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Bis(1*H*-imidazol-3-ium) naphthalene-1,5-disulfonate

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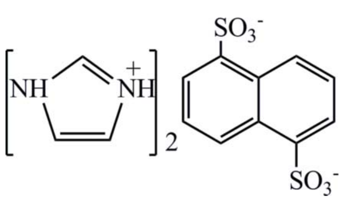
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.095; data-to-parameter ratio = 16.0.

The asymmetric unit of the title organic salt, $2C_3H_5N_2^+\cdot C_{10}H_6O_6S_2^{2-}$, consists of an imidazolium cation and half a naphthalene-1,5-disulfonate dianion, completed to the full dianion through an inversion center. N—H···S and N—H···O hydrogen bonds link cations and anions in the crystal, forming a chain propagating along [101].

Related literature

For general background to structure phase transitions in ferroelectrics, see: Ye *et al.* (2009); Zhang *et al.* (2009).



Experimental

Crystal data

$2C_3H_5N_2^+\cdot C_{10}H_6O_6S_2^{2-}$
M_r = 424.45
Triclinic, $P\bar{1}$
a = 6.6764 (13) Å
b = 6.7958 (14) Å
c = 10.251 (2) Å
α = 93.66 (3)°
β = 103.30 (3)°
γ = 96.77 (3)°
V = 447.48 (16) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 293 K
0.55 × 0.44 × 0.36 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.837, T_{max} = 0.885
4578 measured reflections
2043 independent reflections
1901 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.095
S = 1.13
2043 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···S1[i]	0.86	2.84	3.588 (2)	147
N2—H2A···O3[i]	0.86	1.90	2.745 (2)	168
N1—H1A···O2[ii]	0.86	2.09	2.847 (2)	147

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $x, y+1, z$.

Data collection: *CrystalClear* (Rigaku, 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*.

The author is grateful to the starter fund of Southeast University for the purchase of the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2419).

References

Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Ye, H.-Y., Fu, D.-W., Zhang, Y., Zhang, W., Xiong, R.-G. & Huang, S. D. (2009). *J. Am. Chem. Soc.* **131**, 42–43.
Zhang, W., Cheng, L.-Z., Xiong, R.-G., Nakamura, T. & Huang, S. D. (2009). *J. Am. Chem. Soc.* **131**, 12544–12545.

supplementary materials

Acta Cryst. (2012). E**68**, o1529 [doi:10.1107/S1600536812016972]

Bis(1*H*-imidazol-3-ium) naphthalene-1,5-disulfonate

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Comment

Dielectric-ferroelectric constitute an interesting class of materials, comprising organic ligands, metal-organic coordination compounds, organic-inorganic hybrids and organic salts (Ye *et al.*, 2009; Zhang *et al.*, 2009). Unfortunately, the dielectric constant of the title compound as a function of temperature indicates that the permittivity is basically temperature-independent, below the melting point of the compound. We have found that title compound has no dielectric anomaly from 80 K to 405 K. Herein we describe the crystal structure of this compound.

The asymmetric unit of the title compound consists of an imidazolium cation in general position, and a half naphthalene-1,5-disulfonate anion, close to a inversion center (Fig. 1). The imidazolium ring and the naphthalene ring make a dihedral angle of 69.3°. The cations and anions are connected in the crystal by N—H···S and N—H···O hydrogen bonds, which improve the stability of the crystal structure. These hydrogen bonds link the cations and anions into a chain oriented in the [101] direction (Fig. 2 and Table 1).

Experimental

The title compound was obtained by the addition of naphthalene-1,5-disulfonic acid (2.88 g, 0.01 mol) to a solution of imidazole (1.36 g, 0.02 mol) in water, in the stoichiometric ratio 1:2. Good quality single crystals were obtained by slow evaporation, after two days (yield: 38%).

Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.93 Å, N—H = 0.86 Å and with U_{iso}(H) = 1.2 U_{eq}(carrier atom).

Computing details

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear* (Rigaku, 2005); data reduction: *CrystalClear* (Rigaku, 2005); 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* (Sheldrick, 2008).

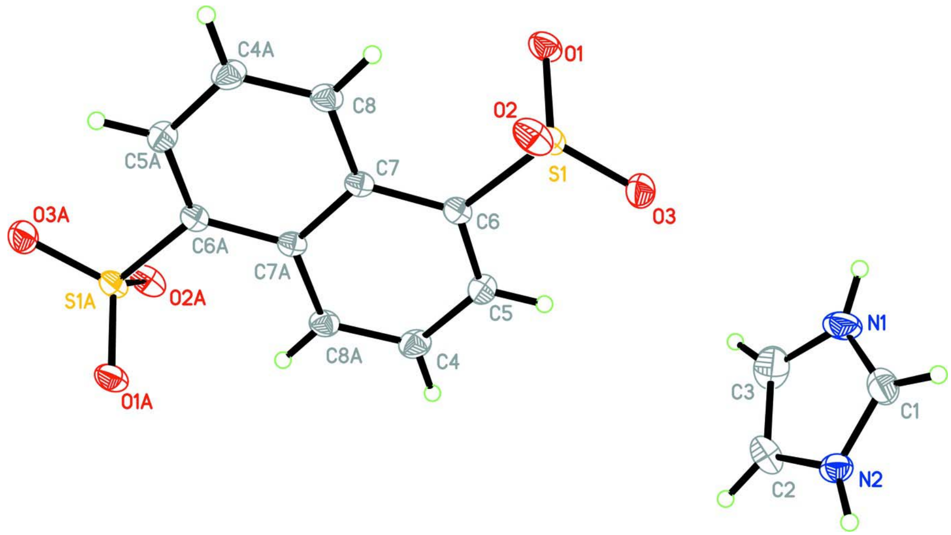

Figure 1

The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

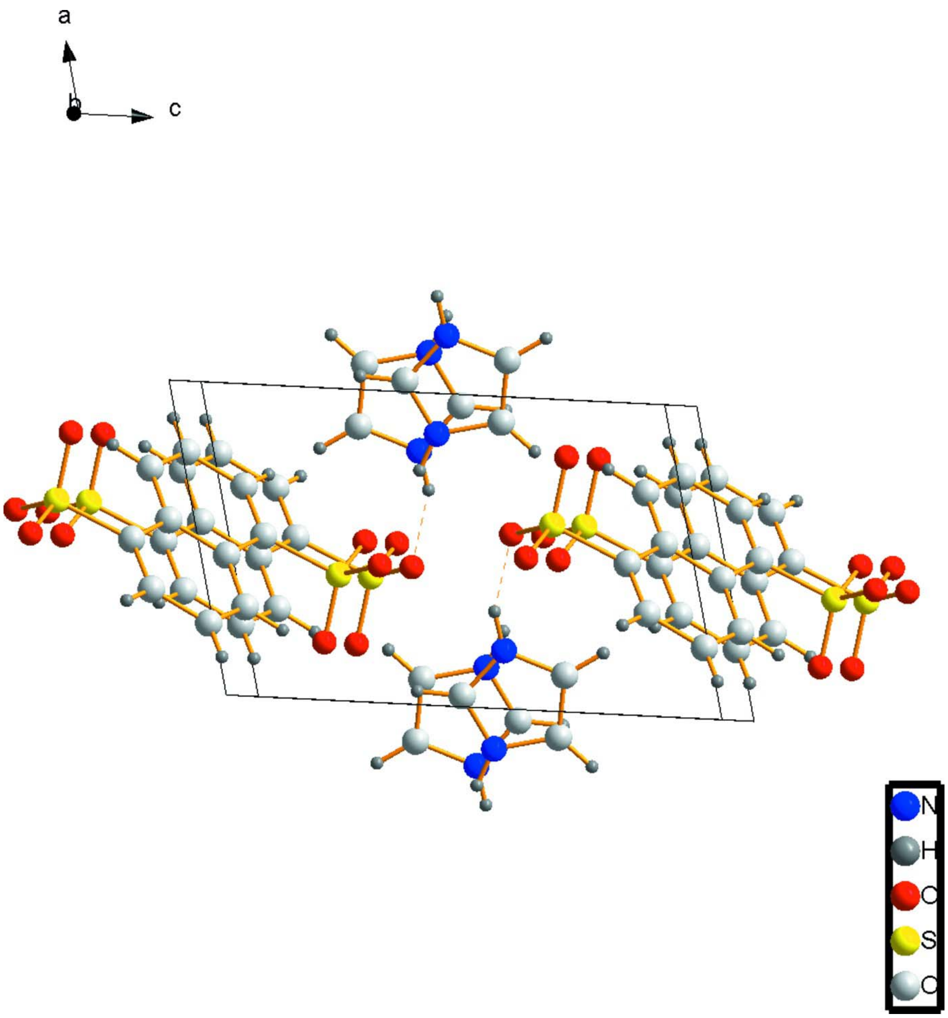

Figure 2

A view of the packing of the title compound, along the *b* axis. Dashed lines indicate hydrogen bonds.

Bis(1*H*-imidazol-3-ium) naphthalene-1,5-disulfonate

Crystal data

$2C_3H_5N_2^+\cdot C_{10}H_6O_6S_2^{2-}$
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Hall symbol: -P 1
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c = 10.251 (2) Å
α = 93.66 (3)°
β = 103.30 (3)°
γ = 96.77 (3)°
V = 447.48 (16) Å^3
Z = 1
F(000) = 220
D_x = 1.575 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
μ = 0.34 mm^{-1}
T = 293 K
Block, colorless
0.55 × 0.44 × 0.36 mm

Data collection

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
CCD_Profile_fitting scans

Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.837, T_{max} = 0.885
4578 measured reflections
2043 independent reflections
1901 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 27.5°, θ_{min} = 3.0°
$h = -8 \rightarrow 8$
$k = -8 \rightarrow 8$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.095$
$S = 1.13$
2043 reflections
128 parameters
0 restraints
0 constraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0312P)^2 + 0.2736P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.473 (17)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.1864 (3)	0.8251 (3)	0.5703 (2)	0.0502 (5)
H1A	0.3103	0.8750	0.5689	0.060*
C1	0.0353 (3)	0.7669 (3)	0.4648 (2)	0.0414 (5)
H1C	0.0430	0.7727	0.3757	0.050*
N2	−0.1299 (2)	0.6987 (2)	0.50561 (17)	0.0339 (4)
H2A	−0.2490	0.6512	0.4542	0.041*
C2	−0.0821 (4)	0.7151 (3)	0.6423 (2)	0.0429 (5)
H2C	−0.1709	0.6782	0.6970	0.051*
C3	0.1172 (4)	0.7945 (4)	0.6829 (3)	0.0561 (7)
H3B	0.1939	0.8233	0.7715	0.067*
S1	0.59698 (6)	0.27214 (7)	0.74446 (4)	0.02816 (18)
O1	0.8155 (2)	0.3366 (2)	0.80260 (13)	0.0360 (3)
O2	0.5600 (2)	0.0983 (2)	0.64608 (13)	0.0381 (4)
O3	0.4864 (2)	0.4326 (2)	0.68915 (14)	0.0399 (4)
C4	0.2276 (3)	0.2277 (3)	1.0055 (2)	0.0349 (4)
H4A	0.1216	0.2937	1.0241	0.042*
C5	0.3273 (3)	0.2901 (3)	0.90549 (19)	0.0317 (4)
H5A	0.2866	0.3968	0.8582	0.038*
C6	0.4841 (3)	0.1945 (3)	0.87756 (16)	0.0253 (4)
C7	0.5517 (2)	0.0313 (2)	0.94962 (16)	0.0239 (3)
C8	0.7149 (3)	−0.0712 (3)	0.92461 (18)	0.0304 (4)
H8A	0.7835	−0.0309	0.8595	0.036*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0278 (8)	0.0370 (10)	0.0858 (15)	−0.0023 (7)	0.0143 (9)	0.0151 (10)

C1	0.0479 (12)	0.0383 (11)	0.0473 (12)	0.0133 (9)	0.0237 (10)	0.0131 (9)
N2	0.0272 (8)	0.0314 (8)	0.0409 (9)	0.0021 (6)	0.0048 (7)	0.0024 (7)
C2	0.0543 (13)	0.0361 (10)	0.0402 (11)	−0.0044 (9)	0.0206 (10)	0.0036 (8)
C3	0.0621 (15)	0.0423 (12)	0.0477 (13)	−0.0113 (11)	−0.0098 (11)	0.0023 (10)
S1	0.0252 (2)	0.0347 (3)	0.0221 (2)	−0.00415 (16)	0.00433 (16)	0.00418 (16)
O1	0.0263 (7)	0.0450 (8)	0.0331 (7)	−0.0064 (5)	0.0048 (5)	0.0061 (6)
O2	0.0400 (8)	0.0454 (8)	0.0260 (7)	−0.0091 (6)	0.0119 (6)	−0.0049 (6)
O3	0.0363 (7)	0.0451 (8)	0.0360 (7)	0.0012 (6)	0.0029 (6)	0.0155 (6)
C4	0.0326 (9)	0.0414 (10)	0.0351 (10)	0.0129 (8)	0.0130 (8)	0.0027 (8)
C5	0.0319 (9)	0.0323 (9)	0.0311 (9)	0.0069 (7)	0.0063 (7)	0.0044 (7)
C6	0.0246 (8)	0.0295 (8)	0.0202 (7)	−0.0008 (6)	0.0047 (6)	0.0000 (6)
C7	0.0210 (7)	0.0287 (8)	0.0200 (7)	0.0000 (6)	0.0038 (6)	−0.0019 (6)
C8	0.0276 (9)	0.0395 (10)	0.0266 (8)	0.0054 (7)	0.0111 (7)	0.0033 (7)

Geometric parameters (Å, º)

N1—C1	1.301 (3)	O3—S1	1.4601 (15)
N1—C3	1.358 (4)	S1—C6	1.7828 (18)
N1—H1A	0.8600	C4—H4A	0.9300
C1—H1C	0.9300	C4—C8^{i}	1.363 (3)
N2—C1	1.312 (3)	C5—H5A	0.9300
N2—C2	1.358 (3)	C5—C4	1.406 (3)
N2—H2A	0.8600	C6—C5	1.369 (3)
C2—C3	1.334 (3)	C6—C7	1.431 (2)
C2—H2C	0.9300	C7—C8	1.422 (2)
C3—H3B	0.9300	C7—C7^{i}	1.428 (3)
O1—S1	1.4464 (14)	C8—C4^{i}	1.363 (3)
O2—S1	1.4621 (15)	C8—H8A	0.9300
C1—N1—C3	109.10 (18)	O1—S1—C6	107.15 (8)
C1—N1—H1A	125.4	O3—S1—C6	106.12 (9)
C3—N1—H1A	125.4	O2—S1—C6	105.93 (8)
N1—C1—N2	108.4 (2)	C8^{i}—C4—C5	120.55 (17)
N1—C1—H1C	125.8	C8^{i}—C4—H4A	119.7
N2—C1—H1C	125.8	C5—C4—H4A	119.7
C1—N2—C2	108.91 (18)	C6—C5—C4	120.21 (17)
C1—N2—H2A	125.5	C6—C5—H5A	119.9
C2—N2—H2A	125.5	C4—C5—H5A	119.9
C3—C2—N2	106.7 (2)	C5—C6—C7	121.20 (16)
C3—C2—H2C	126.7	C5—C6—S1	118.37 (14)
N2—C2—H2C	126.7	C7—C6—S1	120.39 (13)
C2—C3—N1	106.9 (2)	C8—C7—C7^{i}	118.9 (2)
C2—C3—H3B	126.5	C8—C7—C6	123.07 (16)
N1—C3—H3B	126.5	C7^{i}—C7—C6	118.00 (19)
O1—S1—O3	112.88 (9)	C4^{i}—C8—C7	121.10 (17)
O1—S1—O2	112.73 (9)	C4^{i}—C8—H8A	119.5
O3—S1—O2	111.46 (9)	C7—C8—H8A	119.5

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···S1^{ii}	0.86	2.84	3.588 (2)	147
N2—H2*A*···O3^{ii}	0.86	1.90	2.745 (2)	168
N1—H1*A*···O2^{iii}	0.86	2.09	2.847 (2)	147
N1—H1*A*···O2^{iv}	0.86	2.56	3.118 (3)	124

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