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Ethane-1,2-diammonium naphthalene-1,5-disulfonate

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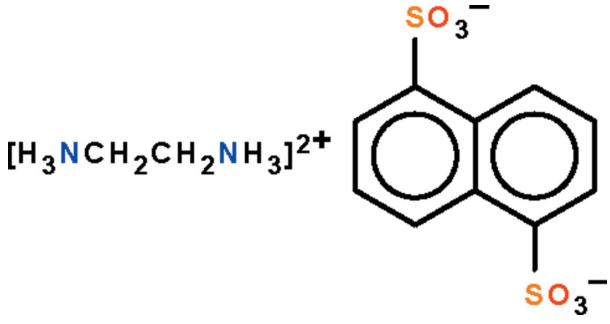
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.031; wR factor = 0.097; data-to-parameter ratio = 15.7.

In the crystal structure of the title salt, $C_2H_{10}N_2^{2+}\cdot C_{10}H_6O_6S_2^{2-}$, both the cation and anion lie on special positions of $\overline{1}$ site symmetry. These are linked by N—H···O and N—H···(O,O) hydrogen bonds, forming a layer structure.

Related literature

For the crystal structures of ammonium 1,5-naphthalenedisulfonates, see, for example: Russel *et al.* (1997); Sakwa & Wheeler (2003); Zhang *et al.* (2004).



Experimental

Crystal data

$C_2H_{10}N_2^{2+}\cdot C_{10}H_6O_6S_2^{2-}$
M_r = 348.39
Monoclinic, $P2_1/c$
a = 11.188 (7) Å
b = 8.230 (4) Å
c = 8.492 (6) Å
β = 100.19 (3)°
V = 769.6 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 293 K
0.31 × 0.27 × 0.23 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.892, T_{max} = 0.919
7310 measured reflections
1759 independent reflections
1599 reflections with $I > 2\sigma(I)$
R_{int} = 0.012

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.097
S = 1.06
1759 reflections
112 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H11···O1	0.87 (1)	2.31 (1)	3.052 (2)	144 (2)
N1—H11···O2	0.87 (1)	2.38 (1)	3.137 (3)	147 (2)
N1—H12···O1^{i}	0.87 (1)	1.93 (1)	2.7800 (19)	164 (2)
N1—H13···O2^{ii}	0.86 (1)	1.94 (1)	2.790 (2)	171 (2)

Symmetry codes: (i) $-x+2, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2622).

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supporting information

Acta Cryst. (2009). E**65**, o2658 [https://doi.org/10.1107/S1600536809039762]

Ethane-1,2-diammonium naphthalene-1,5-disulfonate

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S1. Experimental

To an aqueous solution of sodium naphthalene-1,5-disulfonate (0.58 g, 2 mmol) and ethylenediamine was added cobalt diacetate trihydrate (0.46 g, 2 mmol). The mixture was stirred for 15 min and then filtered. Colorless crystals of the organic salt separated from the solution after a few days. CH&N elemental analysis. Calc. for $C_{10}H_{16}N_2O_6S_2$: C 37.03, H 4.97, N 8.64%; found: C 37.06, H 4.91, N 8.68%.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 to 0.97 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2*U*(C). The ammonium H-atoms were refined with a distance restraint of N–H 0.86±0.01 Å; their temperature factors were refined.

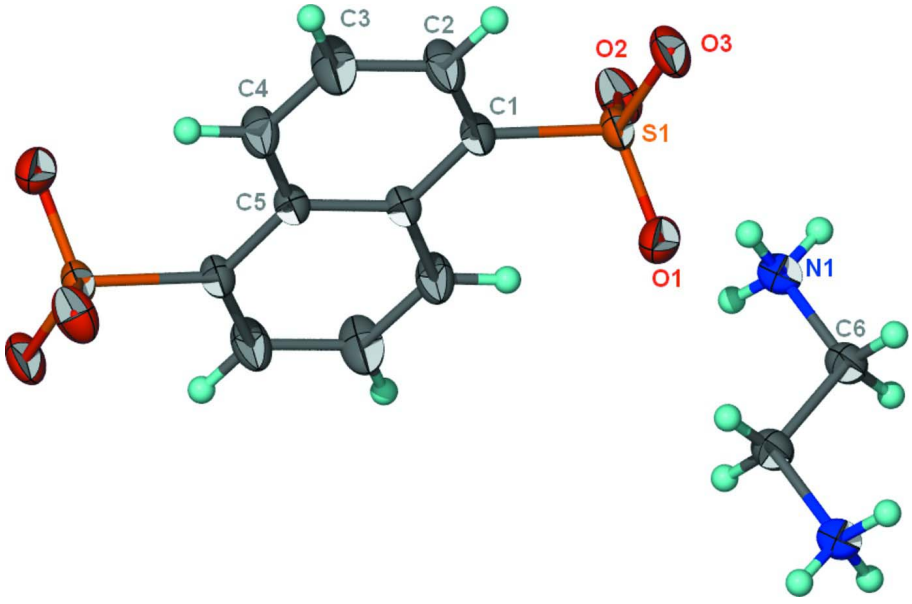

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $[C_{12}H_{10}N_2]$ $[C_{10}H_6O_6S_2]$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Ethane-1,2-diammonium naphthalene-1,5-disulfonate

Crystal data

$C_2H_{10}N_2^{2+}\cdot C_{10}H_6O_6S_2^{2-}$
$M_r = 348.39$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.188\ (7)$ Å
$b = 8.230\ (4)$ Å
$c = 8.492\ (6)$ Å
$\beta = 100.19\ (3)°$
$V = 769.6\ (8)$ Å^3
$Z = 2$
$F(000) = 364$
$D_x = 1.503$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6820 reflections
$\theta = 3.1–27.5°$
$\mu = 0.38$ mm^{-1}
$T = 293$ K
Prism, colorless
0.31 × 0.27 × 0.23 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.892$, $T_{max} = 0.919$
7310 measured reflections
1759 independent reflections
1599 reflections with $I > 2\sigma(I)$
$R_{int} = 0.012$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -14\rightarrow14$
$k = -9\rightarrow10$
$l = -11\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.097$
$S = 1.06$
1759 reflections
112 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2 + 0.1775P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.80614 (3)	0.49980 (4)	0.49518 (4)	0.02704 (14)
O1	0.83952 (9)	0.58324 (13)	0.64845 (12)	0.0385 (3)
O2	0.82188 (9)	0.32459 (13)	0.51712 (14)	0.0415 (3)
O3	0.86701 (9)	0.56466 (15)	0.37277 (13)	0.0406 (3)
N1	0.98833 (11)	0.32604 (14)	0.85576 (14)	0.0297 (3)
C1	0.64836 (11)	0.53300 (16)	0.43172 (15)	0.0262 (3)
C2	0.61199 (13)	0.6030 (2)	0.28556 (18)	0.0388 (3)
H2	0.6693	0.6333	0.2240	0.047*
C3	0.48746 (14)	0.6294 (2)	0.22779 (19)	0.0450 (4)
H3	0.4629	0.6766	0.1278	0.054*
C4	0.40295 (12)	0.58634 (18)	0.31707 (17)	0.0349 (3)
H4	0.3212	0.6047	0.2771	0.042*

C5	0.43711 (11)	0.51406 (14)	0.46991 (16)	0.0239 (3)
C6	1.04788 (12)	0.44939 (17)	0.96990 (16)	0.0310 (3)
H6A	1.0988	0.5190	0.9175	0.037*
H6B	1.0990	0.3962	1.0593	0.037*
H11	0.9543 (15)	0.367 (2)	0.7649 (14)	0.041 (5)*
H12	1.0407 (14)	0.254 (2)	0.835 (2)	0.048 (5)*
H13	0.9362 (13)	0.2720 (19)	0.8978 (19)	0.041 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0183 (2)	0.0338 (2)	0.0301 (2)	0.00095 (10)	0.00700 (14)	0.00333 (11)
O1	0.0296 (5)	0.0519 (6)	0.0336 (5)	−0.0094 (4)	0.0046 (4)	−0.0029 (4)
O2	0.0324 (5)	0.0361 (6)	0.0585 (7)	0.0095 (4)	0.0152 (5)	0.0056 (5)
O3	0.0255 (5)	0.0610 (7)	0.0380 (6)	−0.0009 (5)	0.0130 (4)	0.0098 (5)
N1	0.0320 (6)	0.0295 (6)	0.0288 (5)	0.0020 (5)	0.0085 (4)	0.0005 (4)
C1	0.0195 (6)	0.0303 (6)	0.0293 (6)	0.0013 (5)	0.0058 (4)	0.0031 (5)
C2	0.0265 (6)	0.0556 (9)	0.0362 (7)	0.0008 (6)	0.0110 (5)	0.0172 (6)
C3	0.0312 (7)	0.0663 (10)	0.0371 (8)	0.0055 (7)	0.0056 (6)	0.0266 (7)
C4	0.0230 (6)	0.0473 (8)	0.0336 (7)	0.0040 (6)	0.0027 (5)	0.0126 (6)
C5	0.0207 (6)	0.0249 (6)	0.0268 (6)	0.0012 (4)	0.0060 (5)	0.0026 (4)
C6	0.0294 (7)	0.0322 (6)	0.0325 (7)	0.0010 (6)	0.0087 (5)	−0.0031 (5)

Geometric parameters (Å, º)

S1—O3	1.4421 (12)	C2—H2	0.9300
S1—O1	1.4606 (14)	C3—C4	1.359 (2)
S1—O2	1.4606 (13)	C3—H3	0.9300
S1—C1	1.7733 (17)	C4—C5	1.417 (2)
N1—C6	1.4784 (19)	C4—H4	0.9300
N1—H11	0.867 (9)	C5—C5^{i}	1.428 (3)
N1—H12	0.870 (9)	C5—C1^{i}	1.4300 (18)
N1—H13	0.860 (9)	C6—C6^{ii}	1.516 (3)
C1—C2	1.363 (2)	C6—H6A	0.9700
C1—C5^{i}	1.4300 (18)	C6—H6B	0.9700
C2—C3	1.410 (2)		
O3—S1—O1	112.91 (8)	C3—C2—H2	120.0
O3—S1—O2	113.31 (7)	C4—C3—C2	120.52 (13)
O1—S1—O2	110.14 (7)	C4—C3—H3	119.7
O3—S1—C1	107.19 (7)	C2—C3—H3	119.7
O1—S1—C1	106.39 (7)	C3—C4—C5	121.23 (13)
O2—S1—C1	106.38 (6)	C3—C4—H4	119.4
C6—N1—H11	113.1 (12)	C5—C4—H4	119.4
C6—N1—H12	110.9 (13)	C4—C5—C5^{i}	118.99 (14)
H11—N1—H12	106.8 (17)	C4—C5—C1^{i}	123.28 (12)
C6—N1—H13	110.1 (12)	C5^{i}—C5—C1^{i}	117.73 (15)
H11—N1—H13	110.4 (16)	N1—C6—C6^{ii}	109.58 (15)

H12—N1—H13	105.3 (17)	N1—C6—H6A	109.8
C2—C1—C5^{i}	121.56 (12)	C6^{ii}—C6—H6A	109.8
C2—C1—S1	117.55 (10)	N1—C6—H6B	109.8
C5^{i}—C1—S1	120.89 (10)	C6^{ii}—C6—H6B	109.8
C1—C2—C3	119.96 (13)	H6A—C6—H6B	108.2
C1—C2—H2	120.0		
O3—S1—C1—C2	2.51 (14)	C5^{i}—C1—C2—C3	−0.5 (2)
O1—S1—C1—C2	123.56 (13)	S1—C1—C2—C3	178.79 (14)
O2—S1—C1—C2	−119.01 (13)	C1—C2—C3—C4	0.4 (3)
O3—S1—C1—C5^{i}	−178.25 (11)	C2—C3—C4—C5	0.0 (3)
O1—S1—C1—C5^{i}	−57.19 (13)	C3—C4—C5—C5^{i}	−0.2 (2)
O2—S1—C1—C5^{i}	60.24 (12)	C3—C4—C5—C1^{i}	179.91 (15)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H11···O1	0.87 (1)	2.31 (1)	3.052 (2)	144 (2)
N1—H11···O2	0.87 (1)	2.38 (1)	3.137 (3)	147 (2)
N1—H12···O1^{iii}	0.87 (1)	1.93 (1)	2.7800 (19)	164 (2)
N1—H13···O2^{iv}	0.86 (1)	1.94 (1)	2.790 (2)	171 (2)

Symmetry codes: (iii) −*x*+2, *y*−1/2, −*z*+3/2; (iv) *x*, −*y*+1/2, *z*+1/2.