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4-(4-Nitrobenzenesulfonamido)pyridinium chloride

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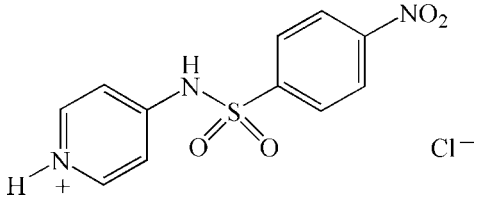
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.107; data-to-parameter ratio = 15.2.

In the title compound, $C_{11}H_{10}N_3O_4S^+\cdot Cl^-$, the benzene ring makes an angle of 89.2 (1)° with the pyridinium ring. The dihedral angle between the nitro group and the benzene ring is 15.7 (1)°. The crystal structure is stabilized by N—H···Cl hydrogen bonds.

Related literature

For zwitterionic forms of *N*-arylbenzenesulfonamides, see: Li *et al.* (2007); Yu & Li (2007). For reference geometric data, see: Allen *et al.* (1987). Damiano *et al.* (2007) describe the use of pyridinium derivatives for the construction of supramolecular architectures.



Experimental

Crystal data

$C_{11}H_{10}N_3O_4S^+\cdot Cl^-$
M_r = 315.73
Monoclinic, $C2/c$
a = 37.942 (8) Å
b = 5.2446 (10) Å
c = 13.713 (3) Å
β = 107.77 (3)°
V = 2598.5 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.47 mm^{-1}
T = 113 (2) K
0.12 × 0.10 × 0.08 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.932, T_{max} = 0.963
9693 measured reflections
2865 independent reflections
2330 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.107
S = 1.06
2865 reflections
189 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Cl1^{i}	0.93 (3)	2.12 (3)	3.039 (2)	171 (3)
N2—H2A···Cl1^{ii}	0.89 (3)	2.18 (3)	3.066 (2)	173 (3)

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2146).

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
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supporting information

Acta Cryst. (2008). E**64**, o2091 [doi:10.1107/S1600536808032054]

4-(4-Nitrobenzenesulfonamido)pyridinium chloride

Hao Zhang, Yu-Xiang Ma, Lin Zhou and Hai-Zhen Mo

S1. Comment

Organic pyridinium salts have been widely used in the construction of supramolecular architectures (Damiano *et al.*, 2007). As part of our ongoing studies of supramolecular chemistry involving the pyridinium rings (Li *et al.*, 2007), the structure of the title compound was determined by X-ray diffraction. In the cations of the title compound the short C—N distance [N2—C1 = 1.394 (3) Å] has a value between those of a typical C═N double and C—N single bond (1.47–1.50 Å and 1.34–1.38 Å, respectively; Allen *et al.*, 1987). This might be indicative of a slight conjugation of the sulphonamide π electrons N with those of the pyridinium ring. The benzene ring exhibits an angle of 89.2 (1)° with the pyridinium ring. The dihedral angle between the nitro group and the benzene ring is 164.3 (1)°. The crystal packing is stabilized by N—H···Cl hydrogen bonds (Table 1). Fig. 2 showing supramolecular chains linked by N—H···Cl hydrogen bonds.

S2. Experimental

A solution of 4-nitrobenzenesulfonyl chloride (2.2 g, 10 mmol) in CH_2Cl_2 (10 ml) was added dropwise to a suspension of 4-aminopyridine (0.9 g, 10 mmol) in CH_2Cl_2 (10 ml) at room temperature with stirring. The reaction mixture was stirred overnight. The yellow solid obtained was washed with warm water to obtain the title compound in a yield of 61.6%. A colorless single-crystal suitable for X-ray analysis was obtained by slow evaporation of an hydrochloric acid (10%) solution at room temperature over a period of a week. Analysis calculated for $C_{11}H_{10}N_3O_4SCl$: C 41.84, H 3.19, N 13.31%; found: C 41.95, H 3.52, N 13.69%.

S3. Refinement

The N-bound H atoms were located in a difference map and their coordinates were refined with $U_{iso}(H) = 1.2U_{eq}(N)$. The C-bound H atoms were positioned geometrically (C—H = 0.95 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

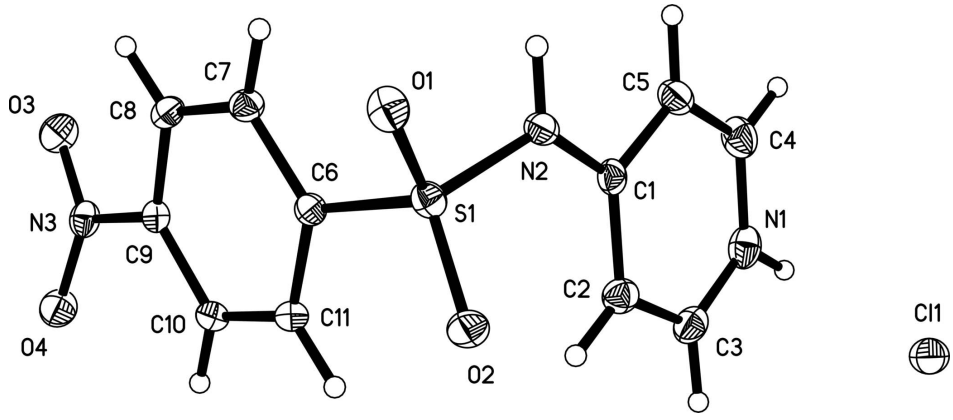

Figure 1

View of one molecule of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level (arbitrary spheres for the H atoms).

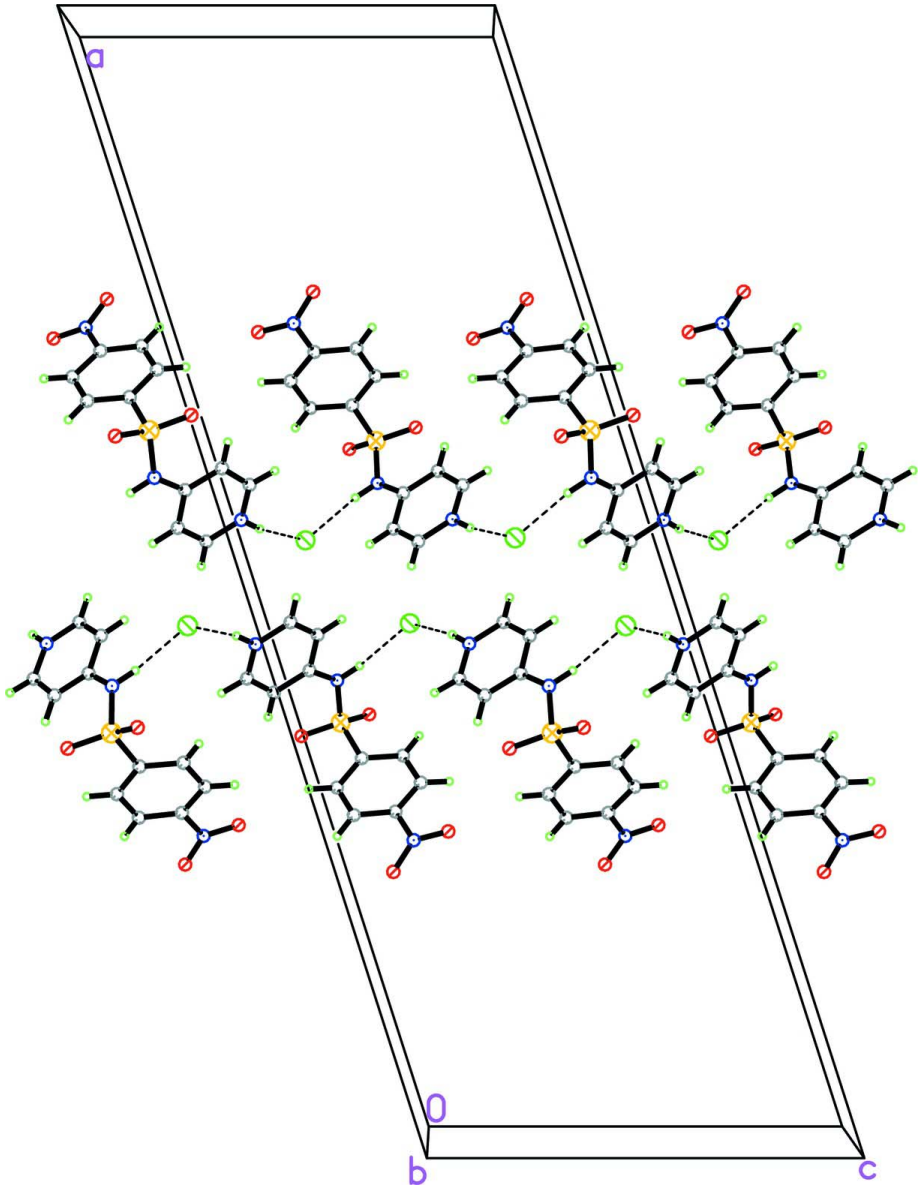

Figure 2

The packing of title compound, view down the *b* axis, showing supramolecular chains linked by N—H···Cl hydrogen bonds which are indicated by dashed lines.

4-(4-Nitrobenzenesulfonamido)pyridinium chloride

Crystal data

$C_{11}H_{10}N_3O_4S^+\cdot Cl^-$
$M_r = 315.73$
Monoclinic, $C2/c$
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$b = 5.2446\ (10)$ Å
$c = 13.713\ (3)$ Å
$\beta = 107.77\ (3)°$
$V = 2598.5\ (9)$ Å^3
$Z = 8$

$F(000) = 1296$
$D_x = 1.614$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3179 reflections
$\theta = 2.6–27.1°$
$\mu = 0.47$ mm^{-1}
$T = 113$ K
Block, colourless
0.12 × 0.10 × 0.08 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Radiation source: Rotating anode
Confocal monochromator
Detector resolution: 7.21 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.932, T_{max} = 0.963
9693 measured reflections
2865 independent reflections
2330 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 27.1°, θ_{min} = 2.3°
h = −35→48
k = −6→6
l = −17→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.107
S = 1.06
2865 reflections
189 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 1.967P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
S1	0.130148 (12)	0.37275 (10)	0.40268 (4)	0.02104 (16)
O1	0.12396 (4)	0.1690 (3)	0.32996 (12)	0.0268 (4)
O2	0.14305 (4)	0.3226 (3)	0.51052 (12)	0.0271 (4)
O3	0.21998 (4)	1.2270 (3)	0.21517 (12)	0.0320 (4)
O4	0.25562 (4)	1.2246 (3)	0.37259 (12)	0.0334 (4)
N1	0.05555 (5)	1.1001 (4)	0.52726 (16)	0.0297 (5)
N2	0.09049 (4)	0.5214 (4)	0.37499 (15)	0.0215 (4)
N3	0.22877 (5)	1.1462 (3)	0.30326 (14)	0.0246 (4)
C1	0.08046 (5)	0.7177 (4)	0.42979 (16)	0.0217 (4)
C2	0.10010 (6)	0.7864 (4)	0.52953 (17)	0.0253 (5)
H2	0.1227	0.7032	0.5645	0.030*
C3	0.08643 (6)	0.9760 (4)	0.57664 (18)	0.0284 (5)
H3	0.0992	1.0196	0.6456	0.034*
C4	0.03605 (6)	1.0410 (5)	0.43021 (19)	0.0323 (5)
H4	0.0141	1.1327	0.3966	0.039*

C5	0.04777 (5)	0.8496 (4)	0.38013 (18)	0.0277 (5)
H5	0.0338	0.8060	0.3120	0.033*
C6	0.16110 (5)	0.5922 (4)	0.37472 (16)	0.0190 (4)
C7	0.15830 (5)	0.6369 (4)	0.27247 (16)	0.0221 (5)
H7	0.1409	0.5446	0.2196	0.027*
C8	0.18104 (5)	0.8169 (4)	0.24842 (16)	0.0225 (4)
H8	0.1797	0.8499	0.1793	0.027*
C9	0.20570 (5)	0.9469 (4)	0.32797 (16)	0.0196 (4)
C10	0.20940 (5)	0.9012 (4)	0.43010 (16)	0.0229 (5)
H10	0.2272	0.9914	0.4827	0.028*
C11	0.18659 (5)	0.7207 (4)	0.45380 (16)	0.0223 (4)
H11	0.1884	0.6856	0.5231	0.027*
Cl1	0.038070 (13)	0.52540 (11)	0.65583 (4)	0.02598 (16)
H1	0.0477 (8)	1.233 (6)	0.561 (2)	0.058 (9)*
H2A	0.0771 (8)	0.504 (6)	0.310 (2)	0.059 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0197 (2)	0.0190 (3)	0.0238 (3)	0.00150 (18)	0.00570 (19)	0.0027 (2)
O1	0.0272 (7)	0.0204 (8)	0.0333 (9)	0.0011 (6)	0.0101 (6)	−0.0028 (7)
O2	0.0281 (7)	0.0289 (9)	0.0233 (9)	0.0018 (6)	0.0062 (6)	0.0100 (7)
O3	0.0388 (8)	0.0284 (9)	0.0310 (10)	−0.0013 (7)	0.0137 (7)	0.0059 (8)
O4	0.0313 (8)	0.0372 (10)	0.0321 (10)	−0.0125 (7)	0.0103 (7)	−0.0109 (8)
N1	0.0333 (10)	0.0246 (11)	0.0368 (12)	−0.0034 (8)	0.0190 (9)	−0.0056 (9)
N2	0.0189 (8)	0.0234 (10)	0.0207 (10)	0.0006 (7)	0.0038 (7)	−0.0008 (8)
N3	0.0261 (8)	0.0216 (10)	0.0287 (11)	−0.0001 (7)	0.0124 (7)	−0.0033 (8)
C1	0.0194 (9)	0.0231 (11)	0.0246 (11)	−0.0038 (8)	0.0097 (8)	0.0007 (9)
C2	0.0272 (10)	0.0249 (12)	0.0236 (12)	−0.0005 (8)	0.0074 (8)	0.0023 (10)
C3	0.0326 (11)	0.0301 (13)	0.0249 (12)	−0.0068 (9)	0.0126 (9)	−0.0016 (10)
C4	0.0261 (10)	0.0329 (14)	0.0392 (15)	0.0050 (9)	0.0117 (10)	−0.0031 (11)
C5	0.0209 (9)	0.0322 (13)	0.0281 (13)	0.0016 (8)	0.0046 (8)	−0.0034 (10)
C6	0.0185 (8)	0.0186 (11)	0.0195 (11)	0.0033 (7)	0.0055 (7)	0.0012 (8)
C7	0.0227 (9)	0.0222 (12)	0.0205 (11)	0.0000 (8)	0.0050 (8)	−0.0036 (9)
C8	0.0260 (9)	0.0239 (12)	0.0183 (11)	0.0013 (8)	0.0081 (8)	−0.0001 (9)
C9	0.0181 (8)	0.0205 (11)	0.0213 (11)	0.0009 (7)	0.0078 (7)	−0.0003 (9)
C10	0.0193 (9)	0.0277 (12)	0.0197 (11)	0.0008 (8)	0.0030 (8)	−0.0008 (9)
C11	0.0206 (9)	0.0275 (12)	0.0176 (11)	0.0011 (8)	0.0041 (7)	0.0013 (9)
Cl1	0.0256 (3)	0.0283 (3)	0.0228 (3)	0.00156 (19)	0.0056 (2)	−0.0007 (2)

Geometric parameters (Å, º)

S1—O1	1.4311 (16)	C2—H2	0.9500
S1—O2	1.4331 (16)	C3—H3	0.9500
S1—N2	1.6332 (17)	C4—C5	1.365 (3)
S1—C6	1.768 (2)	C4—H4	0.9500
O3—N3	1.226 (2)	C5—H5	0.9500
O4—N3	1.233 (2)	C6—C11	1.388 (3)

N1—C3	1.330 (3)	C6—C7	1.393 (3)
N1—C4	1.347 (3)	C7—C8	1.385 (3)
N1—H1	0.93 (3)	C7—H7	0.9500
N2—C1	1.394 (3)	C8—C9	1.381 (3)
N2—H2A	0.89 (3)	C8—H8	0.9500
N3—C9	1.468 (3)	C9—C10	1.385 (3)
C1—C2	1.391 (3)	C10—C11	1.387 (3)
C1—C5	1.402 (3)	C10—H10	0.9500
C2—C3	1.371 (3)	C11—H11	0.9500

O1—S1—O2	120.92 (10)	N1—C4—C5	120.1 (2)
O1—S1—N2	104.52 (10)	N1—C4—H4	120.0
O2—S1—N2	109.13 (10)	C5—C4—H4	120.0
O1—S1—C6	108.27 (10)	C4—C5—C1	119.6 (2)
O2—S1—C6	107.63 (10)	C4—C5—H5	120.2
N2—S1—C6	105.35 (9)	C1—C5—H5	120.2
C3—N1—C4	121.6 (2)	C11—C6—C7	121.73 (19)
C3—N1—H1	118.5 (18)	C11—C6—S1	119.82 (16)
C4—N1—H1	119.9 (18)	C7—C6—S1	118.42 (15)
C1—N2—S1	127.65 (15)	C8—C7—C6	119.50 (19)
C1—N2—H2A	117 (2)	C8—C7—H7	120.3
S1—N2—H2A	112.8 (19)	C6—C7—H7	120.3
O3—N3—O4	123.83 (19)	C9—C8—C7	118.0 (2)
O3—N3—C9	118.12 (18)	C9—C8—H8	121.0
O4—N3—C9	118.04 (18)	C7—C8—H8	121.0
C2—C1—N2	124.68 (19)	C8—C9—C10	123.26 (19)
C2—C1—C5	118.6 (2)	C8—C9—N3	118.51 (19)
N2—C1—C5	116.69 (19)	C10—C9—N3	118.22 (18)
C3—C2—C1	119.0 (2)	C9—C10—C11	118.50 (19)
C3—C2—H2	120.5	C9—C10—H10	120.8
C1—C2—H2	120.5	C11—C10—H10	120.8
N1—C3—C2	121.1 (2)	C10—C11—C6	118.97 (19)
N1—C3—H3	119.5	C10—C11—H11	120.5
C2—C3—H3	119.5	C6—C11—H11	120.5

O1—S1—N2—C1	172.50 (18)	O2—S1—C6—C7	168.84 (15)
O2—S1—N2—C1	41.8 (2)	N2—S1—C6—C7	−74.81 (18)
C6—S1—N2—C1	−73.5 (2)	C11—C6—C7—C8	−1.0 (3)
S1—N2—C1—C2	−14.1 (3)	S1—C6—C7—C8	176.94 (15)
S1—N2—C1—C5	167.25 (16)	C6—C7—C8—C9	−0.4 (3)
N2—C1—C2—C3	−177.14 (19)	C7—C8—C9—C10	1.8 (3)
C5—C1—C2—C3	1.5 (3)	C7—C8—C9—N3	−177.26 (17)
C4—N1—C3—C2	1.5 (3)	O3—N3—C9—C8	15.3 (3)
C1—C2—C3—N1	−2.4 (3)	O4—N3—C9—C8	−165.44 (18)
C3—N1—C4—C5	0.1 (3)	O3—N3—C9—C10	−163.75 (18)
N1—C4—C5—C1	−1.0 (4)	O4—N3—C9—C10	15.5 (3)
C2—C1—C5—C4	0.1 (3)	C8—C9—C10—C11	−1.7 (3)
N2—C1—C5—C4	178.9 (2)	N3—C9—C10—C11	177.29 (17)

O1—S1—C6—C11	−145.42 (16)	C9—C10—C11—C6	0.3 (3)
O2—S1—C6—C11	−13.15 (19)	C7—C6—C11—C10	1.1 (3)
N2—S1—C6—C11	103.20 (18)	S1—C6—C11—C10	−176.88 (15)
O1—S1—C6—C7	36.57 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Cl1^{i}	0.93 (3)	2.12 (3)	3.039 (2)	171 (3)
N2—H2*A*···Cl1^{ii}	0.89 (3)	2.18 (3)	3.066 (2)	173 (3)

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