Bis(2-aminobenzimidazolium) sulfate monohydrate

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In the title hydrated molecular salt, $2\text{C}_7\text{H}_8\text{N}_3^+\cdot\text{SO}_4^{2-}\cdot\text{H}_2\text{O}$, the components are linked by numerous $\text{N}—\text{H}—\text{O}$ and $\text{O}—\text{H}—\text{O}$ hydrogen bonds.

3D view

Chemical scheme

Structure description

2-Aminobenzimidazole has been used for the synthesis of a series of sulfur heterocycles such as $9\text{H}-3\text{-thia}-1,4\text{a,9-triaza-fluorene-2,4-dithione}$ (1): its potassium thiolate salt was used to prepare metal coordination compounds (Peña-Hueso et al., 2008), and is the precursor of the title compound. When compound 1 is dissolved in dimethyl sulfoxide and strong acids are added, instead of producing the protonated derivative, the thia-diazine ring breaks down, producing 2-aminobenzimidazolium sulfate (2): its crystal structural features are the subject of the present paper.

Compound 2 is formed by the transfer of two protons from sulfuric acid to the heterocycle: the crystal has two 2-aminobenzimidazolium cations, one sulfate anion and one water molecule in its asymmetric unit (Fig. 1). There is a small asymmetry in the $\text{S}—\text{O}$ bond lengths of the $\text{SO}_4^{2-}$ ion from 1.4596 (16) to 1.4723 (15) Å, probably caused by the hydrogen bonds around the anion (Gagné & Hawthorne, 2018). Two benzimidazolium cations are stacked in a head-to-tail way, with a distance between $\text{C}_9$ of one molecule and $\text{C}_{18}$ of another of 3.441 (3) Å.

The sulfate ion accepts seven $\text{N}—\text{H}—\text{O}$ hydrogen bonds from four adjacent benzimidazolium cations and one $\text{O}—\text{H}—\text{O}$ link from a water molecule (Table 1, Fig. 2). The water molecule accepts one $\text{N}—\text{H}—\text{O}$ hydrogen bond and forms two $\text{O}—\text{H}—\text{O}$ links to two $\text{SO}_4^{2-}$ ions (Fig. 3). In the extended structure, the benzimidazolium cations form parallel ribbons propagating in the [010] direction (Fig. 4).
The first crystal structure of a 2-aminobenzimidazolium salt was reported with the nitrate anion (Bats et al., 1999) and a related structure with hydrogen sulfate as the counter-ion is also known (You et al., 2009).

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

|                | D—H—A          | D—H | H—A  | D—A  | D—H—A  |
|----------------|-----------------|------|------|------|---------|
| N1—H1—O25"    | 0.81 (4)        | 2.25 | 3   | 2.946 | 144 (3) |
| N3—H3—O22"    | 0.83 (3)        | 1.93 | 3   | 2.749 | 172 (3) |
| N11—H11—O23   | 0.85 (4)        | 1.96 | 4   | 2.786 | 166 (3) |
| N13—H13—O24"  | 0.83 (4)        | 1.91 | 4   | 2.720 | 165 (3) |
| N10—H101—O23" | 0.87 (4)        | 2.03 | 4   | 2.894 | 169 (3) |
| N10—H102—O25" | 0.89 (3)        | 2.00 | 3   | 2.890 | 175 (3) |
| N20—H202—O22" | 0.94 (3)        | 2.09 | 4   | 2.973 | 157 (3) |
| O26—H261—O24" | 0.80 (7)        | 2.22 | 7   | 2.983 | 160 (7) |
| O26—H262—O24" | 0.80 (7)        | 2.14 | 7   | 2.860 | 150 (6) |
| C17—H17—O22   | 0.95            | 2.56 | 2   | 3.272 | 152     |

Symmetry codes: (i) x, y + 1/2, z; (ii) x + 1, y + 1, z; (iii) x + 2, y + 1/2, z; (iv) x + 2, y, z + 1/2; (v) x, y + 3/2, z.

### Table 2
Experimental details.

|                          |                  |
|--------------------------|------------------|
| Crystal data             |                  |
| Chemical formula         | 2C7H8N3⁺·SO4⁻·H2O |
| Mr                       | 382.4            |
| Crystal system, space group | Monoclinic, P21/c |
| Temperature (K)          | 293              |
| a, b, c (Å)              | 12.1115 (2), 10.6282 (2), 17.4772 (3) |
| β (°)                    | 127.723 (1)      |
| V (Å³)                   | 1779.48 (6)      |
| Z                        | 4                |
| Radiation type           | Mo Kα            |
| μ (mm⁻¹)                 | 0.22             |
| Crystal size (mm)        | 0.25 × 0.25 × 0.17 |

### Figure 1
The molecular structure of 2 showing displacement ellipsoids drawn at the 50% probability level.

### Figure 2
Hydrogen-bond environment around the sulfate anion.

### Figure 3
Network of hydrogen bonds (dashed lines) involving the water molecules and sulfate ions.

### Figure 4
The unit-cell packing showing [010] ribbons of cations linked by sulfate anions.

Computer programs: COLLECT (Nonius, 2001), DENZO/SCALEPACK (Otwinowski & Minor, 1997), SHEXL97 (Sheldrick, 2008), CRYSTALS (Betteridge et al., 2003) and CAMERON (Watkin et al., 1996).
Synthesis and crystallization

The decomposition of 9H-3-thia-1,4a,9-triaza-fluorene-2,4-di-thione with dilute aqueous H$_2$SO$_4$ in DMSO afforded the title compound 2, m.p. 287–289°C. IR (KBr), $\nu$ (cm$^{-1}$): 3285 (N—H), 1682 (C≡N), 1520 (C=C), 1478 (C—N). NMR (DMSO-$_d_6$, p.p.m.) $\delta$ $^1$H: 7.27 (H4, H7); 7.09 (H5, H6); 13.18 (N1—H, N3—H); 8.70 (NH$_2$); $\delta$ $^{13}$C: 152.1 (C2); 111.8 (C4, C7); 123.4 (C5, C6); 130.4 (C8, C9). $\delta$ $^{15}$N: −257.1 (N1, N3); −312.9 (N10). Analysis calculated (%) for C$_{16}$H$_{16}$N$_6$SO$_5$: C, 43.97; H, 4.74; N, 21.98. Found: C, 43.50; H, 4.80; N, 21.80. The chemical shifts of C2 (152.1 p.p.m.), C8 and C9 (130.4 p.p.m.) in the $^{13}$C NMR spectrum indicate that the endocyclic nitrogen atoms are protonated, in agreement with the crystal structure.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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full crystallographic data

IUCrData (2022). 7, x220172  [https://doi.org/10.1107/S2414314622001729]

Bis(2-aminobenzimidazolium) sulfate monohydrate

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Crystal data

2C7H8N3+·SO42−·H2O

Mr = 382.4

Monoclinic, P21/c

Hall symbol: -P 2ybc

a = 12.1115 (2) Å

b = 10.6282 (2) Å

c = 17.4772 (3) Å

β = 127.723 (1)°

V = 1779.48 (6) Å³

Z = 4

F(000) = 800

D, = 1.427 Mg m⁻³

Mo Kα radiation, λ = 0.71073 Å

Cell parameters from 4784 reflections

θ = 1–29°

µ = 0.22 mm⁻¹

T = 293 K

Prism, colourless

0.25 × 0.25 × 0.17 mm

Data collection

Nonius KappaCCD
diffractometer

Radiation source: Enraf Nonius FR590

Graphite monochromator

Detector resolution: 9 pixels mm⁻¹

φ & ω scans

9132 measured reflections

4563 independent reflections

2429 reflections with I > 2σ(I)

R(int) = 0.04

θ(max) = 28.7°, θ(min) = 2.1°

h = −15→16

k = −14→14

l = −23→23

Refinement

Refinement on F

Least-squares matrix: full

R[F² > 2σ(F²)] = 0.041

wr(F²) = 0.050

S = 1.03

2429 reflections

265 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: difference Fourier map

H atoms treated by a mixture of independent and constrained refinement

Method, part 1, Chebychev polynomial, (Watkin, 1994, Prince, 1982) [weight] = 1.0/[A₀*T₀(x) + A₁*T₁(x) + ··· + Aₙ₋₁*Tₙ₋₁(x)]

where Aᵢ are the Chebychev coefficients listed below and x = F / Fmax

Method = Robust Weighting (Prince, 1982) W = [weight] * [1-(deltaF/6*sigmaF)²]² Aᵢ are: 0.914 0.838 0.564 0.170 0.849E−01

(Δ/σ)max = 0.0002

Δρmax = 0.25 e Å⁻³

Δρmin = −0.31 e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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. The positions of all NH and OH hydrogen atoms were refined, and all CH were placed at ideal positions.

**Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)**

| Atom | x   | y   | z   | $U_{eq}$/$U_{eq}$ |
|------|-----|-----|-----|------------------|
| C2   | 0.5660 (3) | 0.1533 (2) | −0.12552 (17) | 0.0484 |
| C4   | 0.5449 (3) | 0.1836 (2) | 0.0688 (2) | 0.0626 |
| C5   | 0.6271 (4) | 0.1200 (3) | 0.1556 (2) | 0.0725 |
| C6   | 0.7293 (3) | 0.0372 (3) | 0.1756 (2) | 0.0728 |
| C7   | 0.7524 (3) | 0.0132 (3) | 0.1090 (2) | 0.0682 |
| C8   | 0.6705 (3) | 0.0761 (2) | 0.0224 (18) | 0.0503 |
| C9   | 0.5691 (2) | 0.1616 (2) | 0.00250 (16) | 0.047 |
| C12  | 0.9604 (2) | 0.2887 (2) | 0.21087 (16) | 0.047 |
| C14  | 0.8306 (3) | 0.3839 (3) | −0.0275 (2) | 0.0719 |
| C15  | 0.7199 (4) | 0.4642 (3) | −0.0859 (2) | 0.0819 |
| C16  | 0.6467 (4) | 0.5164 (3) | −0.0557 (2) | 0.0786 |
| C17  | 0.6837 (3) | 0.4930 (3) | 0.03457 (18) | 0.0617 |
| C18  | 0.7951 (2) | 0.4131 (2) | 0.09334 (16) | 0.0479 |
| C19  | 0.8659 (3) | 0.3583 (2) | 0.06268 (17) | 0.0521 |
| H1   | 0.700 (3) | 0.023 (3) | −0.073 (2) | 0.0781* |
| H3   | 0.440 (3) | 0.256 (3) | −0.122 (2) | 0.0603* |
| H4   | 0.476 | 0.2396 | 0.0553 | 0.0818* |
| H5   | 0.6134 | 0.1333 | 0.2013 | 0.0945* |
| H6   | 0.7819 | −0.0041 | 0.2343 | 0.0851* |
| H7   | 0.82 | −0.0425 | 0.1215 | 0.0843* |
| H11  | 0.830 (3) | 0.384 (3) | 0.220 (2) | 0.0595* |
| H13  | 1.021 (3) | 0.235 (3) | 0.136 (2) | 0.0682* |
| H14  | 0.8797 | 0.3482 | −0.0463 | 0.0925* |
| H15  | 0.6943 | 0.4849 | −0.1462 | 0.0986* |
| H16  | 0.5679 | 0.568 | −0.0992 | 0.0857* |
| H17  | 0.6367 | 0.5309 | 0.0569 | 0.0697* |
| H101 | 0.580 (3) | 0.137 (3) | −0.227 (2) | 0.0811* |
| H102 | 0.472 (3) | 0.237 (3) | −0.247 (2) | 0.0806* |
| H201 | 1.041 (3) | 0.247 (3) | 0.339 (2) | 0.07* |
| H202 | 1.115 (3) | 0.183 (3) | 0.301 (2) | 0.0698* |
| H261 | 0.979 (7) | 0.918 (6) | 0.069 (5) | 0.1811* |
| H262 | 0.925 (6) | 0.838 (6) | 0.005 (5) | 0.1804* |
| N1   | 0.6657 (2) | 0.0745 (2) | −0.05947 (16) | 0.0562 |
| N3   | 0.5078 (2) | 0.20819 (19) | −0.08953 (14) | 0.0477 |
| N10  | 0.5301 (3) | 0.1737 (2) | −0.21296 (17) | 0.0601 |
| N11  | 0.85749 (19) | 0.3685 (2) | 0.18649 (14) | 0.0479 |
| N13  | 0.9688 (2) | 0.2826 (2) | 0.13810 (14) | 0.0539 |
| N20  | 1.0417 (2) | 0.2263 (2) | 0.29315 (16) | 0.0582 |
|   | x     | y     | z     | U11  | U22  | U33  | U12  | U13  | U23  |
|---|-------|-------|-------|------|------|------|------|------|------|
| O22 | 0.72767 (16) | 0.64914 (16) | 0.21275 (11) | 0.0506 |
| O23 | 0.72874 (19) | 0.44104 (15) | 0.26788 (13) | 0.0584 |
| O24 | 0.8960 (2) | 0.5933 (2) | 0.37860 (12) | 0.0746 |
| O25 | 0.6554 (2) | 0.61476 (17) | 0.31313 (14) | 0.0657 |
| O26 | 0.9603 (4) | 0.8443 (3) | 0.06107 (18) | 0.1136 |
| S21 | 0.75054 (6) | 0.57563 (5) | 0.29273 (4) | 0.0431 |

**Atomic displacement parameters (Å²)**

|   | U11  | U22  | U33  | U12  | U13  | U23  |
|---|------|------|------|------|------|------|
| C2 | 0.0604 (14) | 0.0435 (12) | 0.0537 (13) | 0.0027 (10) | 0.0411 (12) | −0.0021 (10) |
| C4 | 0.0850 (19) | 0.0550 (15) | 0.0668 (16) | 0.0109 (13) | 0.0563 (16) | 0.0013 (12) |
| C5 | 0.109 (2) | 0.0657 (17) | 0.0641 (17) | 0.0001 (17) | 0.0640 (18) | 0.0001 (14) |
| C6 | 0.087 (2) | 0.0733 (18) | 0.0555 (15) | 0.0049 (16) | 0.0420 (16) | 0.0142 (14) |
| C7 | 0.0703 (17) | 0.0651 (17) | 0.0705 (17) | 0.0194 (14) | 0.0436 (15) | 0.0185 (14) |
| C8 | 0.0577 (14) | 0.0464 (12) | 0.0551 (14) | 0.0050 (11) | 0.0388 (12) | 0.0017 (11) |
| C9 | 0.0580 (13) | 0.0411 (11) | 0.0484 (12) | 0.0015 (10) | 0.0358 (11) | −0.0010 (10) |
| C12 | 0.0421 (11) | 0.0541 (13) | 0.0449 (12) | −0.0005 (10) | 0.0266 (11) | −0.0062 (11) |
| C14 | 0.086 (2) | 0.087 (2) | 0.0555 (16) | 0.0163 (16) | 0.0498 (16) | −0.0027 (14) |
| C15 | 0.107 (3) | 0.085 (2) | 0.0498 (15) | 0.0272 (19) | 0.0461 (17) | 0.0063 (14) |
| C16 | 0.090 (2) | 0.0757 (19) | 0.0485 (15) | 0.0291 (17) | 0.0315 (15) | −0.0001 (14) |
| C17 | 0.0615 (15) | 0.0649 (16) | 0.0475 (14) | 0.0171 (13) | 0.0277 (12) | −0.0065 (12) |
| C18 | 0.0467 (12) | 0.0520 (13) | 0.0425 (12) | 0.0014 (10) | 0.0261 (11) | −0.0085 (10) |
| C19 | 0.0542 (14) | 0.0561 (14) | 0.0480 (13) | 0.0051 (11) | 0.0322 (12) | −0.0054 (11) |
| N1 | 0.0716 (14) | 0.0522 (12) | 0.0658 (13) | 0.0182 (11) | 0.0527 (12) | 0.0089 (10) |
| N3 | 0.0555 (11) | 0.0470 (10) | 0.0480 (11) | 0.0102 (9) | 0.0356 (10) | 0.0018 (9) |
| N10 | 0.0807 (16) | 0.0608 (13) | 0.0583 (13) | 0.0140 (11) | 0.0525 (13) | 0.0042 (10) |
| N11 | 0.0440 (10) | 0.0592 (12) | 0.0450 (10) | 0.0050 (9) | 0.0296 (9) | −0.0045 (9) |
| N13 | 0.0522 (12) | 0.0660 (13) | 0.0499 (11) | 0.0139 (10) | 0.0345 (10) | −0.0004 (10) |
| N20 | 0.0551 (12) | 0.0685 (14) | 0.0502 (12) | 0.0098 (11) | 0.0318 (11) | 0.0020 (11) |
| O22 | 0.0481 (9) | 0.0669 (10) | 0.0421 (8) | 0.0040 (7) | 0.0302 (8) | 0.0120 (7) |
| O23 | 0.0752 (12) | 0.0507 (9) | 0.0791 (12) | −0.0031 (8) | 0.0624 (11) | −0.0046 (8) |
| O24 | 0.0619 (11) | 0.1028 (15) | 0.0410 (9) | −0.0251 (11) | 0.0223 (9) | 0.0111 (9) |
| O25 | 0.0948 (14) | 0.0562 (10) | 0.0907 (13) | 0.0093 (9) | 0.0796 (12) | 0.0092 (9) |
| O26 | 0.144 (2) | 0.148 (3) | 0.0652 (14) | −0.069 (2) | 0.0725 (17) | −0.0286 (16) |
| S21 | 0.0483 (3) | 0.0508 (3) | 0.0396 (3) | −0.0046 (3) | 0.0317 (3) | 0.0008 (2) |

**Geometric parameters (Å, °)**

|   | C2—N1 | C15—H15 | C16—C17 | C17—C18 | C17—H17 | C18—C19 | C18—N11 | C19—N13 | H1—N1 |
|---|-------|---------|---------|---------|---------|---------|---------|---------|-------|
| C2 | 1.336 (3) | C15 | 1.374 (4) | C16 | 0.95 |
| C2 | 1.333 (3) | C16 | 0.931 | C18 | 1.387 (3) |
| C2 | 1.326 (3) | C16 | 0.92 | C19 | 1.389 (3) |
| C4 | 1.380 (4) | C17 | 1.379 (3) | C19 | 0.80 (3) |
C6—H6 0.922  
C7—C8 1.373 (4)  
C7—H7 0.921  
C8—C9 1.390 (3)  
C8—N1 1.396 (3)  
C9—N3 1.386 (3)  
C12—N11 1.343 (3)  
C12—N13 1.338 (3)  
C12—N20 1.321 (3)  
C14—C15 1.376 (4)  
C14—C19 1.385 (4)  
C14—H14 0.919  
C15—C16 1.394 (4)  

N1—C2—N3 109.0 (2)  
N1—C2—N10 125.7 (2)  
N3—C2—N10 125.2 (2)  
C5—C4—C9 117.5 (2)  
C5—C4—H4 121.5  
C9—C4—H4 121  
C4—C5—C6 121.5 (3)  
C4—C5—H5 119.2  
C6—C5—H5 119.3  
C5—C6—C7 121.3 (3)  
C5—C6—H6 119.3  
C7—C6—H6 119.4  
C6—C7—C8 117.2 (3)  
C6—C7—H7 122  
C8—C7—H7 120.8  
C7—C8—C9 121.8 (2)  
C7—C8—N1 132.3 (2)  
C9—C8—N1 106.0 (2)  
C8—C9—C4 120.7 (2)  
C8—C9—N3 106.76 (19)  
C4—C9—N3 132.5 (2)  
N11—C12—N13 109.0 (2)  
N11—C12—N20 126.2 (2)  
N13—C12—N20 124.8 (2)  
C15—C14—C19 116.6 (2)  
C15—C14—H14 122.8  
C19—C14—H14 120.7  
C14—C15—C16 121.6 (3)  
C14—C15—H15 119.2  
C16—C15—H15 119.3  
C15—C16—C17 121.7 (3)  
C15—C16—H16 119.2  
C17—C16—H16 119.1  
C16—C17—C18 116.8 (2)
Hydrogen-bond geometry (Å, °)

| D—H···A | D—H  | H···A  | D···A  | D—H···A |
|---------|-------|--------|--------|---------|
| NC1—H1···O25 | 0.81 (4) | 2.25 (3) | 2.946 (3) | 144 (3) |
| NC3—H3···O22 | 0.83 (3) | 1.93 (3) | 2.749 (3) | 172 (3) |
| NC11—H11···O23 | 0.85 (4) | 1.96 (4) | 2.786 (4) | 166 (3) |
| NC13—H13···O24 | 0.83 (4) | 1.91 (4) | 2.720 (3) | 165 (3) |
| NC10—H101···O23 | 0.87 (4) | 2.03 (4) | 2.894 (5) | 169 (3) |
| NC10—H102···O25 | 0.89 (3) | 2.00 (3) | 2.890 (3) | 175 (3) |
| NC20—H201···O26 | 0.84 (3) | 2.04 (3) | 2.853 (4) | 165 (3) |
| NC20—H202···O22 | 0.93 (4) | 2.09 (4) | 2.973 (4) | 157 (3) |
| OC26—H261···O24 | 0.80 (7) | 2.22 (7) | 2.983 (4) | 160 (7) |
| OC26—H262···O24 | 0.80 (7) | 2.14 (7) | 2.860 (4) | 150 (6) |
| CC17—H17···O22 | 0.95 | 2.56 | 3.272 (3) | 132 |

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