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2-[(*E*)-(Dimethylamino)methyleneamino]-*N*-phenylbenzenesulfonamide

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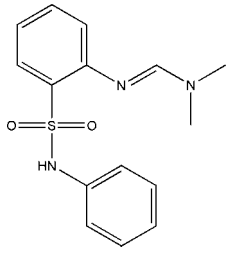
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.082; data-to-parameter ratio = 13.2.

In the title compound, $C_{15}H_{17}N_3O_2S$, all bond lengths and angles are normal. Intramolecular N—H···N hydrogen bonding influences the molecular conformation. The benzene and phenyl rings make a dihedral angle of 75.80 (2)°. In the crystal structure, weak intermolecular C—H···O hydrogen bonds link the molecules into zigzag chains extended along the *b* axis.

Related literature

For a related crystal structure, see: Henschel *et al.* (1996). For applications of sulfonimide derivatives, see: Kamoshita *et al.* (1987) and Zhang *et al.* (2007).



Experimental

Crystal data

$C_{15}H_{17}N_3O_2S$
M_r = 303.38
Monoclinic, $C2/c$
a = 16.297 (3) Å
b = 8.9962 (18) Å
c = 20.314 (4) Å
β = 99.28 (3)°
V = 2939.3 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 153 (2) K
0.47 × 0.43 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.901, T_{max} = 0.956
11196 measured reflections
2583 independent reflections
2470 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.082
S = 1.07
2583 reflections
196 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N2	0.86 (2)	2.249 (19)	2.8899 (18)	131.1 (17)
C11—H11A···O1^{i}	0.95	2.47	3.2724 (19)	143

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

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2317).

References

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Zhang, Z. B., Zhou, S. Y. & Nie, J. (2007). *J. Mol. Catal. A Chem.* **265**, 9–14.

  doi:10.1107/S1600536807050040

supplementary materials

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2-[(*E*)-(Dimethylamino)methyleneamino]-*N*-phenylbenzenesulfonamide

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Comment

Sulfonimide is an important kind of group in organic chemistry. Many compounds containing sulfonimide groups possess a broad spectrum of biological activities and can be widely used as herbicides (Kamoshita *et al.*, 1987). In addition, some compounds containing sulfonimide groups can be used as catalyst (Zhang *et al.*, 2007). Here, we report the crystal structure of (I).

In (I) (Fig. 1), all bond lengths and angles are normal and in a good agreement with those reported previously (Henschel *et al.*, 1996). The two rings - C4—C9 and C10—C15 - are oriented at angle of 75.80 (2)°. The intramolecular N1—H1A···N2 hydrogen bond influences the molecular conformation. In the crystal, the weak intermolecular C—H···O hydrogen bonds link the molecules into zigzag chains extended along the *b* axis.

Experimental

2-Amino-*N*-phenyl-benzenesulfonamide (10 mmol) was added dropwise to the solution of NaOH (25 mmol)in DMF(20 ml) and the mixture was heated under reflux for 2 h. Then the mixture was poured into water and extracted with CH_2Cl_2 (35 ml) and the organic layer was washed with 10% NaCl solution and water. The excess CH_2Cl_2 was removed on a water vacuum pump to obtain the final product (80% yield). Single crystals suitable for X-ray measurements were obtained by recrystallization from methanol at room temperature.

Refinement

All H atoms were found on difference maps. C-bound H atoms were placed in idealized positions (C—H 0.95–0.98 Å) and refined as riding, with U_{iso}(H)= 1.2–1.5Ueq(C). Atom H1A was refined isotropically.

Figures

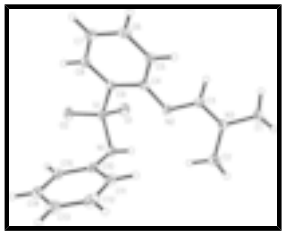
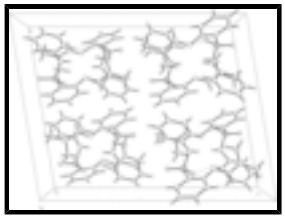


Fig. 1. The molecular structure of (I), with the atom labels and 40% probability displacement ellipsoids.



2-[(*E*)-(Dimethylamino)methyleneamino]-*N*-phenylbenzenesulfonamide

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M_r = 303.38	D_x = 1.371 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 4407 reflections
a = 16.297 (3) Å	θ = 2.9–26.4º
b = 8.9962 (18) Å	μ = 0.23 mm^{-1}
c = 20.314 (4) Å	*T* = 153 (2) K
β = 99.28 (3)º	Block, colourless
V = 2939.3 (10) Å^3	0.47 × 0.43 × 0.20 mm
Z = 8	

Data collection

Rigaku R0AXIS RAPID IP area-detector diffractometer	2583 independent reflections
Radiation source: Rotating Anode	2470 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.014
T = 153(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 3.2º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*h* = −19→19
T_{min} = 0.901, T_{max} = 0.956	*k* = −10→10
11196 measured reflections	*l* = −24→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.032	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.082	$w = 1/[\sigma^2(F_o^2) + (0.0399P)^2 + 3.4264P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max} < 0.001$
2583 reflections	$\Delta\rho_{max}$ = 0.21 e Å^{-3}

196 parameters	$\Delta\rho_{min} = -0.44$ 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	0.15973 (2)	0.20300 (4)	0.133242 (16)	0.02004 (12)
O1	0.12393 (7)	0.31020 (12)	0.17211 (5)	0.0288 (3)
O2	0.15721 (7)	0.22993 (12)	0.06340 (5)	0.0269 (3)
N1	0.25745 (8)	0.18718 (14)	0.16876 (6)	0.0220 (3)
N2	0.16787 (7)	0.03356 (13)	0.26003 (6)	0.0193 (3)
C3	0.14768 (9)	0.01258 (16)	0.31854 (7)	0.0198 (3)
H3A	0.0980	−0.0405	0.3216	0.024*
C1	0.16694 (11)	0.0447 (2)	0.43857 (7)	0.0313 (4)
H1C	0.1143	−0.0100	0.4331	0.047*
H1D	0.1593	0.1429	0.4576	0.047*
H1E	0.2094	−0.0105	0.4686	0.047*
C11	0.35427 (9)	−0.02078 (17)	0.18347 (7)	0.0261 (3)
H11A	0.3415	−0.0350	0.2271	0.031*
C13	0.43044 (10)	−0.09194 (19)	0.09645 (8)	0.0319 (4)
H13A	0.4703	−0.1539	0.0807	0.038*
C2	0.27188 (10)	0.13687 (19)	0.37240 (8)	0.0289 (4)
H2C	0.3060	0.0764	0.3471	0.043*
H2D	0.3013	0.1507	0.4180	0.043*
H2E	0.2614	0.2340	0.3508	0.043*
C14	0.38898 (9)	0.01647 (19)	0.05553 (8)	0.0274 (3)
H14A	0.4000	0.0275	0.0113	0.033*
C6	0.04005 (9)	−0.24517 (18)	0.15244 (8)	0.0248 (3)
H6A	0.0144	−0.3389	0.1563	0.030*
C4	0.12052 (8)	−0.03763 (16)	0.20566 (7)	0.0183 (3)
C15	0.33173 (9)	0.10892 (17)	0.07828 (7)	0.0226 (3)
H15A	0.3050	0.1852	0.0504	0.027*
C10	0.31362 (9)	0.08928 (16)	0.14230 (7)	0.0206 (3)
C12	0.41316 (10)	−0.10926 (18)	0.16082 (8)	0.0317 (4)
H12A	0.4420	−0.1823	0.1894	0.038*
C7	0.03399 (9)	−0.17763 (18)	0.09029 (8)	0.0265 (3)

H7A	0.0043	−0.2245	0.0518	0.032*
C8	0.07166 (9)	−0.04144 (18)	0.08525 (7)	0.0223 (3)
H8A	0.0688	0.0049	0.0429	0.027*
N3	0.19335 (8)	0.06204 (14)	0.37424 (6)	0.0217 (3)
C5	0.08311 (9)	−0.17730 (16)	0.20879 (7)	0.0212 (3)
H5A	0.0874	−0.2265	0.2506	0.025*
C9	0.11380 (8)	0.02794 (16)	0.14199 (7)	0.0183 (3)
H1A	0.2568 (12)	0.168 (2)	0.2103 (10)	0.034 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0241 (2)	0.0200 (2)	0.0155 (2)	0.00066 (14)	0.00152 (14)	0.00187 (13)
O1	0.0367 (6)	0.0235 (6)	0.0263 (6)	0.0051 (5)	0.0050 (5)	−0.0020 (4)
O2	0.0321 (6)	0.0304 (6)	0.0173 (5)	0.0008 (5)	0.0016 (4)	0.0070 (4)
N1	0.0236 (7)	0.0263 (7)	0.0153 (6)	−0.0056 (5)	0.0012 (5)	0.0005 (5)
N2	0.0205 (6)	0.0221 (6)	0.0147 (6)	−0.0008 (5)	0.0013 (5)	0.0011 (5)
C3	0.0193 (7)	0.0201 (7)	0.0198 (7)	−0.0008 (6)	0.0028 (6)	0.0024 (6)
C1	0.0368 (9)	0.0412 (10)	0.0161 (7)	−0.0076 (7)	0.0049 (6)	0.0016 (7)
C11	0.0286 (8)	0.0257 (8)	0.0223 (7)	−0.0077 (6)	−0.0013 (6)	0.0060 (6)
C13	0.0271 (8)	0.0293 (9)	0.0376 (9)	0.0000 (7)	0.0006 (7)	−0.0067 (7)
C2	0.0265 (8)	0.0352 (9)	0.0242 (8)	−0.0098 (7)	0.0016 (6)	−0.0012 (7)
C14	0.0256 (8)	0.0340 (9)	0.0221 (7)	−0.0052 (7)	0.0019 (6)	−0.0038 (6)
C6	0.0192 (7)	0.0247 (8)	0.0316 (8)	−0.0031 (6)	0.0070 (6)	−0.0048 (6)
C4	0.0144 (6)	0.0225 (7)	0.0181 (7)	0.0019 (6)	0.0032 (5)	−0.0011 (6)
C15	0.0223 (7)	0.0249 (8)	0.0192 (7)	−0.0048 (6)	−0.0007 (5)	0.0031 (6)
C10	0.0200 (7)	0.0207 (7)	0.0200 (7)	−0.0078 (6)	−0.0004 (5)	−0.0001 (6)
C12	0.0316 (9)	0.0237 (8)	0.0362 (9)	−0.0020 (7)	−0.0051 (7)	0.0051 (7)
C7	0.0204 (7)	0.0343 (9)	0.0244 (8)	−0.0028 (6)	0.0021 (6)	−0.0102 (7)
C8	0.0181 (7)	0.0315 (8)	0.0171 (7)	0.0018 (6)	0.0020 (5)	−0.0024 (6)
N3	0.0236 (6)	0.0264 (7)	0.0151 (6)	−0.0047 (5)	0.0029 (5)	0.0011 (5)
C5	0.0180 (7)	0.0238 (7)	0.0227 (7)	0.0012 (6)	0.0059 (6)	0.0013 (6)
C9	0.0156 (6)	0.0216 (7)	0.0177 (7)	0.0013 (5)	0.0030 (5)	−0.0004 (5)

Geometric parameters (Å, °)

S1—O1	1.4291 (12)	C2—N3	1.4519 (19)
S1—O2	1.4332 (11)	C2—H2C	0.9800
S1—N1	1.6451 (13)	C2—H2D	0.9800
S1—C9	1.7650 (15)	C2—H2E	0.9800
N1—C10	1.436 (2)	C14—C15	1.384 (2)
N1—H1A	0.86 (2)	C14—H14A	0.9500
N2—C3	1.2972 (18)	C6—C5	1.384 (2)
N2—C4	1.3965 (18)	C6—C7	1.390 (2)
C3—N3	1.3270 (19)	C6—H6A	0.9500
C3—H3A	0.9500	C4—C5	1.403 (2)
C1—N3	1.4487 (18)	C4—C9	1.410 (2)
C1—H1C	0.9800	C15—C10	1.390 (2)
C1—H1D	0.9800	C15—H15A	0.9500

C1—H1E	0.9800	C12—H12A	0.9500
C11—C12	1.382 (2)	C7—C8	1.382 (2)
C11—C10	1.393 (2)	C7—H7A	0.9500
C11—H11A	0.9500	C8—C9	1.391 (2)
C13—C14	1.385 (2)	C8—H8A	0.9500
C13—C12	1.390 (2)	C5—H5A	0.9500
C13—H13A	0.9500		
O1—S1—O2	118.93 (7)	C15—C14—H14A	119.6
O1—S1—N1	105.58 (7)	C13—C14—H14A	119.6
O2—S1—N1	108.65 (7)	C5—C6—C7	120.70 (14)
O1—S1—C9	109.20 (7)	C5—C6—H6A	119.7
O2—S1—C9	107.80 (7)	C7—C6—H6A	119.7
N1—S1—C9	105.96 (6)	N2—C4—C5	124.31 (13)
C10—N1—S1	121.29 (10)	N2—C4—C9	119.01 (13)
C10—N1—H1A	110.7 (13)	C5—C4—C9	116.52 (13)
S1—N1—H1A	106.4 (13)	C14—C15—C10	119.49 (14)
C3—N2—C4	117.93 (12)	C14—C15—H15A	120.3
N2—C3—N3	122.84 (13)	C10—C15—H15A	120.3
N2—C3—H3A	118.6	C15—C10—C11	119.99 (14)
N3—C3—H3A	118.6	C15—C10—N1	121.10 (13)
N3—C1—H1C	109.5	C11—C10—N1	118.77 (13)
N3—C1—H1D	109.5	C11—C12—C13	120.38 (15)
H1C—C1—H1D	109.5	C11—C12—H12A	119.8
N3—C1—H1E	109.5	C13—C12—H12A	119.8
H1C—C1—H1E	109.5	C8—C7—C6	119.18 (14)
H1D—C1—H1E	109.5	C8—C7—H7A	120.4
C12—C11—C10	119.87 (14)	C6—C7—H7A	120.4
C12—C11—H11A	120.1	C7—C8—C9	120.16 (14)
C10—C11—H11A	120.1	C7—C8—H8A	119.9
C14—C13—C12	119.37 (15)	C9—C8—H8A	119.9
C14—C13—H13A	120.3	C3—N3—C1	121.72 (13)
C12—C13—H13A	120.3	C3—N3—C2	120.60 (12)
N3—C2—H2C	109.5	C1—N3—C2	117.68 (12)
N3—C2—H2D	109.5	C6—C5—C4	121.58 (14)
H2C—C2—H2D	109.5	C6—C5—H5A	119.2
N3—C2—H2E	109.5	C4—C5—H5A	119.2
H2C—C2—H2E	109.5	C8—C9—C4	121.84 (14)
H2D—C2—H2E	109.5	C8—C9—S1	118.53 (11)
C15—C14—C13	120.85 (15)	C4—C9—S1	119.63 (11)
O1—S1—N1—C10	−179.13 (11)	N2—C3—N3—C1	176.32 (14)
O2—S1—N1—C10	−50.50 (13)	N2—C3—N3—C2	−3.2 (2)
C9—S1—N1—C10	65.09 (12)	C7—C6—C5—C4	1.3 (2)
C4—N2—C3—N3	172.83 (13)	N2—C4—C5—C6	−176.99 (13)
C12—C13—C14—C15	1.0 (2)	C9—C4—C5—C6	−1.6 (2)
C3—N2—C4—C5	−32.9 (2)	C7—C8—C9—C4	0.8 (2)
C3—N2—C4—C9	151.77 (13)	C7—C8—C9—S1	−179.14 (11)
C13—C14—C15—C10	−2.2 (2)	N2—C4—C9—C8	176.20 (13)
C14—C15—C10—C11	1.3 (2)	C5—C4—C9—C8	0.5 (2)

C14—C15—C10—N1	177.14 (13)	N2—C4—C9—S1	−3.85 (18)
C12—C11—C10—C15	0.7 (2)	C5—C4—C9—S1	−179.51 (10)
C12—C11—C10—N1	−175.25 (13)	O1—S1—C9—C8	119.83 (12)
S1—N1—C10—C15	61.15 (17)	O2—S1—C9—C8	−10.70 (13)
S1—N1—C10—C11	−122.99 (13)	N1—S1—C9—C8	−126.88 (12)
C10—C11—C12—C13	−1.8 (2)	O1—S1—C9—C4	−60.12 (13)
C14—C13—C12—C11	1.0 (2)	O2—S1—C9—C4	169.35 (11)
C5—C6—C7—C8	0.1 (2)	N1—S1—C9—C4	53.17 (13)
C6—C7—C8—C9	−1.1 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···N2	0.86 (2)	2.249 (19)	2.8899 (18)	131.1 (17)
C11—H11A···O1^{i}	0.95	2.47	3.2724 (19)	143

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

Fig. 1

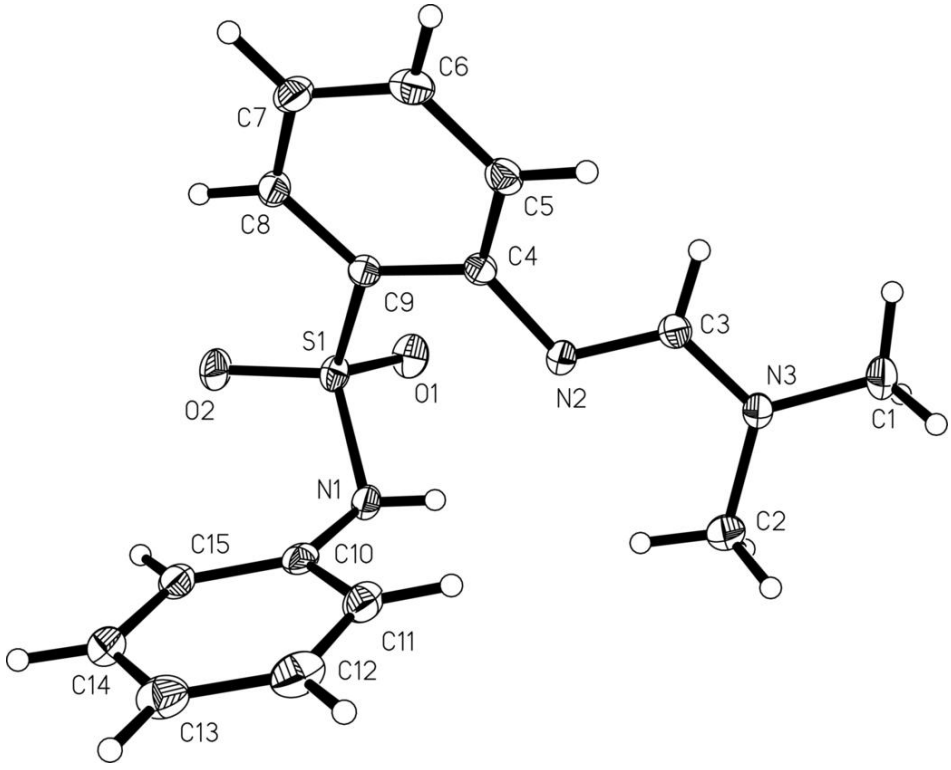
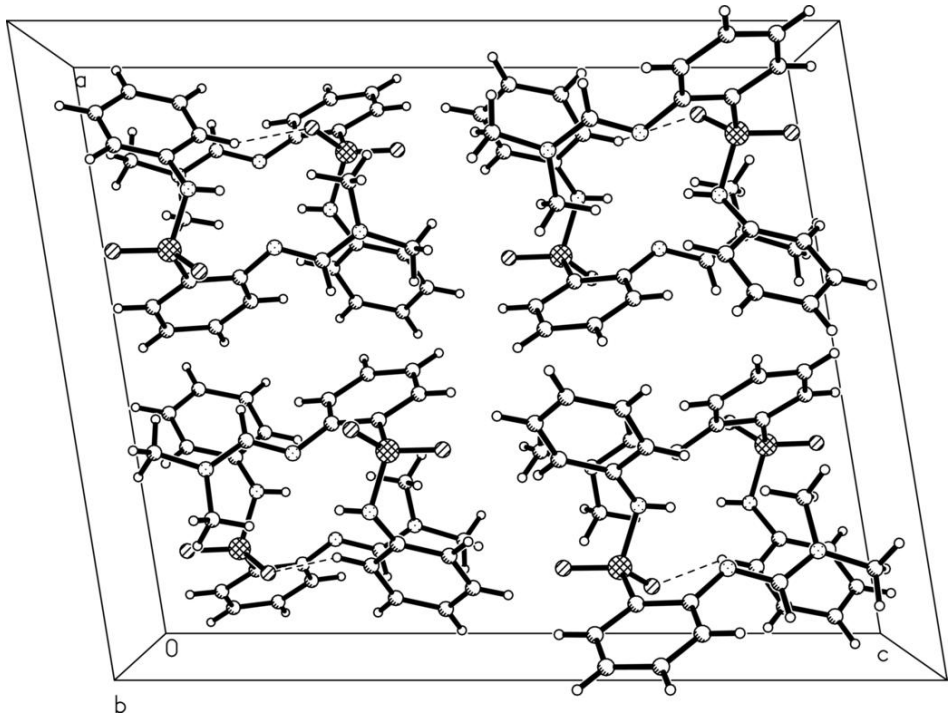


Fig. 2



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2-[(*E*)-(Dimethylamino)methyleneamino]-*N*-phenylbenzenesulfonamide. Corrigendum

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Corrections are made to the name of the author and the address in Zhong [*Acta Cryst.* (2007), E**63**, o4446].

In the paper by Zhong (2007), the author's name and the postcode are given incorrectly. The correct name should be Q. Zong and the postcode should be 314001, as given above.

References

Zhong, Q. (2007). *Acta Cryst.* E**63**, o4446.

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