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4-Nitro-*N*-(4-pyridyl)benzenesulfonamide

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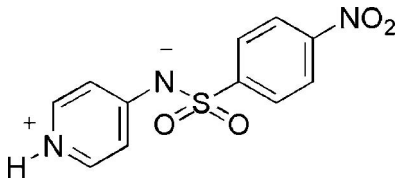
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.005 Å; R factor = 0.046; wR factor = 0.176; data-to-parameter ratio = 13.1.

The title compound, $C_{11}H_9N_3O_4S$, exists as its zwitterion tautomer in the solid state. The molecules are linked by N—H···N hydrogen-bond interactions into supramolecular chains.



Experimental

Crystal data

$C_{11}H_9N_3O_4S$
M_r = 279.27
Monoclinic, $P2_1/c$
a = 13.978 (3) Å
b = 7.5376 (15) Å
c = 12.176 (2) Å
β = 115.34 (3)°
V = 1159.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 113 (2) K
0.16 × 0.14 × 0.12 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.954, T_{max} = 0.966
9190 measured reflections
2262 independent reflections
1889 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.176
S = 1.18
2262 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1^{i}	0.92	1.92	2.816 (3)	165

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

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: HB2464).

References

Bruker (1997). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Rigaku/MSC (2005). *CrystalClear* and *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

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4-Nitro-*N*-(4-pyridyl)benzenesulfonamide

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Comment

The title compound, (I), contains both an acid and a base centre, thus displays a zwitterion structure in the solid state (Fig. 1), *i.e.* nominal proton transfer from the sulfonamide N—H group to the pyridine N atom. The short C3—N1 distance [1.356 (4) Å] indicates that the N1 lone-pair electrons conjugate with pyridinium ring which correlates with the formal contribution of a second, uncharged, tautomer (see scheme) to the overall structure of the molecule. The benzene ring forms an angle of 81.71 (15)° with the pyridinium ring.

In the crystal of (I), molecules are linked by intermolecular N—H···N hydrogen bonds (Table 1), forming chains as shown in Fig. 2, two of which pack face to face to produce an independent molecular layer.

Experimental

A solution of 4-nitrobenzenesulfonyl chloride in CH_2Cl_2 was added dropwise to a suspension of 4-aminopyridine in CH_2Cl_2 at room temperature with stirring. The reaction mixture continued stirring overnight. The yellow solid obtained was washed with warm water in a yield of 77.9%. Yellow blocks of (I) were grown by diffusion of $(^{i}Pr)_2O$ into a DMSO solution.

Refinement

The N-bound H atom was located in a difference map and refined as riding in its as-found relative position. The C-bound H atoms were positioned geometrically (C—H = 0.95 Å) and refined as riding atoms. The constraint U_{iso}(H) = 1.2 U_{eq}(C and N) was applied.

Figures

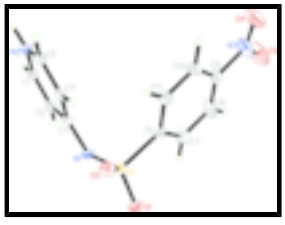


Fig. 1. A view of (I) with displacement ellipsoids drawn at the 50% probability level (arbitrary spheres for the H atoms).

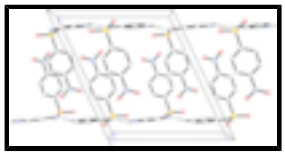


Fig. 2. The packing of (I), view down the *b* axis, showing supramolecular chains linked by N—H···N hydrogen bonds which are indicated by dashed lines.

Fig. 3. The tautomerization in the title compound.

4-Nitro-*N*-(4-pyridyl)benzenesulfonamide

Crystal data

$C_{11}H_9N_3O_4S$	F_{000} = 576
M_r = 279.27	D_x = 1.600 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1893 reflections
a = 13.978 (3) Å	θ = 3.1–25.0º
b = 7.5376 (15) Å	μ = 0.29 mm^{-1}
c = 12.176 (2) Å	T = 113 (2) K
β = 115.34 (3)º	Block, yellow
V = 1159.4 (4) Å^3	0.16 × 0.14 × 0.12 mm
Z = 4	

Data collection

Rigaku Saturn diffractometer	1889 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.050
Monochromator: graphite	θ_{max} = 26.0º
T = 113(2) K	θ_{min} = 1.6º
ω scans	h = −17→17
Absorption correction: multi-scan (CrystalClear; Rigaku/MSC, 2005)	k = −9→9
T_{min} = 0.954, T_{max} = 0.966	l = −13→15
9190 measured reflections	Standard reflections: ?
2262 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difmap and geom
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H-atom parameters constrained
$wR(F^2)$ = 0.176	$w = 1/[\sigma^2(F_o^2) + (0.1054P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.18	$(\Delta/\sigma)_{max}$ = 0.002
2262 reflections	$\Delta\rho_{max}$ = 0.46 e Å^{-3}
173 parameters	$\Delta\rho_{min}$ = −0.65 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	0.16805 (5)	0.66565 (9)	0.10514 (6)	0.0152 (3)
O1	0.17183 (16)	0.6925 (2)	0.22344 (19)	0.0202 (5)
O2	0.11008 (16)	0.7935 (2)	0.01426 (18)	0.0185 (5)
O3	0.68036 (19)	0.5905 (4)	0.2563 (3)	0.0529 (9)
O4	0.63460 (19)	0.7324 (4)	0.0894 (3)	0.0476 (8)
N1	0.13602 (18)	0.4652 (3)	0.0713 (2)	0.0148 (5)
N2	0.11262 (18)	0.2208 (3)	−0.2411 (2)	0.0150 (5)
H2A	0.1072	0.1577	−0.3077	0.018*
N3	0.6147 (2)	0.6614 (4)	0.1659 (3)	0.0351 (8)
C1	0.1198 (2)	0.1267 (4)	−0.1438 (2)	0.0159 (6)
H1	0.1211	0.0008	−0.1462	0.019*
C2	0.1250 (2)	0.2084 (4)	−0.0440 (3)	0.0167 (6)
H2	0.1292	0.1392	0.0231	0.020*
C3	0.1245 (2)	0.3942 (4)	−0.0360 (3)	0.0142 (6)
C4	0.1143 (2)	0.4876 (4)	−0.1408 (3)	0.0163 (6)
H4	0.1110	0.6135	−0.1421	0.020*
C5	0.1091 (2)	0.3984 (4)	−0.2388 (3)	0.0163 (6)
H5	0.1028	0.4632	−0.3085	0.020*
C6	0.3010 (2)	0.6735 (3)	0.1231 (3)	0.0159 (6)
C7	0.3796 (2)	0.6078 (4)	0.2301 (3)	0.0251 (7)
H7	0.3625	0.5661	0.2932	0.030*
C8	0.4834 (3)	0.6038 (4)	0.2442 (3)	0.0295 (8)
H8	0.5384	0.5597	0.3169	0.035*
C9	0.5048 (2)	0.6640 (4)	0.1521 (3)	0.0239 (7)
C10	0.4278 (2)	0.7273 (4)	0.0444 (3)	0.0264 (7)
H10	0.4456	0.7664	−0.0187	0.032*
C11	0.3243 (2)	0.7329 (4)	0.0300 (3)	0.0236 (7)
H11	0.2698	0.7771	−0.0431	0.028*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

S1	0.0197 (4)	0.0117 (4)	0.0171 (5)	−0.0007 (2)	0.0107 (3)	−0.0005 (3)
O1	0.0291 (12)	0.0163 (10)	0.0213 (12)	−0.0018 (8)	0.0165 (9)	−0.0049 (8)
O2	0.0224 (11)	0.0125 (9)	0.0222 (12)	0.0026 (8)	0.0111 (9)	0.0029 (8)
O3	0.0219 (14)	0.067 (2)	0.062 (2)	0.0105 (12)	0.0109 (13)	0.0292 (16)
O4	0.0268 (13)	0.074 (2)	0.0473 (17)	−0.0041 (14)	0.0207 (13)	0.0090 (16)
N1	0.0216 (12)	0.0114 (11)	0.0166 (13)	−0.0014 (9)	0.0133 (10)	−0.0031 (9)
N2	0.0171 (12)	0.0154 (12)	0.0140 (12)	0.0002 (9)	0.0081 (10)	−0.0012 (10)
N3	0.0210 (15)	0.0327 (16)	0.050 (2)	−0.0023 (12)	0.0140 (15)	0.0035 (14)
C1	0.0161 (14)	0.0119 (13)	0.0198 (16)	−0.0013 (10)	0.0076 (12)	−0.0023 (11)
C2	0.0153 (14)	0.0137 (13)	0.0219 (16)	0.0000 (10)	0.0086 (12)	0.0043 (12)
C3	0.0109 (13)	0.0150 (13)	0.0162 (15)	−0.0005 (10)	0.0054 (11)	0.0007 (11)
C4	0.0165 (14)	0.0130 (13)	0.0217 (16)	0.0017 (10)	0.0105 (12)	0.0027 (11)
C5	0.0168 (14)	0.0165 (14)	0.0173 (15)	0.0007 (11)	0.0089 (12)	0.0012 (12)
C6	0.0203 (15)	0.0129 (13)	0.0157 (15)	−0.0022 (10)	0.0088 (12)	−0.0030 (11)
C7	0.0274 (17)	0.0270 (16)	0.0202 (16)	−0.0018 (13)	0.0097 (13)	0.0054 (14)
C8	0.0206 (16)	0.0281 (17)	0.0329 (19)	−0.0011 (13)	0.0049 (14)	0.0087 (15)
C9	0.0163 (16)	0.0236 (16)	0.0308 (19)	−0.0031 (12)	0.0090 (14)	−0.0024 (13)
C10	0.0271 (17)	0.0342 (18)	0.0204 (17)	−0.0049 (14)	0.0126 (14)	0.0042 (14)
C11	0.0196 (15)	0.0300 (17)	0.0202 (16)	−0.0010 (13)	0.0077 (13)	0.0036 (14)

Geometric parameters (Å, °)

S1—O2	1.429 (2)	C3—C4	1.410 (4)
S1—O1	1.433 (2)	C4—C5	1.345 (4)
S1—N1	1.580 (2)	C4—H4	0.9500
S1—C6	1.776 (3)	C5—H5	0.9500
O3—N3	1.214 (4)	C6—C11	1.381 (4)
O4—N3	1.206 (4)	C6—C7	1.388 (4)
N1—C3	1.356 (4)	C7—C8	1.387 (4)
N2—C5	1.340 (4)	C7—H7	0.9500
N2—C1	1.348 (4)	C8—C9	1.357 (5)
N2—H2A	0.9151	C8—H8	0.9500
N3—C9	1.472 (4)	C9—C10	1.377 (4)
C1—C2	1.336 (4)	C10—C11	1.382 (4)
C1—H1	0.9500	C10—H10	0.9500
C2—C3	1.404 (4)	C11—H11	0.9500
C2—H2	0.9500		
O2—S1—O1	116.62 (12)	C5—C4—H4	120.0
O2—S1—N1	116.06 (12)	C3—C4—H4	120.0
O1—S1—N1	106.36 (12)	N2—C5—C4	122.0 (3)
O2—S1—C6	106.82 (13)	N2—C5—H5	119.0
O1—S1—C6	106.57 (14)	C4—C5—H5	119.0
N1—S1—C6	103.20 (12)	C11—C6—C7	121.1 (3)
C3—N1—S1	122.2 (2)	C11—C6—S1	120.8 (2)
C5—N2—C1	119.8 (2)	C7—C6—S1	118.0 (2)
C5—N2—H2A	123.3	C8—C7—C6	119.3 (3)
C1—N2—H2A	116.9	C8—C7—H7	120.3
O4—N3—O3	124.1 (3)	C6—C7—H7	120.3
O4—N3—C9	118.7 (3)	C9—C8—C7	118.7 (3)

O3—N3—C9	117.2 (3)	C9—C8—H8	120.7
C2—C1—N2	120.8 (3)	C7—C8—H8	120.7
C2—C1—H1	119.6	C8—C9—C10	122.9 (3)
N2—C1—H1	119.6	C8—C9—N3	119.3 (3)
C1—C2—C3	121.5 (3)	C10—C9—N3	117.7 (3)
C1—C2—H2	119.2	C9—C10—C11	118.7 (3)
C3—C2—H2	119.2	C9—C10—H10	120.6
N1—C3—C2	117.3 (2)	C11—C10—H10	120.6
N1—C3—C4	126.8 (3)	C6—C11—C10	119.2 (3)
C2—C3—C4	115.9 (3)	C6—C11—H11	120.4
C5—C4—C3	120.0 (3)	C10—C11—H11	120.4
O2—S1—N1—C3	48.1 (3)	O1—S1—C6—C7	34.0 (3)
O1—S1—N1—C3	179.6 (2)	N1—S1—C6—C7	−77.8 (3)
C6—S1—N1—C3	−68.4 (2)	C11—C6—C7—C8	0.7 (5)
C5—N2—C1—C2	−1.0 (4)	S1—C6—C7—C8	176.7 (2)
N2—C1—C2—C3	−0.7 (4)	C6—C7—C8—C9	−0.2 (5)
S1—N1—C3—C2	162.8 (2)	C7—C8—C9—C10	−0.8 (5)
S1—N1—C3—C4	−15.6 (4)	C7—C8—C9—N3	179.7 (3)
C1—C2—C3—N1	−176.4 (2)	O4—N3—C9—C8	−172.1 (3)
C1—C2—C3—C4	2.2 (4)	O3—N3—C9—C8	6.1 (4)
N1—C3—C4—C5	176.4 (3)	O4—N3—C9—C10	8.3 (5)
C2—C3—C4—C5	−2.1 (4)	O3—N3—C9—C10	−173.5 (3)
C1—N2—C5—C4	1.1 (4)	C8—C9—C10—C11	1.2 (5)
C3—C4—C5—N2	0.5 (4)	N3—C9—C10—C11	−179.3 (3)
O2—S1—C6—C11	−24.7 (3)	C7—C6—C11—C10	−0.3 (4)
O1—S1—C6—C11	−150.0 (2)	S1—C6—C11—C10	−176.2 (2)
N1—S1—C6—C11	98.2 (2)	C9—C10—C11—C6	−0.6 (5)
O2—S1—C6—C7	159.3 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···N1^{i}	0.92	1.92	2.816 (3)	165

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

Fig. 1

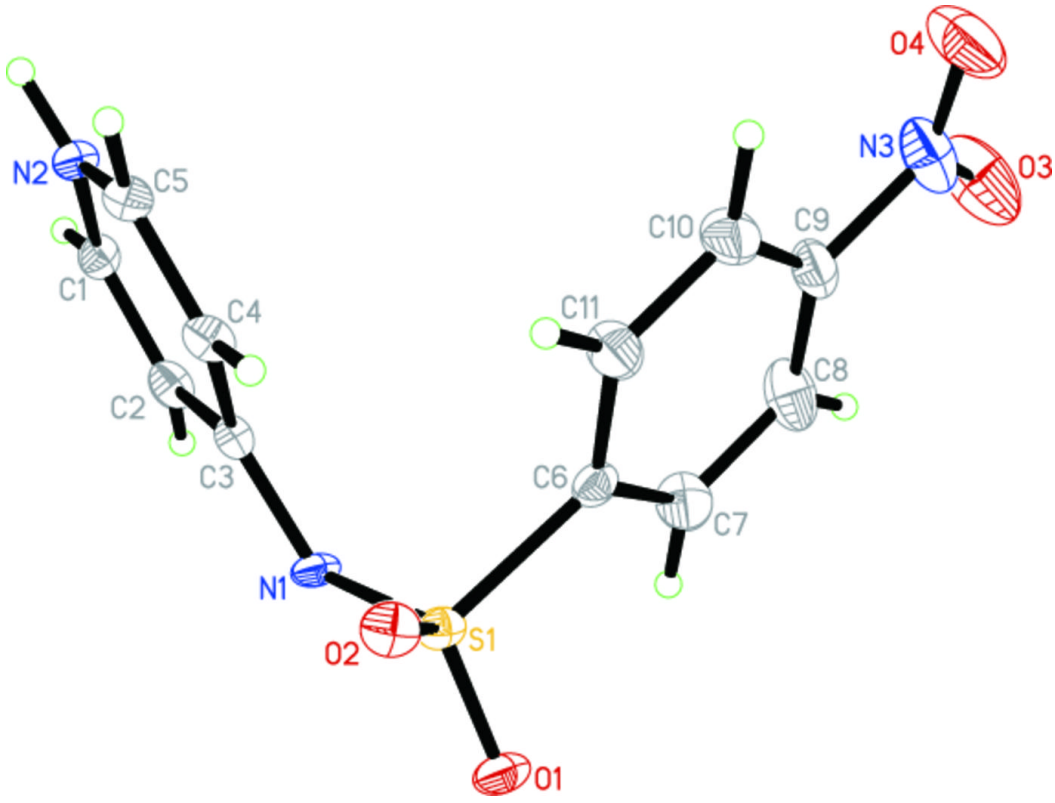


Fig. 2

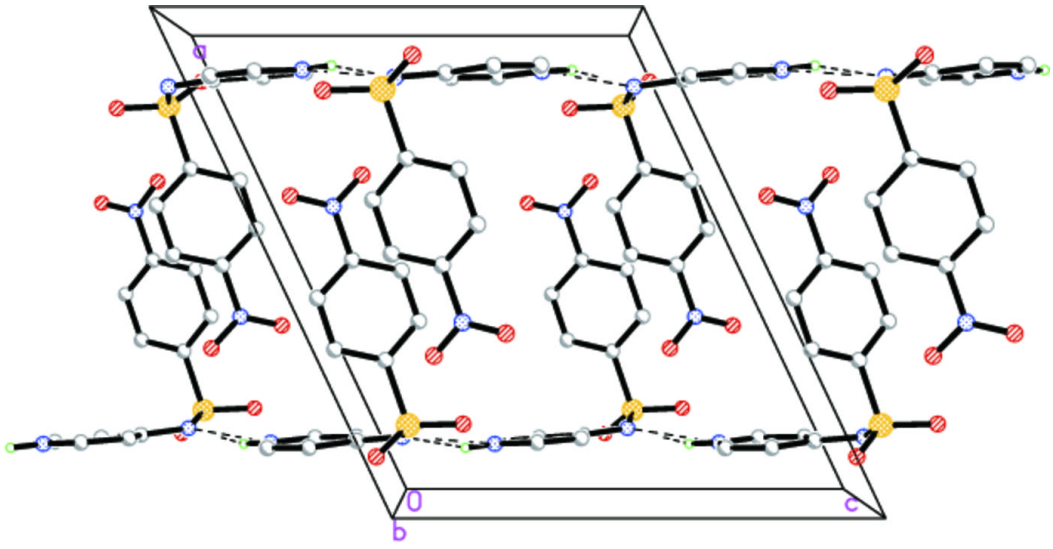
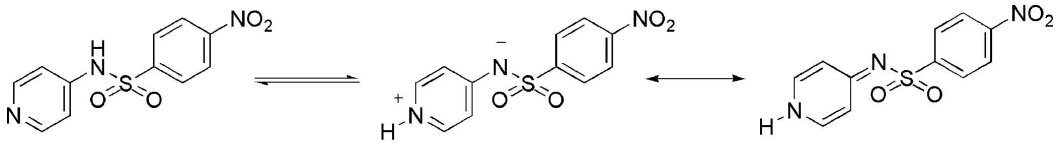


Fig. 3



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