

**[(Amino)(5-amino-4-aminocarbonyl-1*H*-imidazol-3-ium-4-yl)methylene]oxonium 5-amino-4-aminocarbonyl-1*H*-imidazolium sulfate hydrogen sulfate**

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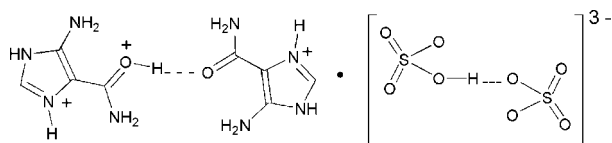
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Key indicators: single-crystal X-ray study; *T* = 223 K; mean  $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$ ; disorder in main residue; *R* factor = 0.030; *wR* factor = 0.075; data-to-parameter ratio = 9.2.

The asymmetric unit of the title compound,  $\text{C}_4\text{H}_8\text{N}_4\text{O}^{2+} \cdot \text{C}_4\text{H}_7\text{N}_4\text{O}^+ \cdot \text{SO}_4^{2-} \cdot \text{HSO}_4^-$ , contains one half of an  $\text{O}-\text{H} \cdots \text{O}$  hydrogen-bonded dimer-like unit, *viz.* a  $\text{C}_4\text{H}_8\text{N}_4\text{O}^{2+} \cdot \text{C}_4\text{H}_7\text{N}_4\text{O}^+$  unit and one half of an  $\text{SO}_4^{2-} \cdot \text{HSO}_4^-$  unit. Each of these dimeric units lies on an inversion centre, with the O-bound H atoms disordered across inversion centres. The cations and part of the anions are arranged in layers parallel to the ( $\bar{1}20$ ) plane through a combination of  $\text{N}-\text{H} \cdots \text{O}$ ,  $\text{N}-\text{H} \cdots \text{S}$  and  $\text{O}-\text{H} \cdots \text{S}$  hydrogen bonds

**Related literature**

For the synthesis, see: Asai (1974). For general background, see: Sandbhor *et al.* (2004); Materazzi *et al.* (2004). For related structures, see: Banerjee *et al.* (1991, 1999); Adamiak *et al.* (1979); Dey *et al.* (2006); Hemamalini *et al.* (2005); Huo *et al.* (2005).



**Experimental**

*Crystal data*

$\text{C}_4\text{H}_8\text{N}_4\text{O}^{2+} \cdot \text{C}_4\text{H}_7\text{N}_4\text{O}^+ \cdot \text{SO}_4^{2-} \cdot \text{HSO}_4^-$   
*M<sub>r</sub>* = 448.41  
Triclinic, *P* $\bar{1}$   
*a* = 6.0731 (16)  $\text{ \AA}$   
*b* = 7.929 (3)  $\text{ \AA}$   
*c* = 9.257 (3)  $\text{ \AA}$   
 $\alpha$  = 113.841 (6)°

$\beta$  = 92.660 (5)°  
 $\gamma$  = 92.220 (5)°  
*V* = 406.5 (2)  $\text{ \AA}^3$   
*Z* = 1

Mo *K* $\alpha$  radiation  
 $\mu$  = 0.41  $\text{ mm}^{-1}$   
*T* = 223 (2) K  
0.50  $\times$  0.45  $\times$  0.23 mm

*Data collection*

Rigaku Mercury diffractometer  
Absorption correction: multi-scan (Jacobson, 1998)  
*T*<sub>min</sub> = 0.823, *T*<sub>max</sub> = 0.913

3859 measured reflections  
1469 independent reflections  
1376 reflections with *I* > 2 $\sigma$ (*I*)  
*R*<sub>int</sub> = 0.017

*Refinement*

$R[F^2 > 2\sigma(F^2)] = 0.030$   
*wR*(*F*<sup>2</sup>) = 0.075  
*S* = 1.10  
1469 reflections  
159 parameters  
1 restraint

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.25 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.40 \text{ e \AA}^{-3}$

**Table 1**  
Hydrogen-bond geometry ( $\text{ \AA}$ , °).

<i>D</i> — <i>H</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i> ⋯ <i>A</i>
N1—H1⋯O5 <sup>i</sup>	0.85 (3)	1.87 (3)	2.718 (2)	171 (3)
N2—H2⋯O3	0.86 (2)	1.83 (2)	2.656 (2)	160 (2)
N2—H2⋯S1	0.86 (2)	2.84 (2)	3.668 (2)	162 (2)
N3—H3 <i>B</i> ⋯O4 <sup>ii</sup>	0.86 (3)	2.18 (3)	2.975 (2)	152 (2)
N3—H3 <i>A</i> ⋯O2	0.88 (3)	2.06 (3)	2.898 (2)	157 (2)
N4—H4 <i>B</i> ⋯O2 <sup>i</sup>	0.87 (3)	2.05 (3)	2.925 (2)	178 (2)
N4—H4 <i>A</i> ⋯O4 <sup>iii</sup>	0.87 (3)	2.32 (3)	3.020 (2)	138 (2)
N4—H4 <i>A</i> ⋯O1	0.87 (3)	2.31 (3)	2.888 (2)	124 (2)
O1—H1O⋯O1 <sup>iv</sup>	0.84 (5)	1.61 (5)	2.448 (3)	174 (7)
O4—H4O⋯O4 <sup>v</sup>	0.83 (3)	1.65 (3)	2.469 (3)	169 (7)
O4—H4O⋯S1 <sup>v</sup>	0.83 (3)	2.72 (5)	3.424 (2)	144 (6)

Symmetry codes: (i) *x, y, z* + 1; (ii) *x* + 1, *y, z*; (iii)  $-x + 1, -y + 1, -z + 1$ ; (iv)  $-x + 2, -y + 1, -z + 1$ ; (v)  $-x, -y + 1, -z$ .

Data collection: *CrystalClear* (Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MS, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2490).

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**supplementary materials**

*Acta Cryst.* (2007). E63, o4662-o4663 [ doi:10.1107/S1600536807056590 ]

**[(Amino)(5-amino-4-aminocarbonyl-1*H*-imidazol-3-ium-4-yl)methylene]oxonium 5-amino-4-aminocarbonyl-1*H*-imidazolium sulfate hydrogen sulfate**

**L.-P. Lv, X.-J. Li, W.-W. Li, W.-B. Yu and X.-C. Hu**

### Comment

The chemistry of imidazole compounds has been of much interest due to the presence of such heterocycle in a large variety of biologically important molecules. For example, some imidazole derivatives have shown interesting antifungal and anti-tumour properties (Sandbhor *et al.*, 2004). In living systems, the imidazole ring is an essential metal binding site, since imidazole units are bound to metal ions in almost all copper- and zinc-metalloproteins and in nickel-containing urease (Materazzi *et al.*, 2004). A component of the title compound, 5-amino-1*H*-imidazole-4-carboxamide, is useful as an important intermediate in preparing guanine and xanthine, which are themselves useful for the preparation of pharmaceuticals (Asai, 1974). Also, it is useful as an additive in the fermentation of microorganisms, and used in the treatment of liver function disorders. We report here the crystal structure of the title compound.

The asymmetric unit of the title compound contains one half each of O—H $\cdots$ O hydrogen-bonded C<sub>4</sub>H<sub>8</sub>N<sub>4</sub>O<sup>2+</sup>·C<sub>4</sub>H<sub>7</sub>N<sub>4</sub>O<sup>+</sup> cationic units, and SO<sub>4</sub><sup>2-</sup>·HSO<sub>4</sub><sup>-</sup> anionic units. Each of these hydrogen-bonded dimer-like units lie on inversion centres (Fig. 1). The O-bound H atoms of these units are disordered across the inversion centres. The imidazolium ring is planar to within  $\pm 0.003$  (1) Å. The amino and carboxamide groups are coplanar with the imidazolium ring, with atoms N4 and O1 deviating from the imidazolium plane by 0.018 (3) Å and 0.039 (3) Å, respectively. The C4=O1 bond length of 1.283 (2) Å is significantly longer compared to the corresponding distance (1.230 (3)–1.255 (4) Å) observed in structures containing oxonium ion (Banerjee *et al.*, 1991, 1999; Adamiak *et al.*, 1979; Dey *et al.*, 2006). The geometric parameters of the sulfate anion are consistent with the reported data (Hemamalini *et al.*, 2005; Huo *et al.*, 2005). The O—S—O bond angles (Table 1) of the sulfate group, in the range 105.36 (8)–112.17 (8)°, indicate a distorted tetrahedron.

The cationic units and part of the anionic units are arranged in layers parallel to the ( $\bar{1}$  2 0) plane through a combination of N—H $\cdots$ O, N—H $\cdots$ S and O—H $\cdots$ S hydrogen bonds (Table 2).

### Experimental

The title compound was prepared according to the literature method (Asai, 1974). Crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution at room temperature (m.p. 443–445 K).

### Refinement

All H atoms were located in a difference map. Atoms H1O and H4O are disordered across inversion centres and they were refined with site occupancies of 0.50. The O4—H4O distance was restrained to 0.85 (3) Å. Atom H3 was included in the riding model approximation, with C—H = 0.94 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Figures

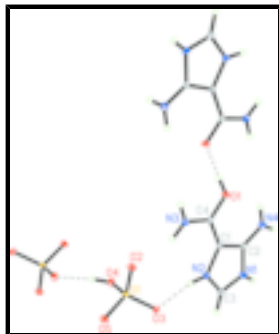
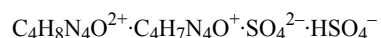


Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 20% probability level. Unlabelled atoms are related to other labelled atoms by the symmetry operation  $(2-x, 1-y, 1-z)$  in cationic units and  $(-x, 1-y, -z)$  in anionic units. Hydrogen bonds are shown as dashed lines.

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*Crystal data*



$M_r = 448.41$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 6.0731$  (16) Å

$b = 7.929$  (3) Å

$c = 9.257$  (3) Å

$\alpha = 113.841$  (6)°

$\beta = 92.660$  (5)°

$\gamma = 92.220$  (5)°

$V = 406.5$  (2) Å<sup>3</sup>

$Z = 1$

$F_{000} = 232$

$D_x = 1.832$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71070$  Å

Cell parameters from 3859 reflections

$\theta = 3.4$ – $25.3$ °

$\mu = 0.41$  mm<sup>-1</sup>

$T = 223$  (2) K

Block, colourless

$0.50 \times 0.45 \times 0.23$  mm

*Data collection*

Rigaku Mercury diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 223$ (2) K

$\omega$  scans

Absorption correction: multi-scan (Jacobson, 1998)

$T_{\min} = 0.823$ ,  $T_{\max} = 0.913$

3859 measured reflections

1469 independent reflections

1376 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.017$

$\theta_{\text{max}} = 25.3$ °

$\theta_{\text{min}} = 3.4$ °

$h = -7 \rightarrow 7$

$k = -9 \rightarrow 8$

$l = -11 \rightarrow 11$

Standard reflections: ?

*Refinement*

Refinement on  $F^2$

Secondary atom site location: difference Fourier map

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.030$$

$$wR(F^2) = 0.075$$

$$S = 1.10$$

1469 reflections

159 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0351P)^2 + 0.2509P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.25 \text{ e } \text{Å}^{-3}$$

$$\Delta\rho_{\min} = -0.40 \text{ e } \text{Å}^{-3}$$

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  $F^2 > 2\sigma(F^2)$  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 ( $\text{Å}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
O1	0.8662 (2)	0.59705 (19)	0.58585 (16)	0.0255 (3)	
H1O	0.959 (10)	0.536 (8)	0.525 (8)	0.047 (17)*	0.50
N1	0.3241 (3)	0.8526 (2)	0.82081 (19)	0.0223 (4)	
H1	0.256 (4)	0.864 (4)	0.902 (3)	0.048 (8)*	
N2	0.3694 (2)	0.8362 (2)	0.58551 (19)	0.0195 (3)	
H2	0.335 (4)	0.848 (3)	0.499 (3)	0.031 (6)*	
N3	0.7272 (3)	0.6588 (2)	0.38140 (19)	0.0222 (4)	
H3A	0.617 (4)	0.695 (3)	0.337 (3)	0.036 (6)*	
H3B	0.841 (4)	0.616 (3)	0.328 (3)	0.031 (6)*	
N4	0.6298 (3)	0.7035 (2)	0.8699 (2)	0.0266 (4)	
H4A	0.743 (4)	0.642 (3)	0.831 (3)	0.037 (7)*	
H4B	0.574 (4)	0.709 (3)	0.957 (3)	0.037 (6)*	
C1	0.5441 (3)	0.7481 (2)	0.6234 (2)	0.0175 (4)	
C2	0.5134 (3)	0.7603 (2)	0.7755 (2)	0.0180 (4)	
C3	0.2418 (3)	0.8952 (3)	0.7039 (2)	0.0224 (4)	
H3	0.1126	0.9577	0.7065	0.027*	
C4	0.7185 (3)	0.6652 (2)	0.5253 (2)	0.0185 (4)	
S1	0.20015 (7)	0.76780 (6)	0.17903 (5)	0.01807 (16)	
O2	0.4304 (2)	0.72426 (19)	0.15779 (16)	0.0276 (3)	
O3	0.1683 (2)	0.88383 (18)	0.34502 (14)	0.0238 (3)	

## supplementary materials

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O4	0.0598 (2)	0.58928 (18)	0.14092 (16)	0.0250 (3)	
H4O	0.037 (11)	0.528 (9)	0.045 (4)	0.057 (18)*	0.50
O5	0.1189 (2)	0.85258 (19)	0.07560 (15)	0.0265 (3)	

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0224 (7)	0.0334 (8)	0.0223 (7)	0.0122 (6)	0.0052 (6)	0.0118 (6)
N1	0.0227 (8)	0.0243 (8)	0.0206 (8)	0.0060 (6)	0.0085 (7)	0.0088 (7)
N2	0.0203 (8)	0.0213 (8)	0.0186 (8)	0.0042 (6)	0.0014 (6)	0.0096 (6)
N3	0.0194 (8)	0.0293 (9)	0.0204 (8)	0.0057 (7)	0.0068 (7)	0.0119 (7)
N4	0.0301 (9)	0.0341 (10)	0.0205 (9)	0.0121 (8)	0.0068 (7)	0.0148 (8)
C1	0.0171 (9)	0.0183 (9)	0.0184 (9)	0.0026 (7)	0.0017 (7)	0.0087 (7)
C2	0.0187 (8)	0.0158 (8)	0.0190 (9)	0.0008 (7)	0.0025 (7)	0.0065 (7)
C3	0.0205 (9)	0.0217 (9)	0.0245 (10)	0.0055 (7)	0.0042 (8)	0.0082 (8)
C4	0.0179 (9)	0.0170 (9)	0.0196 (9)	-0.0010 (7)	0.0015 (7)	0.0067 (7)
S1	0.0193 (3)	0.0215 (3)	0.0153 (2)	0.00434 (18)	0.00328 (17)	0.00899 (19)
O2	0.0208 (7)	0.0379 (8)	0.0298 (8)	0.0085 (6)	0.0068 (6)	0.0185 (6)
O3	0.0313 (7)	0.0239 (7)	0.0155 (6)	0.0060 (6)	0.0030 (5)	0.0066 (5)
O4	0.0301 (7)	0.0245 (7)	0.0190 (7)	-0.0029 (6)	0.0026 (6)	0.0077 (6)
O5	0.0293 (7)	0.0357 (8)	0.0234 (7)	0.0101 (6)	0.0068 (6)	0.0199 (6)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

O1—C4	1.283 (2)	N4—C2	1.324 (2)
O1—H1O	0.84 (5)	N4—H4A	0.87 (3)
N1—C3	1.339 (3)	N4—H4B	0.87 (3)
N1—C2	1.377 (2)	C1—C2	1.393 (2)
N1—H1	0.85 (3)	C1—C4	1.429 (2)
N2—C3	1.309 (2)	C3—H3	0.94
N2—C1	1.399 (2)	S1—O5	1.4540 (13)
N2—H2	0.86 (2)	S1—O2	1.4568 (14)
N3—C4	1.316 (2)	S1—O3	1.4641 (13)
N3—H3A	0.88 (3)	S1—O4	1.5263 (15)
N3—H3B	0.86 (3)	O4—H4O	0.83 (3)
C4—O1—H1O	116 (5)	N4—C2—N1	121.98 (17)
C3—N1—C2	109.38 (16)	N4—C2—C1	131.95 (17)
C3—N1—H1	123.9 (18)	N1—C2—C1	106.07 (15)
C2—N1—H1	125.9 (18)	N2—C3—N1	109.33 (16)
C3—N2—C1	109.21 (16)	N2—C3—H3	125.3
C3—N2—H2	120.8 (16)	N1—C3—H3	125.3
C1—N2—H2	129.8 (16)	O1—C4—N3	121.99 (17)
C4—N3—H3A	121.1 (16)	O1—C4—C1	115.94 (16)
C4—N3—H3B	119.6 (15)	N3—C4—C1	122.07 (17)
H3A—N3—H3B	119 (2)	O5—S1—O2	112.17 (8)
C2—N4—H4A	116.3 (16)	O5—S1—O3	111.19 (8)
C2—N4—H4B	118.8 (16)	O2—S1—O3	110.78 (8)
H4A—N4—H4B	124 (2)	O5—S1—O4	108.28 (8)

C2—C1—N2	106.00 (15)	O2—S1—O4	108.77 (8)
C2—C1—C4	127.66 (16)	O3—S1—O4	105.36 (8)
N2—C1—C4	126.34 (16)	S1—O4—H4O	112 (5)
C3—N2—C1—C2	-0.6 (2)	C4—C1—C2—N1	179.67 (17)
C3—N2—C1—C4	-179.96 (17)	C1—N2—C3—N1	0.7 (2)
C3—N1—C2—N4	179.34 (17)	C2—N1—C3—N2	-0.4 (2)
C3—N1—C2—C1	0.0 (2)	C2—C1—C4—O1	-1.4 (3)
N2—C1—C2—N4	-178.85 (19)	N2—C1—C4—O1	177.80 (16)
C4—C1—C2—N4	0.5 (3)	C2—C1—C4—N3	178.53 (17)
N2—C1—C2—N1	0.35 (19)	N2—C1—C4—N3	-2.3 (3)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1 $\cdots$ O5 <sup>i</sup>	0.85 (3)	1.87 (3)	2.718 (2)	171 (3)
N2—H2 $\cdots$ O3	0.86 (2)	1.83 (2)	2.656 (2)	160 (2)
N2—H2 $\cdots$ S1	0.86 (2)	2.84 (2)	3.668 (2)	162 (2)
N3—H3B $\cdots$ O4 <sup>ii</sup>	0.86 (3)	2.18 (3)	2.975 (2)	152 (2)
N3—H3A $\cdots$ O2	0.88 (3)	2.06 (3)	2.898 (2)	157 (2)
N4—H4B $\cdots$ O2 <sup>i</sup>	0.87 (3)	2.05 (3)	2.925 (2)	178 (2)
N4—H4A $\cdots$ O4 <sup>iii</sup>	0.87 (3)	2.32 (3)	3.020 (2)	138 (2)
N4—H4A $\cdots$ O1	0.87 (3)	2.31 (3)	2.888 (2)	124 (2)
O1—H1O $\cdots$ O1 <sup>iv</sup>	0.84 (5)	1.61 (5)	2.448 (3)	174 (7)
O4—H4O $\cdots$ O4 <sup>v</sup>	0.83 (3)	1.65 (3)	2.469 (3)	169 (7)
O4—H4O $\cdots$ S1 <sup>v</sup>	0.83 (3)	2.72 (5)	3.424 (2)	144 (6)

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



Fig. 1

