.38 e Å^{-3}
273 parameters	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.34132 (3)	0.03077 (7)	0.05542 (4)	0.0478 (2)
S2	0.29039 (3)	0.01230 (7)	0.20435 (4)	0.0471 (2)
O1	0.31699 (8)	−0.0994 (2)	0.04417 (15)	0.0689 (6)
O2	0.33162 (8)	0.1314 (2)	−0.00784 (12)	0.0633 (6)
O3	0.31436 (8)	−0.1187 (2)	0.21575 (15)	0.0674 (6)
O4	0.29099 (8)	0.1039 (2)	0.27150 (12)	0.0622 (6)
O5	0.45481 (10)	0.4127 (3)	0.30077 (16)	0.0813 (7)
O6	0.43517 (11)	0.6151 (3)	0.2557 (2)	0.0969 (9)
N1	0.32225 (8)	0.1017 (2)	0.13871 (14)	0.0455 (5)
N2	0.42661 (11)	0.4927 (3)	0.25742 (18)	0.0634 (7)
C1	0.57602 (13)	−0.0289 (4)	0.1548 (2)	0.0845 (12)
H1A	0.5890	−0.0989	0.1223	0.127*
H1B	0.5838	−0.0537	0.2120	0.127*
H1C	0.5927	0.0572	0.1465	0.127*
C2	0.51728 (11)	−0.0150 (3)	0.12921 (18)	0.0570 (8)
C3	0.48381 (12)	−0.1222 (3)	0.1399 (2)	0.0617 (8)
H3	0.4978	−0.2045	0.1625	0.074*
C4	0.43021 (11)	−0.1092 (3)	0.11752 (18)	0.0536 (7)
H4	0.4081	−0.1818	0.1254	0.064*
C5	0.40961 (10)	0.0117 (3)	0.08350 (16)	0.0431 (6)
C6	0.44203 (11)	0.1200 (3)	0.07136 (19)	0.0537 (7)
H6	0.4280	0.2015	0.0478	0.064*
C7	0.49557 (12)	0.1052 (3)	0.0948 (2)	0.0620 (8)
H7	0.5176	0.1782	0.0872	0.074*
C8	0.07156 (13)	−0.0322 (4)	0.0105 (2)	0.0814 (11)
H8A	0.0479	0.0263	0.0339	0.122*
H8B	0.0592	−0.1255	0.0098	0.122*
H8C	0.0731	−0.0031	−0.0447	0.122*
C9	0.12544 (11)	−0.0235 (3)	0.06152 (19)	0.0551 (7)
C10	0.14279 (11)	0.0960 (3)	0.10178 (19)	0.0558 (7)
H10	0.1203	0.1713	0.0983	0.067*
C11	0.19262 (11)	0.1071 (3)	0.14717 (19)	0.0504 (7)
H11	0.2035	0.1884	0.1745	0.061*

C12	0.22587 (10)	−0.0044 (3)	0.15123 (17)	0.0423 (6)
C13	0.20953 (11)	−0.1263 (3)	0.1129 (2)	0.0552 (7)
H13	0.2320	−0.2017	0.1164	0.066*
C14	0.15919 (12)	−0.1345 (3)	0.0691 (2)	0.0623 (8)
H14	0.1477	−0.2172	0.0440	0.075*
C15	0.32900 (10)	0.2488 (3)	0.14926 (16)	0.0413 (6)
C16	0.37314 (10)	0.2977 (3)	0.19917 (16)	0.0439 (6)
H16	0.3979	0.2381	0.2276	0.053*
C17	0.37934 (11)	0.4383 (3)	0.20555 (17)	0.0488 (7)
C18	0.34264 (13)	0.5292 (3)	0.1651 (2)	0.0578 (8)
H18	0.3476	0.6236	0.1709	0.069*
C19	0.29890 (13)	0.4776 (3)	0.1165 (2)	0.0590 (8)
H19	0.2737	0.5374	0.0891	0.071*
C20	0.29180 (11)	0.3376 (3)	0.10773 (17)	0.0515 (7)
H20	0.2621	0.3030	0.0741	0.062*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0391 (4)	0.0508 (4)	0.0521 (4)	0.0014 (3)	0.0031 (3)	−0.0106 (3)
S2	0.0430 (4)	0.0439 (4)	0.0527 (4)	−0.0060 (3)	0.0027 (3)	0.0035 (3)
O1	0.0535 (12)	0.0619 (13)	0.0912 (16)	−0.0088 (10)	0.0116 (11)	−0.0322 (12)
O2	0.0585 (12)	0.0803 (15)	0.0480 (11)	0.0216 (11)	−0.0003 (9)	0.0024 (10)
O3	0.0549 (12)	0.0501 (12)	0.0906 (16)	−0.0005 (10)	−0.0071 (11)	0.0180 (11)
O4	0.0652 (13)	0.0710 (14)	0.0502 (12)	−0.0182 (11)	0.0094 (10)	−0.0056 (10)
O5	0.0628 (14)	0.0954 (19)	0.0800 (17)	−0.0226 (14)	−0.0046 (13)	−0.0121 (15)
O6	0.0918 (19)	0.0619 (16)	0.139 (2)	−0.0401 (14)	0.0265 (17)	−0.0284 (15)
N1	0.0429 (12)	0.0388 (12)	0.0560 (14)	−0.0062 (9)	0.0114 (10)	−0.0061 (10)
N2	0.0565 (16)	0.0652 (18)	0.0715 (19)	−0.0204 (14)	0.0192 (14)	−0.0170 (14)
C1	0.0491 (19)	0.119 (3)	0.080 (3)	0.011 (2)	−0.0039 (17)	−0.021 (2)
C2	0.0439 (15)	0.076 (2)	0.0498 (17)	0.0085 (15)	0.0036 (13)	−0.0135 (15)
C3	0.0615 (19)	0.0579 (19)	0.0633 (19)	0.0173 (15)	0.0029 (15)	0.0076 (15)
C4	0.0518 (16)	0.0456 (16)	0.0637 (18)	0.0020 (12)	0.0102 (14)	0.0074 (13)
C5	0.0405 (14)	0.0442 (14)	0.0447 (14)	0.0026 (11)	0.0077 (11)	−0.0005 (11)
C6	0.0497 (16)	0.0452 (16)	0.0658 (19)	0.0022 (12)	0.0081 (14)	0.0076 (13)
C7	0.0480 (17)	0.0643 (19)	0.075 (2)	−0.0111 (14)	0.0142 (15)	−0.0034 (16)
C8	0.0517 (19)	0.109 (3)	0.080 (2)	−0.0089 (19)	0.0004 (17)	0.005 (2)
C9	0.0436 (15)	0.0660 (19)	0.0568 (18)	−0.0067 (14)	0.0111 (13)	0.0050 (15)
C10	0.0449 (16)	0.0517 (16)	0.073 (2)	0.0050 (13)	0.0157 (14)	0.0081 (15)
C11	0.0493 (16)	0.0389 (14)	0.0654 (18)	−0.0048 (12)	0.0160 (13)	−0.0052 (13)
C12	0.0381 (13)	0.0394 (13)	0.0504 (15)	−0.0047 (11)	0.0100 (11)	0.0003 (11)
C13	0.0447 (15)	0.0406 (15)	0.081 (2)	−0.0020 (12)	0.0129 (14)	−0.0058 (14)
C14	0.0524 (17)	0.0541 (18)	0.080 (2)	−0.0151 (14)	0.0096 (16)	−0.0190 (16)
C15	0.0406 (13)	0.0373 (13)	0.0471 (15)	−0.0035 (10)	0.0109 (11)	−0.0034 (11)
C16	0.0412 (14)	0.0440 (14)	0.0471 (15)	−0.0018 (11)	0.0096 (11)	0.0002 (12)
C17	0.0509 (15)	0.0477 (15)	0.0510 (16)	−0.0139 (13)	0.0183 (13)	−0.0092 (13)
C18	0.071 (2)	0.0370 (15)	0.071 (2)	0.0008 (14)	0.0272 (17)	0.0011 (14)
C19	0.0645 (19)	0.0500 (17)	0.0631 (19)	0.0145 (14)	0.0123 (16)	0.0057 (14)

C20	0.0469 (15)	0.0554 (17)	0.0514 (16)	0.0041 (13)	0.0059 (13)	−0.0022 (13)

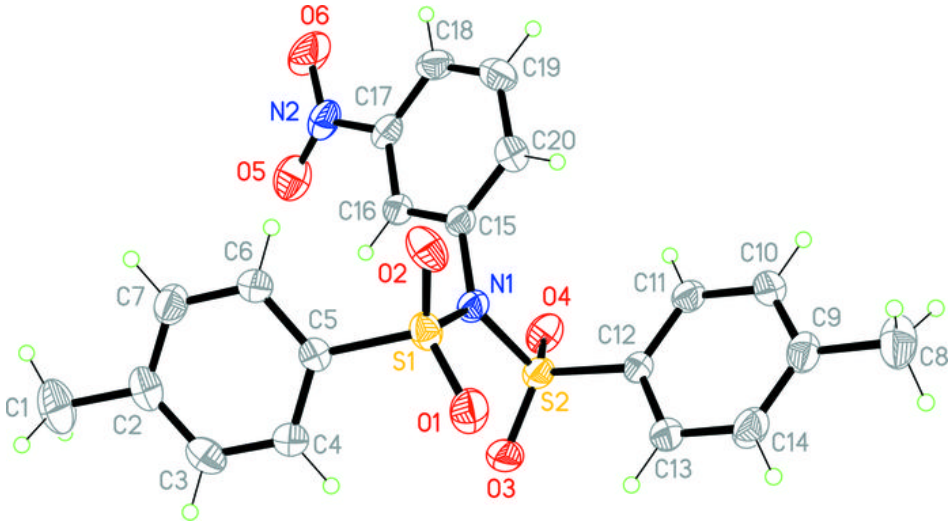
Geometric parameters (Å, °)

S1—O1	1.411 (2)	C7—H7	0.9300
S1—O2	1.421 (2)	C8—C9	1.502 (4)
S1—N1	1.679 (2)	C8—H8A	0.9600
S1—C5	1.755 (3)	C8—H8B	0.9600
S2—O3	1.415 (2)	C8—H8C	0.9600
S2—O4	1.418 (2)	C9—C10	1.375 (4)
S2—N1	1.700 (2)	C9—C14	1.379 (4)
S2—C12	1.754 (3)	C10—C11	1.380 (4)
O5—N2	1.213 (4)	C10—H10	0.9300
O6—N2	1.211 (3)	C11—C12	1.376 (4)
N1—C15	1.448 (3)	C11—H11	0.9300
N2—C17	1.467 (4)	C12—C13	1.376 (4)
C1—C2	1.509 (4)	C13—C14	1.379 (4)
C1—H1A	0.9600	C13—H13	0.9300
C1—H1B	0.9600	C14—H14	0.9300
C1—H1C	0.9600	C15—C16	1.374 (4)
C2—C7	1.377 (4)	C15—C20	1.384 (4)
C2—C3	1.383 (4)	C16—C17	1.378 (4)
C3—C4	1.376 (4)	C16—H16	0.9300
C3—H3	0.9300	C17—C18	1.383 (4)
C4—C5	1.370 (4)	C18—C19	1.366 (5)
C4—H4	0.9300	C18—H18	0.9300
C5—C6	1.380 (4)	C19—C20	1.378 (4)
C6—C7	1.378 (4)	C19—H19	0.9300
C6—H6	0.9300	C20—H20	0.9300
O1—S1—O2	120.07 (14)	C9—C8—H8A	109.5
O1—S1—N1	106.96 (13)	C9—C8—H8B	109.5
O2—S1—N1	106.03 (12)	H8A—C8—H8B	109.5
O1—S1—C5	110.14 (13)	C9—C8—H8C	109.5
O2—S1—C5	108.27 (13)	H8A—C8—H8C	109.5
N1—S1—C5	104.16 (12)	H8B—C8—H8C	109.5
O3—S2—O4	120.91 (14)	C10—C9—C14	117.9 (3)
O3—S2—N1	107.36 (13)	C10—C9—C8	120.9 (3)
O4—S2—N1	103.34 (12)	C14—C9—C8	121.2 (3)
O3—S2—C12	109.90 (12)	C9—C10—C11	121.8 (3)
O4—S2—C12	109.52 (13)	C9—C10—H10	119.1
N1—S2—C12	104.36 (12)	C11—C10—H10	119.1
C15—N1—S1	117.25 (17)	C12—C11—C10	118.8 (3)
C15—N1—S2	119.33 (17)	C12—C11—H11	120.6
S1—N1—S2	123.13 (13)	C10—C11—H11	120.6
O6—N2—O5	123.4 (3)	C11—C12—C13	121.0 (3)
O6—N2—C17	118.6 (3)	C11—C12—S2	118.9 (2)
O5—N2—C17	118.1 (3)	C13—C12—S2	120.1 (2)
C2—C1—H1A	109.5	C12—C13—C14	118.7 (3)
C2—C1—H1B	109.5	C12—C13—H13	120.7

H1A—C1—H1B	109.5	C14—C13—H13	120.7
C2—C1—H1C	109.5	C13—C14—C9	121.8 (3)
H1A—C1—H1C	109.5	C13—C14—H14	119.1
H1B—C1—H1C	109.5	C9—C14—H14	119.1
C7—C2—C3	118.2 (3)	C16—C15—C20	121.2 (2)
C7—C2—C1	120.8 (3)	C16—C15—N1	119.0 (2)
C3—C2—C1	121.0 (3)	C20—C15—N1	119.8 (2)
C4—C3—C2	121.1 (3)	C15—C16—C17	117.6 (3)
C4—C3—H3	119.4	C15—C16—H16	121.2
C2—C3—H3	119.4	C17—C16—H16	121.2
C5—C4—C3	119.5 (3)	C16—C17—C18	122.4 (3)
C5—C4—H4	120.2	C16—C17—N2	118.5 (3)
C3—C4—H4	120.2	C18—C17—N2	119.1 (3)
C4—C5—C6	120.7 (3)	C19—C18—C17	118.7 (3)
C4—C5—S1	120.2 (2)	C19—C18—H18	120.7
C6—C5—S1	119.1 (2)	C17—C18—H18	120.7
C7—C6—C5	118.9 (3)	C18—C19—C20	120.4 (3)
C7—C6—H6	120.6	C18—C19—H19	119.8
C5—C6—H6	120.6	C20—C19—H19	119.8
C2—C7—C6	121.6 (3)	C19—C20—C15	119.7 (3)
C2—C7—H7	119.2	C19—C20—H20	120.1
C6—C7—H7	119.2	C15—C20—H20	120.1
O1—S1—N1—C15	−162.34 (19)	C10—C11—C12—C13	−1.9 (4)
O2—S1—N1—C15	−33.1 (2)	C10—C11—C12—S2	176.7 (2)
C5—S1—N1—C15	81.0 (2)	O3—S2—C12—C11	168.2 (2)
O1—S1—N1—S2	11.4 (2)	O4—S2—C12—C11	33.1 (3)
O2—S1—N1—S2	140.62 (16)	N1—S2—C12—C11	−77.0 (2)
C5—S1—N1—S2	−105.25 (16)	O3—S2—C12—C13	−13.3 (3)
O3—S2—N1—C15	−145.6 (2)	O4—S2—C12—C13	−148.4 (2)
O4—S2—N1—C15	−16.7 (2)	N1—S2—C12—C13	101.5 (2)
C12—S2—N1—C15	97.8 (2)	C11—C12—C13—C14	0.8 (4)
O3—S2—N1—S1	40.84 (19)	S2—C12—C13—C14	−177.7 (2)
O4—S2—N1—S1	169.69 (15)	C12—C13—C14—C9	1.3 (5)
C12—S2—N1—S1	−75.78 (17)	C10—C9—C14—C13	−2.4 (5)
C7—C2—C3—C4	−0.6 (5)	C8—C9—C14—C13	177.3 (3)
C1—C2—C3—C4	179.2 (3)	S1—N1—C15—C16	−96.1 (3)
C2—C3—C4—C5	0.5 (5)	S2—N1—C15—C16	89.9 (3)
C3—C4—C5—C6	0.1 (4)	S1—N1—C15—C20	82.4 (3)
C3—C4—C5—S1	−179.4 (2)	S2—N1—C15—C20	−91.6 (3)
O1—S1—C5—C4	−21.6 (3)	C20—C15—C16—C17	−0.8 (4)
O2—S1—C5—C4	−154.7 (2)	N1—C15—C16—C17	177.7 (2)
N1—S1—C5—C4	92.8 (2)	C15—C16—C17—C18	1.2 (4)
O1—S1—C5—C6	158.9 (2)	C15—C16—C17—N2	−179.0 (2)
O2—S1—C5—C6	25.8 (3)	O6—N2—C17—C16	171.6 (3)
N1—S1—C5—C6	−86.8 (2)	O5—N2—C17—C16	−9.4 (4)
C4—C5—C6—C7	−0.6 (4)	O6—N2—C17—C18	−8.6 (4)
S1—C5—C6—C7	178.9 (2)	O5—N2—C17—C18	170.5 (3)
C3—C2—C7—C6	0.1 (5)	C16—C17—C18—C19	−0.6 (4)
C1—C2—C7—C6	−179.7 (3)	N2—C17—C18—C19	179.6 (3)

C5—C6—C7—C2	0.5 (5)	C17—C18—C19—C20	−0.4 (5)
C14—C9—C10—C11	1.3 (5)	C18—C19—C20—C15	0.7 (5)
C8—C9—C10—C11	−178.3 (3)	C16—C15—C20—C19	−0.1 (4)
C9—C10—C11—C12	0.7 (4)	N1—C15—C20—C19	−178.6 (2)

Fig. 1


O6
C18
C19
N2
C17
C20
O5
C16
C15
O2
N1
O4
C6
C7
C5
S1
C11
C10
C12
C9
C8
C1
C2
O1
S2
C4
C14
C3
C13
O3