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4-Methyl-*N*-(2,4-dimethylphenyl)-benzenesulfonamide

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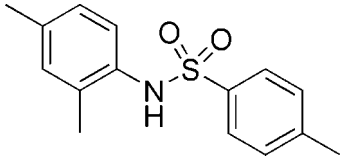
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.122; data-to-parameter ratio = 13.6.

The title compound, $C_{15}H_{17}NO_2S$, crystallizes with two independent molecules in the asymmetric unit. The molecules are linked into dimers *via* N—H···O hydrogen bonds.

Related literature

For *N*-arylbenzenesulfonamides, see: Yu *et al.* (2007); Xing *et al.* (2006); Yu (2006); Xing & Zeng (2005).



Experimental

Crystal data

$C_{15}H_{17}NO_2S$
M_r = 275.36
Triclinic, $P\overline{1}$
a = 9.751 (2) Å
b = 10.867 (2) Å
c = 14.255 (3) Å
α = 100.857 (18)°
β = 98.929 (12)°
γ = 105.55 (2)°
V = 1395.0 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 113 (2) K
0.14 × 0.12 × 0.10 mm

Data collection

Rigaku Saturn CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.954, T_{max} = 0.977
8460 measured reflections
4834 independent reflections
4053 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.122
S = 1.04
4834 reflections
355 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.80 (2)	2.18 (2)	2.959 (2)	162.3 (19)
N2—H2···O4^{ii}	0.84 (2)	2.09 (2)	2.924 (2)	170.7 (19)

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2005).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2496).

References

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supplementary materials

Acta Cryst. (2007). E**63**, o4004 [**doi:10.1107/S1600536807043012**]

4-Methyl-*N*-(2,4-dimethylphenyl)benzenesulfonamide

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Comment

The amide N atom has a pyramidal conformation, but the pyramid is somewhat shallower than expected for pure sp^3 hybrdization. The dihedral angle between the xylene and phenyl ring is 56.23 (9) ° and 46.90 (9) °, respectively, for the two molecules in the asymmetric unit.

In the crystal of (I), strong N—H···O interactions (Table 1) link the molecules into dimers. No significant aromatic interactions were detected.

Experimental

A solution of 4-methylbenzenesulfonyl chloride in CH_2Cl_2 was added dropwise to a mixture of 2,4-xylidine and triethylamine in CH_2Cl_2 at room temperature with stirring. The reaction mixture continued stirring overnight. The resulting solid was purified by recrystallization from methanol. Colourless blocks of the title compound were grown by natural evaporation of a THF solution.

Refinement

The N-bound H atoms were refined freely while the other H atoms were positioned geometrically (C—H = 0.95–0.98 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C)

Figures

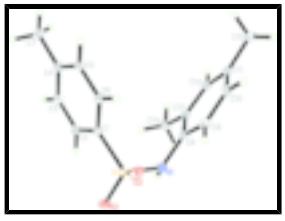


Fig. 1. The molecular structure of molecule one of (I) with the atom-numbering scheme and 30% probability displacement ellipsoids.

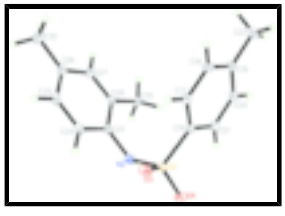


Fig. 2. The molecular structure of molecule two of (I) with the atom-numbering scheme and 30% probability displacement ellipsoids.

4-Methyl-*N*-(2,4-dimethylphenyl)benzenesulfonamide

Crystal data

$C_{15}H_{17}NO_2S$	$Z = 4$
$M_r = 275.36$	$F_{000} = 584$
Triclinic, $P\overline{1}$	$D_x = 1.311$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.751$ (2) Å	Cell parameters from 4328 reflections
$b = 10.867$ (2) Å	$\theta = 2.3$–22.5°
$c = 14.255$ (3) Å	$\mu = 0.23$ mm^{-1}
$\alpha = 100.857$ (18)°	$T = 113$ (2) K
$\beta = 98.929$ (12)°	Block, colorless
$\gamma = 105.55$ (2)°	0.14 × 0.12 × 0.10 mm
$V = 1395.0$ (5) Å^3	

Data collection

Rigaku Saturn CCD diffractometer	4834 independent reflections
Radiation source: rotating anode	4053 reflections with $I > 2\sigma(I)$
Monochromator: confocal	$R_{int} = 0.024$
Detector resolution: 7.31 pixels mm^{-1}	$\theta_{max} = 25.0^\circ$
$T = 113(2)$ K	$\theta_{min} = 2.0^\circ$
/w and /f scans	$h = -11 \rightarrow 9$
Absorption correction: multi-scan (CrystalClear; Rigaku/MSC, 2005)	$k = -11 \rightarrow 12$
$T_{min} = 0.954$, $T_{max} = 0.977$	$l = -14 \rightarrow 16$
8460 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
$R[F^2 > 2\sigma(F^2)] = 0.039$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.122$	$w = 1/[\sigma^2(F_o^2) + (0.0873P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.003$
4834 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
355 parameters	$\Delta\rho_{min} = -0.49$ 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	0.99861 (4)	0.21397 (4)	0.48505 (3)	0.02170 (15)
S2	0.52165 (4)	0.51812 (4)	0.16455 (3)	0.02119 (15)
O1	1.04014 (14)	0.16014 (12)	0.56601 (10)	0.0291 (3)
O2	1.09376 (12)	0.33231 (12)	0.47333 (11)	0.0294 (3)
O3	0.60365 (13)	0.52113 (13)	0.25760 (9)	0.0271 (3)
O4	0.58597 (13)	0.60377 (12)	0.10697 (10)	0.0267 (3)
N1	0.97222 (16)	0.09642 (15)	0.38792 (12)	0.0219 (4)
H1	0.950 (2)	0.025 (2)	0.3991 (16)	0.026*
N2	0.47811 (16)	0.36973 (15)	0.09422 (12)	0.0222 (4)
H2	0.449 (2)	0.373 (2)	0.0364 (16)	0.027*
C1	0.82853 (17)	0.23973 (16)	0.48879 (13)	0.0188 (4)
C2	0.72827 (19)	0.15748 (18)	0.52647 (14)	0.0246 (4)
H2A	0.7519	0.0891	0.5518	0.029*
C3	0.5941 (2)	0.17591 (18)	0.52674 (15)	0.0274 (4)
H3	0.5258	0.1202	0.5533	0.033*
C4	0.55629 (18)	0.27407 (18)	0.48901 (14)	0.0255 (4)
C5	0.65850 (19)	0.35555 (18)	0.45131 (14)	0.0253 (4)
H5	0.6346	0.4232	0.4251	0.030*
C6	0.79475 (19)	0.33916 (17)	0.45152 (14)	0.0220 (4)
H6	0.8643	0.3957	0.4263	0.026*
C7	0.4073 (2)	0.2904 (2)	0.48753 (17)	0.0378 (5)
H7A	0.3330	0.2116	0.4451	0.057*
H7B	0.4021	0.3674	0.4625	0.057*
H7C	0.3900	0.3028	0.5541	0.057*
C8	0.90083 (18)	0.10413 (17)	0.29432 (13)	0.0207 (4)
C9	0.9645 (2)	0.20598 (18)	0.25386 (15)	0.0279 (4)
H9	1.0553	0.2688	0.2877	0.034*
C10	0.8961 (2)	0.21609 (19)	0.16472 (15)	0.0290 (5)
H10	0.9391	0.2879	0.1388	0.035*
C11	0.7658 (2)	0.12334 (18)	0.11204 (14)	0.0257 (4)
C12	0.7065 (2)	0.02065 (18)	0.15271 (14)	0.0252 (4)
H12	0.6188	−0.0449	0.1165	0.030*
C13	0.76901 (18)	0.00868 (17)	0.24418 (14)	0.0221 (4)

C14	0.6958 (2)	−0.10155 (18)	0.28635 (15)	0.0293 (5)
H14A	0.5965	−0.1459	0.2474	0.044*
H14B	0.6920	−0.0660	0.3540	0.044*
H14C	0.7512	−0.1647	0.2851	0.044*
C15	0.6898 (2)	0.1361 (2)	0.01624 (15)	0.0336 (5)
H15A	0.6297	0.0488	−0.0234	0.050*
H15B	0.7624	0.1757	−0.0186	0.050*
H15C	0.6275	0.1922	0.0282	0.050*
C16	0.35716 (18)	0.54699 (16)	0.18285 (13)	0.0200 (4)
C17	0.30726 (19)	0.52371 (17)	0.26574 (14)	0.0238 (4)
H17	0.3640	0.4980	0.3144	0.029*
C18	0.1732 (2)	0.53847 (18)	0.27648 (15)	0.0277 (4)
H18	0.1393	0.5239	0.3336	0.033*
C19	0.08758 (19)	0.57402 (17)	0.20552 (15)	0.0268 (4)
C20	0.1407 (2)	0.59738 (18)	0.12346 (15)	0.0280 (4)
H20	0.0840	0.6230	0.0747	0.034*
C21	0.2741 (2)	0.58418 (18)	0.11117 (14)	0.0248 (4)
H21	0.3088	0.6003	0.0545	0.030*
C22	−0.0588 (2)	0.5874 (2)	0.21815 (18)	0.0400 (6)
H22A	−0.1172	0.5069	0.2320	0.060*
H22B	−0.1095	0.6013	0.1580	0.060*
H22C	−0.0449	0.6627	0.2727	0.060*
C23	0.39989 (18)	0.25998 (17)	0.12776 (13)	0.0208 (4)
C24	0.4748 (2)	0.21941 (18)	0.20114 (14)	0.0265 (4)
H24	0.5759	0.2628	0.2268	0.032*
C25	0.4034 (2)	0.11667 (19)	0.23699 (14)	0.0285 (4)
H25	0.4556	0.0906	0.2877	0.034*
C26	0.2558 (2)	0.05089 (18)	0.19958 (14)	0.0267 (4)
C27	0.1837 (2)	0.09080 (17)	0.12456 (14)	0.0246 (4)
H27	0.0834	0.0451	0.0976	0.029*
C28	0.25167 (19)	0.19451 (17)	0.08714 (13)	0.0220 (4)
C29	0.16798 (19)	0.23170 (18)	0.00476 (14)	0.0255 (4)
H29A	0.1834	0.3268	0.0215	0.038*
H29B	0.0638	0.1848	−0.0057	0.038*
H29C	0.2022	0.2077	−0.0552	0.038*
C30	0.1759 (3)	−0.0604 (2)	0.23838 (16)	0.0373 (5)
H30A	0.1465	−0.0248	0.2978	0.056*
H30B	0.2400	−0.1129	0.2538	0.056*
H30C	0.0891	−0.1162	0.1889	0.056*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0180 (2)	0.0201 (3)	0.0249 (3)	0.00807 (18)	−0.00054 (18)	0.0015 (2)
S2	0.0174 (2)	0.0254 (3)	0.0196 (3)	0.00492 (18)	0.00459 (18)	0.0045 (2)
O1	0.0329 (7)	0.0271 (7)	0.0263 (8)	0.0163 (6)	−0.0048 (6)	0.0029 (6)
O2	0.0178 (6)	0.0220 (7)	0.0436 (9)	0.0036 (5)	0.0034 (6)	0.0028 (6)
O3	0.0206 (6)	0.0362 (8)	0.0218 (7)	0.0070 (5)	0.0018 (5)	0.0054 (6)

O4	0.0230 (6)	0.0286 (7)	0.0246 (8)	0.0005 (5)	0.0074 (5)	0.0064 (6)
N1	0.0225 (8)	0.0182 (8)	0.0249 (9)	0.0081 (6)	0.0035 (6)	0.0035 (7)
N2	0.0233 (8)	0.0267 (9)	0.0186 (9)	0.0102 (7)	0.0062 (6)	0.0050 (7)
C1	0.0186 (8)	0.0179 (9)	0.0172 (9)	0.0065 (7)	0.0003 (7)	−0.0008 (7)
C2	0.0299 (10)	0.0212 (9)	0.0236 (11)	0.0084 (8)	0.0060 (8)	0.0067 (8)
C3	0.0261 (9)	0.0238 (10)	0.0289 (11)	0.0025 (8)	0.0102 (8)	0.0024 (9)
C4	0.0220 (9)	0.0273 (10)	0.0231 (10)	0.0093 (8)	0.0028 (8)	−0.0047 (8)
C5	0.0285 (9)	0.0261 (10)	0.0236 (11)	0.0146 (8)	0.0025 (8)	0.0053 (8)
C6	0.0229 (9)	0.0216 (9)	0.0214 (10)	0.0072 (7)	0.0043 (7)	0.0048 (8)
C7	0.0240 (10)	0.0428 (12)	0.0445 (14)	0.0137 (9)	0.0073 (9)	0.0007 (11)
C8	0.0201 (8)	0.0217 (9)	0.0226 (10)	0.0112 (7)	0.0063 (7)	0.0026 (8)
C9	0.0255 (9)	0.0278 (10)	0.0315 (12)	0.0075 (8)	0.0108 (8)	0.0068 (9)
C10	0.0341 (10)	0.0307 (11)	0.0304 (12)	0.0134 (9)	0.0166 (9)	0.0137 (9)
C11	0.0345 (10)	0.0301 (10)	0.0211 (10)	0.0206 (8)	0.0117 (8)	0.0067 (8)
C12	0.0262 (9)	0.0252 (10)	0.0253 (11)	0.0123 (8)	0.0050 (8)	0.0028 (8)
C13	0.0229 (9)	0.0219 (9)	0.0239 (10)	0.0118 (7)	0.0062 (7)	0.0031 (8)
C14	0.0286 (10)	0.0260 (10)	0.0279 (11)	0.0030 (8)	−0.0017 (8)	0.0080 (9)
C15	0.0444 (11)	0.0435 (12)	0.0260 (12)	0.0289 (10)	0.0129 (9)	0.0128 (10)
C16	0.0199 (8)	0.0172 (9)	0.0207 (10)	0.0046 (7)	0.0048 (7)	0.0007 (7)
C17	0.0241 (9)	0.0222 (9)	0.0225 (10)	0.0051 (7)	0.0044 (7)	0.0028 (8)
C18	0.0280 (10)	0.0266 (10)	0.0268 (11)	0.0053 (8)	0.0125 (8)	0.0016 (8)
C19	0.0233 (9)	0.0200 (9)	0.0345 (12)	0.0072 (7)	0.0071 (8)	−0.0010 (8)
C20	0.0297 (10)	0.0240 (10)	0.0320 (12)	0.0125 (8)	0.0040 (8)	0.0070 (9)
C21	0.0284 (9)	0.0228 (9)	0.0245 (11)	0.0087 (8)	0.0072 (8)	0.0065 (8)
C22	0.0277 (10)	0.0416 (13)	0.0525 (15)	0.0151 (9)	0.0134 (10)	0.0056 (11)
C23	0.0249 (9)	0.0196 (9)	0.0205 (10)	0.0105 (7)	0.0082 (7)	0.0029 (8)
C24	0.0271 (9)	0.0299 (10)	0.0242 (11)	0.0142 (8)	0.0053 (8)	0.0027 (9)
C25	0.0426 (11)	0.0298 (10)	0.0196 (10)	0.0216 (9)	0.0065 (8)	0.0065 (8)
C26	0.0421 (11)	0.0222 (10)	0.0207 (10)	0.0162 (8)	0.0126 (8)	0.0029 (8)
C27	0.0293 (10)	0.0193 (9)	0.0256 (11)	0.0096 (8)	0.0081 (8)	0.0015 (8)
C28	0.0262 (9)	0.0220 (9)	0.0200 (10)	0.0127 (7)	0.0055 (7)	0.0023 (8)
C29	0.0237 (9)	0.0242 (10)	0.0273 (11)	0.0064 (7)	0.0016 (8)	0.0076 (8)
C30	0.0550 (13)	0.0315 (11)	0.0304 (13)	0.0156 (10)	0.0136 (10)	0.0123 (10)

Geometric parameters (Å, °)

S1—O2	1.4255 (14)	C14—H14A	0.9800
S1—O1	1.4402 (14)	C14—H14B	0.9800
S1—N1	1.6315 (16)	C14—H14C	0.9800
S1—C1	1.7613 (16)	C15—H15A	0.9800
S2—O3	1.4285 (14)	C15—H15B	0.9800
S2—O4	1.4380 (13)	C15—H15C	0.9800
S2—N2	1.6363 (16)	C16—C17	1.386 (3)
S2—C16	1.7630 (17)	C16—C21	1.392 (3)
N1—C8	1.434 (2)	C17—C18	1.387 (3)
N1—H1	0.80 (2)	C17—H17	0.9500
N2—C23	1.440 (2)	C18—C19	1.389 (3)
N2—H2	0.84 (2)	C18—H18	0.9500
C1—C6	1.382 (3)	C19—C20	1.390 (3)

C1—C2	1.385 (2)	C19—C22	1.508 (2)
C2—C3	1.376 (3)	C20—C21	1.380 (3)
C2—H2A	0.9500	C20—H20	0.9500
C3—C4	1.389 (3)	C21—H21	0.9500
C3—H3	0.9500	C22—H22A	0.9800
C4—C5	1.392 (3)	C22—H22B	0.9800
C4—C7	1.507 (2)	C22—H22C	0.9800
C5—C6	1.387 (2)	C23—C24	1.390 (3)
C5—H5	0.9500	C23—C28	1.401 (3)
C6—H6	0.9500	C24—C25	1.379 (3)
C7—H7A	0.9800	C24—H24	0.9500
C7—H7B	0.9800	C25—C26	1.391 (3)
C7—H7C	0.9800	C25—H25	0.9500
C8—C9	1.388 (3)	C26—C27	1.389 (3)
C8—C13	1.400 (2)	C26—C30	1.502 (3)
C9—C10	1.378 (3)	C27—C28	1.389 (3)
C9—H9	0.9500	C27—H27	0.9500
C10—C11	1.388 (3)	C28—C29	1.506 (2)
C10—H10	0.9500	C29—H29A	0.9800
C11—C12	1.385 (3)	C29—H29B	0.9800
C11—C15	1.499 (3)	C29—H29C	0.9800
C12—C13	1.396 (3)	C30—H30A	0.9800
C12—H12	0.9500	C30—H30B	0.9800
C13—C14	1.501 (3)	C30—H30C	0.9800
O2—S1—O1	119.70 (8)	C13—C14—H14C	109.5
O2—S1—N1	108.97 (9)	H14A—C14—H14C	109.5
O1—S1—N1	104.75 (8)	H14B—C14—H14C	109.5
O2—S1—C1	107.15 (8)	C11—C15—H15A	109.5
O1—S1—C1	108.99 (9)	C11—C15—H15B	109.5
N1—S1—C1	106.62 (8)	H15A—C15—H15B	109.5
O3—S2—O4	119.67 (8)	C11—C15—H15C	109.5
O3—S2—N2	108.76 (9)	H15A—C15—H15C	109.5
O4—S2—N2	104.71 (8)	H15B—C15—H15C	109.5
O3—S2—C16	107.60 (8)	C17—C16—C21	120.70 (16)
O4—S2—C16	108.58 (8)	C17—C16—S2	119.35 (14)
N2—S2—C16	106.89 (8)	C21—C16—S2	119.80 (14)
C8—N1—S1	120.42 (12)	C16—C17—C18	118.98 (18)
C8—N1—H1	115.2 (16)	C16—C17—H17	120.5
S1—N1—H1	112.2 (15)	C18—C17—H17	120.5
C23—N2—S2	118.80 (12)	C17—C18—C19	121.43 (18)
C23—N2—H2	118.4 (14)	C17—C18—H18	119.3
S2—N2—H2	108.0 (14)	C19—C18—H18	119.3
C6—C1—C2	120.67 (16)	C18—C19—C20	118.31 (17)
C6—C1—S1	119.77 (14)	C18—C19—C22	120.44 (18)
C2—C1—S1	119.54 (14)	C20—C19—C22	121.25 (19)
C3—C2—C1	119.24 (17)	C21—C20—C19	121.47 (18)
C3—C2—H2A	120.4	C21—C20—H20	119.3
C1—C2—H2A	120.4	C19—C20—H20	119.3
C2—C3—C4	121.51 (17)	C20—C21—C16	119.10 (18)

C2—C3—H3	119.2	C20—C21—H21	120.5
C4—C3—H3	119.2	C16—C21—H21	120.5
C3—C4—C5	118.36 (16)	C19—C22—H22A	109.5
C3—C4—C7	120.71 (17)	C19—C22—H22B	109.5
C5—C4—C7	120.92 (18)	H22A—C22—H22B	109.5
C6—C5—C4	120.81 (17)	C19—C22—H22C	109.5
C6—C5—H5	119.6	H22A—C22—H22C	109.5
C4—C5—H5	119.6	H22B—C22—H22C	109.5
C1—C6—C5	119.40 (16)	C24—C23—C28	120.43 (17)
C1—C6—H6	120.3	C24—C23—N2	118.57 (16)
C5—C6—H6	120.3	C28—C23—N2	121.00 (16)
C4—C7—H7A	109.5	C25—C24—C23	120.51 (17)
C4—C7—H7B	109.5	C25—C24—H24	119.7
H7A—C7—H7B	109.5	C23—C24—H24	119.7
C4—C7—H7C	109.5	C24—C25—C26	120.61 (18)
H7A—C7—H7C	109.5	C24—C25—H25	119.7
H7B—C7—H7C	109.5	C26—C25—H25	119.7
C9—C8—C13	120.61 (18)	C27—C26—C25	117.98 (18)
C9—C8—N1	119.38 (16)	C27—C26—C30	120.67 (18)
C13—C8—N1	120.01 (16)	C25—C26—C30	121.34 (19)
C10—C9—C8	120.12 (17)	C28—C27—C26	123.02 (17)
C10—C9—H9	119.9	C28—C27—H27	118.5
C8—C9—H9	119.9	C26—C27—H27	118.5
C9—C10—C11	121.30 (18)	C27—C28—C23	117.41 (17)
C9—C10—H10	119.3	C27—C28—C29	120.43 (16)
C11—C10—H10	119.3	C23—C28—C29	122.15 (16)
C12—C11—C10	117.48 (18)	C28—C29—H29A	109.5
C12—C11—C15	121.24 (18)	C28—C29—H29B	109.5
C10—C11—C15	121.26 (18)	H29A—C29—H29B	109.5
C11—C12—C13	123.30 (17)	C28—C29—H29C	109.5
C11—C12—H12	118.3	H29A—C29—H29C	109.5
C13—C12—H12	118.4	H29B—C29—H29C	109.5
C12—C13—C8	117.13 (17)	C26—C30—H30A	109.5
C12—C13—C14	120.78 (16)	C26—C30—H30B	109.5
C8—C13—C14	122.08 (17)	H30A—C30—H30B	109.5
C13—C14—H14A	109.5	C26—C30—H30C	109.5
C13—C14—H14B	109.5	H30A—C30—H30C	109.5
H14A—C14—H14B	109.5	H30B—C30—H30C	109.5
O2—S1—N1—C8	−63.64 (14)	N1—C8—C13—C12	−178.94 (14)
O1—S1—N1—C8	167.15 (13)	C9—C8—C13—C14	−179.00 (16)
C1—S1—N1—C8	51.70 (15)	N1—C8—C13—C14	1.7 (2)
O3—S2—N2—C23	55.80 (14)	O3—S2—C16—C17	−21.43 (16)
O4—S2—N2—C23	−175.18 (12)	O4—S2—C16—C17	−152.30 (14)
C16—S2—N2—C23	−60.10 (15)	N2—S2—C16—C17	95.24 (15)
O2—S1—C1—C6	19.94 (17)	O3—S2—C16—C21	162.88 (14)
O1—S1—C1—C6	150.82 (14)	O4—S2—C16—C21	32.00 (16)
N1—S1—C1—C6	−96.61 (15)	N2—S2—C16—C21	−80.45 (16)
O2—S1—C1—C2	−161.97 (14)	C21—C16—C17—C18	−0.2 (3)
O1—S1—C1—C2	−31.09 (16)	S2—C16—C17—C18	−175.87 (13)

N1—S1—C1—C2	81.48 (16)	C16—C17—C18—C19	1.0 (3)
C6—C1—C2—C3	−0.2 (3)	C17—C18—C19—C20	−1.3 (3)
S1—C1—C2—C3	−178.25 (14)	C17—C18—C19—C22	179.04 (17)
C1—C2—C3—C4	0.8 (3)	C18—C19—C20—C21	0.9 (3)
C2—C3—C4—C5	−0.7 (3)	C22—C19—C20—C21	−179.44 (17)
C2—C3—C4—C7	178.36 (17)	C19—C20—C21—C16	−0.2 (3)
C3—C4—C5—C6	−0.1 (3)	C17—C16—C21—C20	−0.2 (3)
C7—C4—C5—C6	−179.10 (17)	S2—C16—C21—C20	175.47 (13)
C2—C1—C6—C5	−0.5 (3)	S2—N2—C23—C24	−73.77 (18)
S1—C1—C6—C5	177.53 (13)	S2—N2—C23—C28	106.65 (17)
C4—C5—C6—C1	0.7 (3)	C28—C23—C24—C25	−1.9 (3)
S1—N1—C8—C9	62.40 (19)	N2—C23—C24—C25	178.54 (15)
S1—N1—C8—C13	−118.28 (16)	C23—C24—C25—C26	0.7 (3)
C13—C8—C9—C10	1.8 (3)	C24—C25—C26—C27	0.9 (3)
N1—C8—C9—C10	−178.92 (15)	C24—C25—C26—C30	−179.42 (16)
C8—C9—C10—C11	−2.2 (3)	C25—C26—C27—C28	−1.4 (3)
C9—C10—C11—C12	0.4 (3)	C30—C26—C27—C28	178.87 (16)
C9—C10—C11—C15	178.56 (16)	C26—C27—C28—C23	0.3 (3)
C10—C11—C12—C13	1.9 (3)	C26—C27—C28—C29	179.13 (16)
C15—C11—C12—C13	−176.30 (16)	C24—C23—C28—C27	1.3 (2)
C11—C12—C13—C8	−2.2 (3)	N2—C23—C28—C27	−179.10 (15)
C11—C12—C13—C14	177.15 (16)	C24—C23—C28—C29	−177.47 (16)
C9—C8—C13—C12	0.4 (2)	N2—C23—C28—C29	2.1 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.80 (2)	2.18 (2)	2.959 (2)	162.3 (19)
N2—H2···O4^{ii}	0.84 (2)	2.09 (2)	2.924 (2)	170.7 (19)

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

Fig. 1

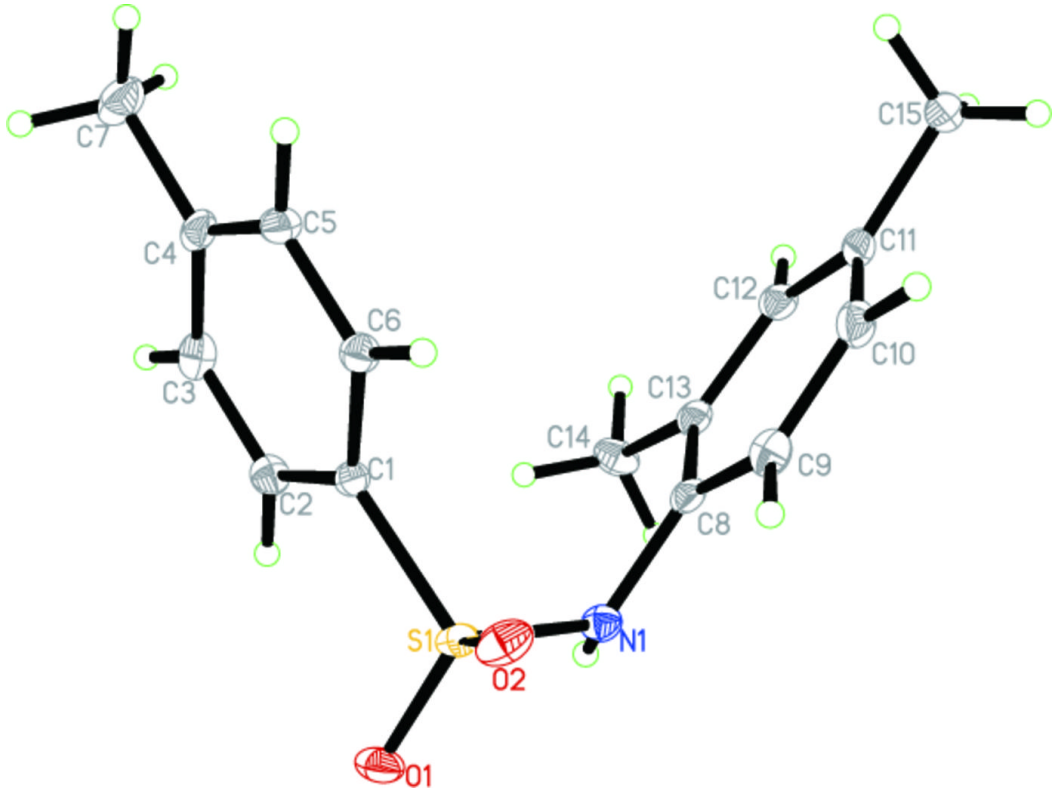
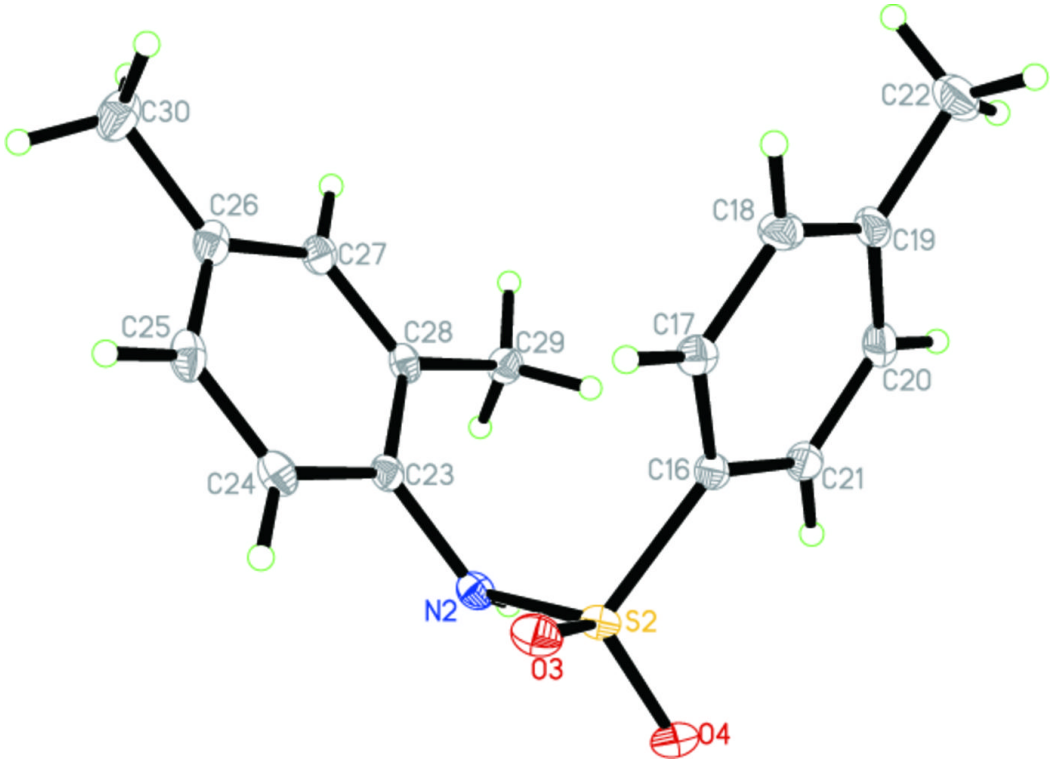


Fig. 2


C30
C26
C27
C25
C28
C29
C24
C23
C22
C18
C19
C17
C20
C16
C21
N2
S2
O3
O4