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(*E*)-2-Methyl-*N*-[4-(methylsulfonyl)-benzylidene]aniline

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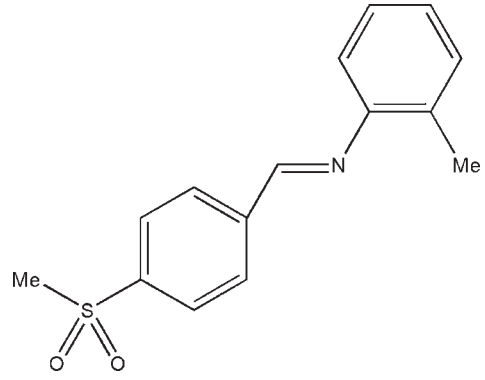
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.044; wR factor = 0.151; data-to-parameter ratio = 15.1.

Molecules of the title compound, $C_{15}H_{15}NO_2S$, display an E configuration with respect to the C=N double bond. The crystal structure is stabilized by weak C—H···O hydrogen bonds. The dihedral angle between the two aromatic ring planes is 50.41 (12)°.

Related literature

For background to Schiff base compounds in coordination chemistry, see: Shao *et al.* (2004).



Experimental

Crystal data

$C_{15}H_{15}NO_2S$
M_r = 273.34
Monoclinic, $P2_1/c$
a = 11.445 (2) Å
b = 7.8770 (16) Å
c = 16.132 (3) Å
β = 98.65 (3)°
V = 1437.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.936, T_{max} = 0.957
2745 measured reflections
2607 independent reflections
1898 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.151
S = 1.00
2607 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···O1^{i}	0.93	2.55	3.274 (3)	135

Symmetry code: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CAD-4 Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* .

This project was sponsored by ShanDong province Science & Technology Innovation Foundation.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2256).

References

Enraf–Nonius (1989). *CAD-4 Software*. Enraf–Nonius, Delft, The Netherlands.
Shao, S.-C., You, Z.-L., Fan, S.-H., Tang, L.-L., Xiong, Z.-D. & Zhu, H.-L. (2004). *Acta Cryst.* E**60**, o2183–o2184.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2009). E**65**, o3072 [doi:10.1107/S1600536809047199]

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S1. Comment

Schiff base compounds have attracted attention for the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular archtectures(Shao *et al.*, 2004). As an extension of work on the structural characterization of Schiff base compounds, the crystal structure of the title compound(I), Figure 1, is reported here. The molecule displays a trans-configuration with respect to the C=N double bond. the crystal structure is stabilized by weak C—H···O hydrogen bonds(Figure 2). The dihedral angle between two aromatic ring planes is 50.41 (12)°.

S2. Experimental

4-(methylsulfonyl)benzaldehyde (0.184g) and o-toluidine (0.107g) were dissolved in acetonitrile (20 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. After keeping the solution in air for 10 d, yellow block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

S3. Refinement

All the H atoms attached to C atoms were placed in geometrical positions and constrained to ride on their parent atoms with C-H distance in the range 0.93-0.98 Å, They were treated as riding atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

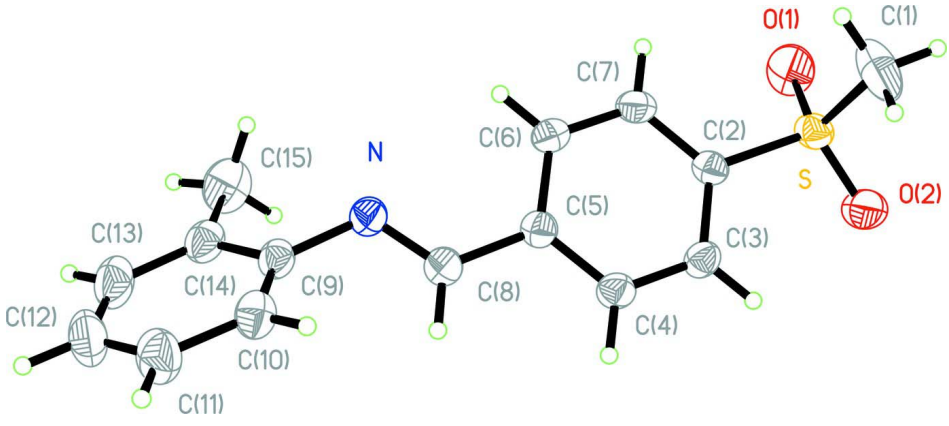

Figure 1

The structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level.

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c = 16.132 (3) Å
β = 98.65 (3)°
V = 1437.8 (5) Å^3
Z = 4
F(000) = 576
D_x = 1.263 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 25 reflections
θ = 9–14°
μ = 0.22 mm^{-1}
T = 293 K
Block, yellow
0.30 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.936, T_{max} = 0.957
2745 measured reflections

2607 independent reflections
1898 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 25.3°, θ_{min} = 1.8°
h = 0→13
k = 0→9
l = −19→19
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.151
S = 1.00
2607 reflections
173 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.09P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.052 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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	0.43428 (5)	0.25210 (8)	0.34889 (3)	0.0539 (3)
N1	0.01690 (16)	0.3139 (2)	0.60356 (12)	0.0527 (5)
O1	0.35995 (19)	0.2305 (3)	0.27085 (11)	0.0941 (8)
C1	0.5014 (3)	0.4515 (4)	0.3496 (2)	0.1056 (12)
H1B	0.5521	0.4550	0.3074	0.158*
H1C	0.5472	0.4715	0.4036	0.158*
H1D	0.4417	0.5375	0.3383	0.158*

C2	0.3445 (2)	0.2644 (3)	0.42882 (13)	0.0447 (5)
O2	0.52410 (16)	0.1283 (3)	0.37209 (12)	0.0867 (7)
C3	0.38513 (18)	0.1981 (3)	0.50701 (13)	0.0487 (5)
H3A	0.4603	0.1507	0.5183	0.058*
C4	0.31293 (19)	0.2031 (3)	0.56824 (13)	0.0503 (6)
H4A	0.3397	0.1583	0.6210	0.060*
C5	0.20111 (19)	0.2740 (3)	0.55184 (13)	0.0463 (5)
C6	0.1612 (2)	0.3412 (3)	0.47238 (14)	0.0569 (6)
H6A	0.0865	0.3898	0.4610	0.068*
C7	0.2329 (2)	0.3353 (3)	0.41107 (14)	0.0569 (6)
H7A	0.2064	0.3788	0.3580	0.068*
C8	0.12384 (19)	0.2695 (3)	0.61761 (14)	0.0499 (6)
H8A	0.1553	0.2328	0.6711	0.060*
C9	−0.05118 (19)	0.3031 (3)	0.67002 (15)	0.0504 (6)
C10	−0.0096 (2)	0.3600 (3)	0.75031 (16)	0.0617 (6)
H10A	0.0659	0.4057	0.7623	0.074*
C11	−0.0797 (3)	0.3492 (4)	0.81250 (18)	0.0807 (9)
H11A	−0.0511	0.3865	0.8664	0.097*
C12	−0.1918 (3)	0.2837 (4)	0.7949 (2)	0.0881 (10)
H12A	−0.2392	0.2764	0.8367	0.106*
C13	−0.2333 (2)	0.2291 (4)	0.7156 (2)	0.0805 (9)
H13A	−0.3090	0.1833	0.7047	0.097*
C14	−0.1664 (2)	0.2396 (3)	0.65064 (18)	0.0613 (7)
C15	−0.2132 (3)	0.1814 (4)	0.5632 (2)	0.0894 (9)
H15A	−0.2931	0.1428	0.5611	0.134*
H15B	−0.1652	0.0901	0.5478	0.134*
H15C	−0.2111	0.2741	0.5248	0.134*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0647 (4)	0.0564 (4)	0.0429 (4)	0.0082 (3)	0.0156 (3)	0.0032 (2)
N1	0.0492 (11)	0.0500 (11)	0.0603 (12)	0.0039 (9)	0.0122 (9)	0.0041 (9)
O1	0.0922 (14)	0.147 (2)	0.0427 (10)	0.0062 (13)	0.0097 (10)	−0.0103 (11)
C1	0.122 (3)	0.078 (2)	0.135 (3)	−0.0203 (19)	0.078 (2)	−0.001 (2)
C2	0.0524 (12)	0.0402 (11)	0.0421 (11)	0.0007 (9)	0.0093 (9)	0.0013 (9)
O2	0.0940 (13)	0.0980 (16)	0.0764 (12)	0.0453 (12)	0.0395 (11)	0.0257 (11)
C3	0.0436 (11)	0.0587 (13)	0.0426 (11)	0.0065 (10)	0.0019 (9)	−0.0034 (10)
C4	0.0516 (13)	0.0598 (14)	0.0382 (11)	0.0046 (10)	0.0027 (9)	0.0003 (10)
C5	0.0489 (12)	0.0460 (13)	0.0444 (11)	0.0005 (9)	0.0078 (9)	−0.0020 (9)
C6	0.0546 (13)	0.0590 (15)	0.0575 (13)	0.0161 (11)	0.0097 (11)	0.0139 (11)
C7	0.0635 (14)	0.0605 (15)	0.0470 (12)	0.0131 (12)	0.0099 (11)	0.0144 (11)
C8	0.0501 (13)	0.0504 (13)	0.0490 (12)	0.0003 (10)	0.0069 (10)	−0.0014 (10)
C9	0.0466 (12)	0.0421 (11)	0.0642 (14)	0.0031 (9)	0.0140 (10)	0.0026 (10)
C10	0.0569 (13)	0.0595 (15)	0.0708 (15)	0.0010 (12)	0.0159 (11)	−0.0064 (12)
C11	0.087 (2)	0.085 (2)	0.0760 (19)	0.0097 (17)	0.0301 (15)	−0.0102 (15)
C12	0.082 (2)	0.096 (2)	0.098 (2)	0.0081 (18)	0.0495 (19)	0.0055 (19)
C13	0.0546 (16)	0.0719 (19)	0.121 (3)	−0.0029 (13)	0.0317 (17)	0.0098 (18)

C14	0.0500 (13)	0.0496 (14)	0.0848 (18)	0.0007 (11)	0.0124 (12)	0.0043 (12)
C15	0.0661 (17)	0.091 (2)	0.106 (2)	−0.0196 (16)	−0.0010 (16)	−0.0162 (19)

Geometric parameters (Å, º)

S1—O1	1.420 (2)	C6—H6A	0.9300
S1—O2	1.4257 (18)	C7—H7A	0.9300
S1—C1	1.747 (3)	C8—H8A	0.9300
S1—C2	1.768 (2)	C9—C10	1.385 (3)
N1—C8	1.260 (3)	C9—C14	1.401 (3)
N1—C9	1.420 (3)	C10—C11	1.378 (3)
C1—H1B	0.9600	C10—H10A	0.9300
C1—H1C	0.9600	C11—C12	1.372 (4)
C1—H1D	0.9600	C11—H11A	0.9300
C2—C3	1.380 (3)	C12—C13	1.364 (5)
C2—C7	1.384 (3)	C12—H12A	0.9300
C3—C4	1.380 (3)	C13—C14	1.391 (4)
C3—H3A	0.9300	C13—H13A	0.9300
C4—C5	1.385 (3)	C14—C15	1.503 (4)
C4—H4A	0.9300	C15—H15A	0.9600
C5—C6	1.398 (3)	C15—H15B	0.9600
C5—C8	1.480 (3)	C15—H15C	0.9600
C6—C7	1.377 (3)		
O1—S1—O2	117.58 (13)	C6—C7—H7A	120.1
O1—S1—C1	108.53 (17)	C2—C7—H7A	120.1
O2—S1—C1	108.33 (16)	N1—C8—C5	122.2 (2)
O1—S1—C2	108.46 (12)	N1—C8—H8A	118.9
O2—S1—C2	108.73 (10)	C5—C8—H8A	118.9
C1—S1—C2	104.42 (12)	C10—C9—C14	120.2 (2)
C8—N1—C9	118.4 (2)	C10—C9—N1	122.4 (2)
S1—C1—H1B	109.5	C14—C9—N1	117.3 (2)
S1—C1—H1C	109.5	C11—C10—C9	120.3 (2)
H1B—C1—H1C	109.5	C11—C10—H10A	119.8
S1—C1—H1D	109.5	C9—C10—H10A	119.8
H1B—C1—H1D	109.5	C12—C11—C10	120.0 (3)
H1C—C1—H1D	109.5	C12—C11—H11A	120.0
C3—C2—C7	121.0 (2)	C10—C11—H11A	120.0
C3—C2—S1	119.54 (17)	C13—C12—C11	119.7 (3)
C7—C2—S1	119.39 (16)	C13—C12—H12A	120.1
C2—C3—C4	119.2 (2)	C11—C12—H12A	120.1
C2—C3—H3A	120.4	C12—C13—C14	122.2 (3)
C4—C3—H3A	120.4	C12—C13—H13A	118.9
C3—C4—C5	120.7 (2)	C14—C13—H13A	118.9
C3—C4—H4A	119.7	C13—C14—C9	117.4 (3)
C5—C4—H4A	119.7	C13—C14—C15	122.0 (3)
C4—C5—C6	119.5 (2)	C9—C14—C15	120.6 (2)
C4—C5—C8	119.21 (19)	C14—C15—H15A	109.5

C6—C5—C8	121.2 (2)	C14—C15—H15B	109.5
C7—C6—C5	119.9 (2)	H15A—C15—H15B	109.5
C7—C6—H6A	120.1	C14—C15—H15C	109.5
C5—C6—H6A	120.1	H15A—C15—H15C	109.5
C6—C7—C2	119.7 (2)	H15B—C15—H15C	109.5
O1—S1—C2—C3	145.99 (19)	C9—N1—C8—C5	179.03 (19)
O2—S1—C2—C3	17.0 (2)	C4—C5—C8—N1	−171.7 (2)
C1—S1—C2—C3	−98.4 (2)	C6—C5—C8—N1	5.3 (3)
O1—S1—C2—C7	−31.9 (2)	C8—N1—C9—C10	45.4 (3)
O2—S1—C2—C7	−160.84 (19)	C8—N1—C9—C14	−137.8 (2)
C1—S1—C2—C7	83.7 (2)	C14—C9—C10—C11	2.2 (4)
C7—C2—C3—C4	0.0 (3)	N1—C9—C10—C11	179.0 (2)
S1—C2—C3—C4	−177.84 (16)	C9—C10—C11—C12	−0.7 (4)
C2—C3—C4—C5	−0.2 (3)	C10—C11—C12—C13	0.1 (5)
C3—C4—C5—C6	0.0 (3)	C11—C12—C13—C14	−1.0 (5)
C3—C4—C5—C8	177.0 (2)	C12—C13—C14—C9	2.4 (4)
C4—C5—C6—C7	0.5 (4)	C12—C13—C14—C15	−179.1 (3)
C8—C5—C6—C7	−176.5 (2)	C10—C9—C14—C13	−3.0 (3)
C5—C6—C7—C2	−0.7 (4)	N1—C9—C14—C13	−179.9 (2)
C3—C2—C7—C6	0.4 (4)	C10—C9—C14—C15	178.5 (2)
S1—C2—C7—C6	178.29 (19)	N1—C9—C14—C15	1.6 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*A*···O1^{i}	0.93	2.55	3.274 (3)	135

Symmetry code: (i) *x*, −*y*+1/2, *z*+1/2.