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A zwitterionic form of *N*-(4-pyridyl)-benzenesulfonamide

Hai-Jun Yu,[a]* Jin-Zhe Chen,[b] Jim Simpson,[c] Jiang-Sheng Li[d] and Guo-Yi Bai[e]

[a]Chemical Engineering Department, Shijiazhuang Vocational Technology Institute, Shijiazhuang, People's Republic of China, [b]Computer Center, Hebei University Affiliated Hospital, Baoding, People's Republic of China, [c]Department of Chemistry, University of Otago, PO Box 56, Dunedin, New Zealand, [d]School of Pharmaceutical Science and Technology, Tianjin University, Tianjin, People's Republic of China, and [e]College of Chemistry and Environmental Science, Hebei University, Baoding, People's Republic of China
Correspondence e-mail: yuhaijun64@yahoo.com.cn

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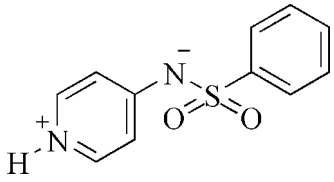
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.044; wR factor = 0.124; data-to-parameter ratio = 11.9.

The title compound, $C_{11}H_{10}N_2O_2S$, crystallizes as a zwitterionic tautomer, *N*-(4-pyridinio)benzenesulfonamidate, with the pyridine N atom protonated and the amide N atom deprotonated. There is evidence for conjugation between the anionic N atom and the pyridinium ring. In the crystal structure, intermolecular N—H···N hydrogen bonds link the molecules into chains along the *c* axis. Weak C—H···O and C—H···π interactions further stabilize the structure.

Related literature

For the preparation of the compound see Li (2007). Aryl sulfonamides with the amide N atom deprotonated have been reported previously, both as salts with suitable cations (Heren *et al.*, 2006; Hannan & Talukdar, 1992) and in zwitterionic forms (Amendola *et al.*, 2005; Lindley *et al.*, 1977; Schaumann *et al.*, 1975).



Experimental

Crystal data

$C_{11}H_{10}N_2O_2S$
M_r = 234.27
Monoclinic, $P2_1/c$
a = 12.238 (6) Å
b = 7.459 (4) Å
c = 12.124 (6) Å
β = 110.231 (7)°
V = 1038.5 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 294 (2) K
0.20 × 0.16 × 0.12 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.943, T_{max} = 0.965
5733 measured reflections
2139 independent reflections
1685 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.124
S = 1.07
2139 reflections
180 parameters
73 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

Cg is the centroid of the pyridinium ring.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N2^{i}	0.82 (3)	1.99 (3)	2.795 (3)	170 (3)
C2—H2···O2^{ii}	0.93	2.52	3.168 (3)	128
C5—H5···O1^{iii}	0.93	2.60	3.221 (3)	125
C4—H4···O1^{iii}	0.93	2.61	3.232 (3)	125
C5—H5···O2^{i}	0.93	2.43	3.075 (3)	126
C9—H9···Cg^{iv}	0.93	2.71	3.603 (8)	161

Symmetry codes: (i) $x, -y-\frac{1}{2}, z+\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $x, y-1, z$; (iv) $-x, -y, -z+2$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2469).

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supplementary materials

Acta Cryst. (2007). E**63**, o3720 [**doi:10.1107/S1600536807037713**]

A zwitterionic form of *N*-(4-pyridyl)benzenesulfonamide

H.-J. Yu, J.-Z. Chen, J. Simpson, J.-S. Li and G.-Y. Bai

Comment

In the solid state *N*-(4-pyridyl)benzenesulfonamide exists as a zwitterion with the pyridine N protonated and the amide N deprotonated, Fig. 1. The short N2—C3 bond, 1.333 (3) Å, indicates a degree of conjugation between the deprotonated N atom and the pyridinium ring. The angle between the pyridinium ring and the major disorder component of the benzene ring is 84.5 (3)°. Aryl sulphonamides with the amide N atom deprotonated have been reported previously, both as salts with suitable cations (Heren *et al.*, 2006; Hannan & Talukdar, 1992) and in zwitterionic forms (Amendola *et al.*, 2005.; Lindley *et al.*, 1977; Schaumann *et al.*, 1975).

Intermolecular N—H···N hydrogen bonds link the molecules into chains along the *c* axis. Weak C—H···O interactions and a C9—H9···*Cg* π-interaction (C9···*Cg* = 3.603 (8) Å, C9—H9···*Cg* = 161°) further stabilize the structure (*Cg* is the centroid of the pyridinium ring).

Experimental

The title compound was prepared using the method of Li (2007). Colourless single crystals were grown by slow evaporation of a solution in methanol.

Refinement

All H-atoms bound to carbon were refined using a riding model with d(C—H) = 0.93 Å and with U_{iso}(H) = 1.2 U_{eq}(C). The H atom on the N atom of the pyridinium ring was located in a difference map and refined with the distance restraint N—H =0.82 (3) Å and with U_{iso}(H) = 1.5 U_{eq}(N). The benzene ring is disordered and the two disorder components were refined as rigid groups; their site occupancies refined to 0.56 (4) and 0.44 (4) respectively.

Figures

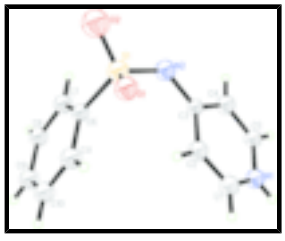

Fig. 1. The molecular structure with the atom-numbering scheme and 30% probability displacement ellipsoids. Only the major component of the disordered benzene ring is shown.

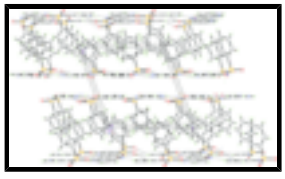

Fig. 2. Packing diagram with hydrogen bonds drawn as dashed lines.

N-(4-pyridinio)benzenesulfonamidate

Crystal data

$C_{11}H_{10}N_2O_2S$	F_{000} = 488
M_r = 234.27	D_x = 1.498 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2352 reflections
a = 12.238 (6) Å	θ = 3.3–26.5º
b = 7.459 (4) Å	μ = 0.30 mm^{-1}
c = 12.124 (6) Å	T = 294 (2) K
β = 110.231 (7)º	Block, colourless
V = 1038.5 (8) Å^3	0.20 × 0.16 × 0.12 mm
Z = 4	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	2139 independent reflections
Radiation source: fine-focus sealed tube	1685 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.033
T = 294(2) K	θ_{max} = 26.5º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −15→11
T_{min} = 0.943, T_{max} = 0.965	k = −9→7
5733 measured reflections	l = −14→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.044	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.124	$w = 1/[\sigma^2(F_o^2) + (0.0572P)^2 + 0.6075P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.001
2139 reflections	$\Delta\rho_{max}$ = 0.40 e Å^{-3}
180 parameters	$\Delta\rho_{min}$ = −0.32 e Å^{-3}
73 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}	Occ. (<1)
S1	0.31544 (6)	0.16315 (8)	0.92018 (5)	0.0360 (2)	
O1	0.37860 (16)	0.2910 (2)	1.00505 (15)	0.0434 (5)	
O2	0.31798 (19)	0.1853 (2)	0.80497 (15)	0.0525 (5)	
N1	0.37226 (18)	−0.2772 (3)	1.26144 (18)	0.0359 (5)	
N2	0.35106 (17)	−0.0376 (3)	0.95349 (16)	0.0335 (5)	
C6	0.1697 (5)	0.1746 (11)	0.9082 (8)	0.030 (3)	0.59 (4)
C7	0.0798 (9)	0.0865 (11)	0.8225 (7)	0.053 (2)	0.59 (4)
H7	0.0953	0.0206	0.7644	0.063*	0.59 (4)
C8	−0.0333 (7)	0.0967 (12)	0.8235 (11)	0.061 (3)	0.59 (4)
H8	−0.0934	0.0377	0.7662	0.074*	0.59 (4)
C9	−0.0565 (4)	0.1951 (14)	0.9103 (13)	0.058 (2)	0.59 (4)
H9	−0.1321	0.2020	0.9110	0.069*	0.59 (4)
C10	0.0334 (9)	0.2833 (14)	0.9960 (9)	0.064 (2)	0.59 (4)
H10	0.0179	0.3492	1.0541	0.077*	0.59 (4)
C11	0.1465 (6)	0.2731 (11)	0.9950 (7)	0.060 (3)	0.59 (4)
H11	0.2066	0.3321	1.0523	0.072*	0.59 (4)
C1	0.3656 (2)	−0.1014 (3)	1.2553 (2)	0.0374 (6)	
H1	0.3650	−0.0370	1.3207	0.045*	
C2	0.3596 (2)	−0.0120 (3)	1.15722 (19)	0.0342 (5)	
H2	0.3545	0.1125	1.1553	0.041*	
C3	0.36113 (19)	−0.1056 (3)	1.05825 (19)	0.0289 (5)	
C4	0.3726 (2)	−0.2902 (3)	1.0710 (2)	0.0353 (5)	
H4	0.3777	−0.3587	1.0089	0.042*	
C5	0.3765 (2)	−0.3719 (3)	1.1703 (2)	0.0347 (5)	
H5	0.3823	−0.4961	1.1756	0.042*	
C6'	0.1758 (6)	0.180 (2)	0.9147 (12)	0.057 (7)	0.41 (4)
C7'	0.1019 (13)	0.090 (2)	0.8167 (11)	0.066 (4)	0.41 (4)
H7'	0.1320	0.0348	0.7646	0.079*	0.41 (4)
C8'	−0.0169 (11)	0.0831 (17)	0.7966 (13)	0.071 (4)	0.41 (4)
H8'	−0.0664	0.0232	0.7310	0.086*	0.41 (4)
C9'	−0.0619 (5)	0.1657 (18)	0.8744 (17)	0.051 (3)	0.41 (4)
H9'	−0.1414	0.1610	0.8610	0.062*	0.41 (4)
C10'	0.0120 (11)	0.2552 (18)	0.9724 (13)	0.043 (3)	0.41 (4)

H10'	−0.0181	0.3105	1.0245	0.051*	0.41 (4)
C11'	0.1309 (9)	0.2622 (16)	0.9925 (9)	0.034 (3)	0.41 (4)
H11'	0.1803	0.3221	1.0581	0.041*	0.41 (4)
H1A	0.375 (3)	−0.329 (4)	1.322 (3)	0.057 (9)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0568 (4)	0.0243 (3)	0.0332 (3)	−0.0001 (3)	0.0234 (3)	0.0018 (2)
O1	0.0572 (11)	0.0299 (9)	0.0479 (10)	−0.0077 (8)	0.0244 (9)	−0.0067 (8)
O2	0.0938 (15)	0.0371 (10)	0.0399 (10)	0.0064 (10)	0.0401 (10)	0.0112 (8)
N1	0.0484 (13)	0.0345 (11)	0.0257 (10)	−0.0010 (9)	0.0141 (9)	0.0041 (9)
N2	0.0531 (12)	0.0253 (10)	0.0277 (10)	0.0026 (9)	0.0210 (9)	0.0008 (8)
C6	0.039 (3)	0.020 (3)	0.028 (3)	0.002 (2)	0.008 (2)	0.003 (2)
C7	0.051 (4)	0.057 (4)	0.046 (3)	−0.002 (3)	0.011 (3)	−0.012 (3)
C8	0.051 (3)	0.076 (4)	0.052 (4)	−0.006 (3)	0.011 (3)	−0.016 (3)
C9	0.055 (3)	0.062 (4)	0.051 (4)	0.001 (3)	0.013 (3)	−0.009 (3)
C10	0.055 (4)	0.060 (4)	0.072 (4)	−0.003 (3)	0.014 (3)	−0.010 (3)
C11	0.056 (4)	0.061 (5)	0.068 (5)	0.001 (3)	0.028 (3)	−0.002 (3)
C1	0.0530 (15)	0.0360 (13)	0.0255 (11)	−0.0030 (11)	0.0165 (10)	−0.0040 (10)
C2	0.0491 (14)	0.0263 (11)	0.0291 (12)	−0.0019 (10)	0.0161 (10)	−0.0033 (9)
C3	0.0338 (12)	0.0280 (11)	0.0269 (11)	−0.0011 (9)	0.0130 (9)	−0.0004 (9)
C4	0.0520 (15)	0.0292 (12)	0.0282 (11)	0.0031 (10)	0.0184 (10)	−0.0021 (10)
C5	0.0454 (14)	0.0276 (12)	0.0327 (12)	0.0033 (10)	0.0156 (10)	0.0009 (10)
C6'	0.068 (8)	0.048 (8)	0.049 (8)	−0.001 (5)	0.015 (4)	0.003 (4)
C7'	0.055 (5)	0.071 (6)	0.068 (6)	−0.006 (4)	0.017 (4)	0.001 (4)
C8'	0.064 (5)	0.080 (5)	0.073 (5)	−0.002 (4)	0.028 (4)	−0.007 (4)
C9'	0.045 (4)	0.058 (4)	0.048 (5)	0.001 (3)	0.012 (3)	−0.006 (4)
C10'	0.035 (4)	0.042 (4)	0.051 (5)	−0.003 (3)	0.016 (3)	−0.012 (3)
C11'	0.032 (4)	0.032 (4)	0.039 (4)	−0.003 (3)	0.011 (3)	−0.010 (3)

Geometric parameters (Å, °)

S1—O2	1.4174 (19)	C1—C2	1.343 (3)
S1—O1	1.4195 (18)	C1—H1	0.9300
S1—N2	1.573 (2)	C2—C3	1.394 (3)
S1—C6'	1.692 (5)	C2—H2	0.9300
S1—C6	1.742 (4)	C3—C4	1.387 (3)
N1—C1	1.315 (3)	C4—C5	1.335 (3)
N1—C5	1.328 (3)	C4—H4	0.9300
N1—H1A	0.82 (3)	C5—H5	0.9300
N2—C3	1.333 (3)	C6'—C7'	1.3900
C6—C7	1.3900	C6'—C11'	1.3900
C6—C11	1.3900	C7'—C8'	1.3900
C7—C8	1.3900	C7'—H7'	0.9300
C7—H7	0.9300	C8'—C9'	1.3900
C8—C9	1.3900	C8'—H8'	0.9300
C8—H8	0.9300	C9'—C10'	1.3900
C9—C10	1.3900	C9'—H9'	0.9300

C9—H9	0.9300	C10'—C11'	1.3900
C10—C11	1.3900	C10'—H10'	0.9300
C10—H10	0.9300	C11'—H11'	0.9300
C11—H11	0.9300		
O2—S1—O1	116.35 (12)	N1—C1—H1	119.0
O2—S1—N2	105.41 (11)	C2—C1—H1	119.0
O1—S1—N2	114.85 (11)	C1—C2—C3	120.0 (2)
O2—S1—C6'	108.6 (5)	C1—C2—H2	120.0
O1—S1—C6'	105.6 (4)	C3—C2—H2	120.0
N2—S1—C6'	105.4 (5)	N2—C3—C4	117.2 (2)
O2—S1—C6	106.4 (3)	N2—C3—C2	127.2 (2)
O1—S1—C6	108.2 (3)	C4—C3—C2	115.6 (2)
N2—S1—C6	104.7 (3)	C5—C4—C3	121.6 (2)
C1—N1—C5	120.2 (2)	C5—C4—H4	119.2
C1—N1—H1A	120 (2)	C3—C4—H4	119.2
C5—N1—H1A	119 (2)	N1—C5—C4	120.5 (2)
C3—N2—S1	122.23 (16)	N1—C5—H5	119.7
C7—C6—C11	120.0	C4—C5—H5	119.7
C7—C6—S1	124.2 (6)	C7'—C6'—C11'	120.0
C11—C6—S1	115.7 (6)	C7'—C6'—S1	110.4 (9)
C6—C7—C8	120.0	C11'—C6'—S1	129.6 (9)
C6—C7—H7	120.0	C8'—C7'—C6'	120.0
C8—C7—H7	120.0	C8'—C7'—H7'	120.0
C7—C8—C9	120.0	C6'—C7'—H7'	120.0
C7—C8—H8	120.0	C7'—C8'—C9'	120.0
C9—C8—H8	120.0	C7'—C8'—H8'	120.0
C8—C9—C10	120.0	C9'—C8'—H8'	120.0
C8—C9—H9	120.0	C10'—C9'—C8'	120.0
C10—C9—H9	120.0	C10'—C9'—H9'	120.0
C11—C10—C9	120.0	C8'—C9'—H9'	120.0
C11—C10—H10	120.0	C9'—C10'—C11'	120.0
C9—C10—H10	120.0	C9'—C10'—H10'	120.0
C10—C11—C6	120.0	C11'—C10'—H10'	120.0
C10—C11—H11	120.0	C10'—C11'—C6'	120.0
C6—C11—H11	120.0	C10'—C11'—H11'	120.0
N1—C1—C2	122.0 (2)	C6'—C11'—H11'	120.0
O2—S1—N2—C3	178.12 (19)	S1—N2—C3—C2	−10.0 (3)
O1—S1—N2—C3	48.7 (2)	C1—C2—C3—N2	177.0 (2)
C6'—S1—N2—C3	−67.1 (5)	C1—C2—C3—C4	−1.9 (3)
C6—S1—N2—C3	−69.8 (3)	N2—C3—C4—C5	−176.1 (2)
O2—S1—C6—C7	45.2 (5)	C2—C3—C4—C5	2.9 (4)
O1—S1—C6—C7	170.9 (4)	C1—N1—C5—C4	−0.9 (4)
N2—S1—C6—C7	−66.2 (5)	C3—C4—C5—N1	−1.6 (4)
C6'—S1—C6—C7	−173 (18)	O2—S1—C6'—C7'	41.3 (6)
O2—S1—C6—C11	−137.9 (4)	O1—S1—C6'—C7'	166.7 (5)
O1—S1—C6—C11	−12.1 (5)	N2—S1—C6'—C7'	−71.3 (6)
N2—S1—C6—C11	110.8 (4)	C6—S1—C6'—C7'	3(17)
C6'—S1—C6—C11	4(17)	O2—S1—C6'—C11'	−140.4 (9)

C11—C6—C7—C8	0.0	O1—S1—C6'—C11'	−14.9 (11)
S1—C6—C7—C8	176.9 (6)	N2—S1—C6'—C11'	107.0 (9)
C6—C7—C8—C9	0.0	C6—S1—C6'—C11'	−179 (18)
C7—C8—C9—C10	0.0	C11'—C6'—C7'—C8'	0.0
C8—C9—C10—C11	0.0	S1—C6'—C7'—C8'	178.5 (10)
C9—C10—C11—C6	0.0	C6'—C7'—C8'—C9'	0.0
C7—C6—C11—C10	0.0	C7'—C8'—C9'—C10'	0.0
S1—C6—C11—C10	−177.1 (6)	C8'—C9'—C10'—C11'	0.0
C5—N1—C1—C2	1.9 (4)	C9'—C10'—C11'—C6'	0.0
N1—C1—C2—C3	−0.4 (4)	C7'—C6'—C11'—C10'	0.0
S1—N2—C3—C4	168.89 (18)	S1—C6'—C11'—C10'	−178.2 (13)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···N2^{i}	0.82 (3)	1.99 (3)	2.795 (3)	170 (3)
C2—H2···O2^{ii}	0.93	2.52	3.168 (3)	128
C5—H5···O1^{iii}	0.93	2.60	3.221 (3)	125
C4—H4···O1^{iii}	0.93	2.61	3.232 (3)	125
C5—H5···O2^{i}	0.93	2.43	3.075 (3)	126
C9—H9···Cg^{iv}	0.93	2.71	3.603 (8)	161

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

Fig. 1

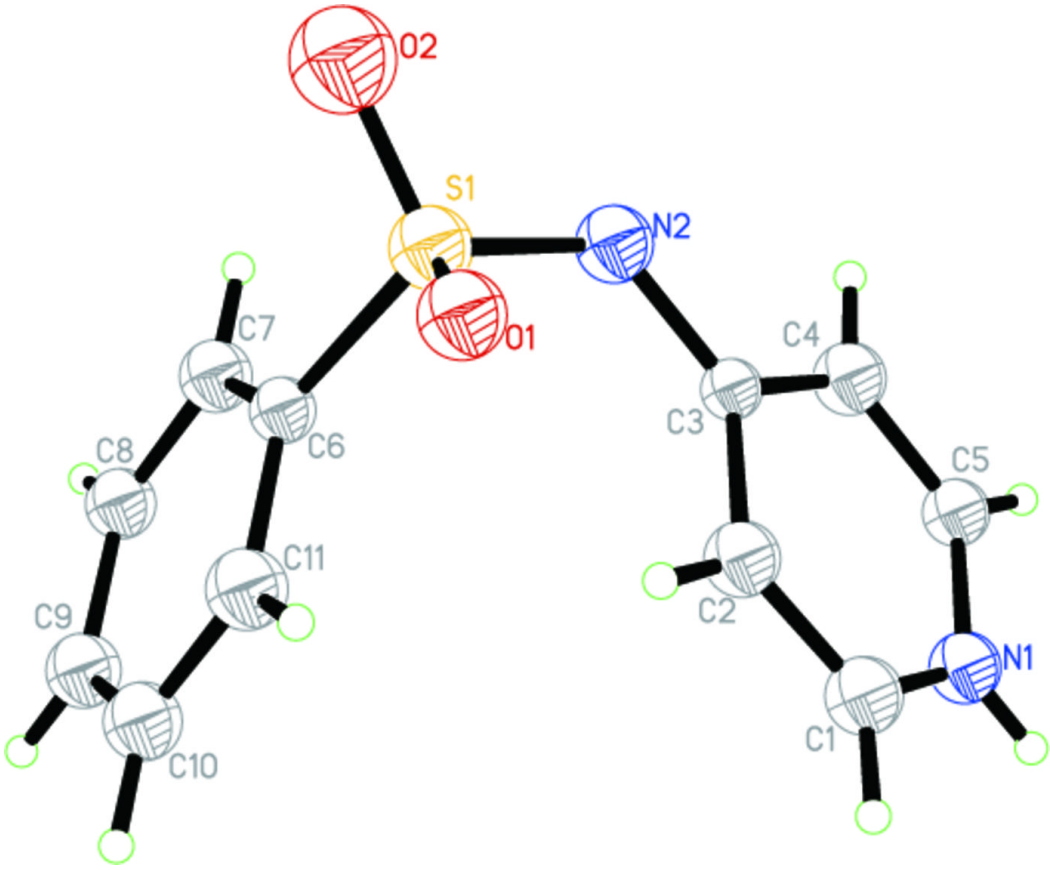

Fig. 2