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Guanidinium 4-hydroxy-3-carboxybenzenesulfonate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.112
Data-to-parameter ratio = 12.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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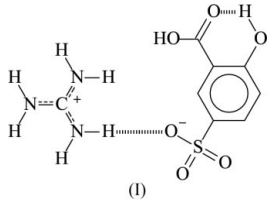
The anions of guanidinium 4-hydroxy-3-carboxybenzenesulfonate, $CH_6N_3^+\cdot C_7H_5O_6S^-$, are linked into a linear chain by a short $O_{carboxyl}\cdots O_{sulfonate}$ interaction of 2.611 (2) Å; the hydroxyl group is linked intramolecularly to the carbonyl O atom, also by a short hydrogen bond [O···O = 2.601 (2) Å]. Adjacent chains are connected into a three-dimensional network structure through hydrogen-bonding interactions with the cation.

Comment

The crystal structure of guanidinium 3-carboxybenzenesulfonate contains two symmetry-independent formula units; one anion is linked across an inversion center through the carboxylic acid —CO_2H unit [O—H···O 2.662 (4) Å] into a dianionic entity. In the other anion, the carboxylic acid unit is linked to the sulfonate group of an adjacent anion [O—H···O 2.684 (4) Å], forming a linear chain (Videnova-Adrabińska *et al.*, 2001). The cations interact with the anions to furnish a three-dimensional network. With the introduction of a hydroxyl group in the 4-position of the aromatic ring, the resulting compound, (I) (scheme and Fig. 1), also features a similarly linked chain, but the chain (Fig. 2) is connected by a stronger hydrogen bond [2.611 (2) Å]. The hydroxy H atom serves no function other than to form an internal hydrogen bond.



(I)

The cations and anions are linked into a tightly held three-dimensional network structure that is marginally more compact compared with guanidinium 3-carboxybenzenesulfonate (Videnova-Adrabińska *et al.*, 2001), as noted from its higher density. The 4-hydroxy-3-carboxybenzenesulfonate anion has recently been characterized as its dihydrated 4,4′-bipyridinium salt (Muthiah *et al.*, 2003).

Experimental

Equimolar quantities of guanidine hydrochloride (0.02 g, 0.2 mmol) and sodium 4-hydroxy-3-carboxybenzenesulfonate (0.05 g, 0.2 mmol) were dissolved in a small volume of water and the solvent was allowed to evaporate over several days. CH&N analysis for $C_8H_{11}N_3O_6$ (found/calc): C 34.88 (34.65), H 4.20 (4.00), N 15.24% (15.16%).

Crystal data

$CH_6N_3^+\cdot C_7H_5O_6S^-$	$Z = 2$
$M_r = 277.26$	$D_x = 1.583$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.4072$ (6) Å	Cell parameters from 2298 reflections
$b = 8.6995$ (7) Å	$\theta = 2.5$–$28.0°$
$c = 10.2525$ (8) Å	$\mu = 0.30$ mm^{-1}
$\alpha = 87.205$ (1)°	$T = 298$ (2) K
$\beta = 74.517$ (1)°	Plate, colorless
$\gamma = 66.277$ (1)°	0.31 × 0.13 × 0.05 mm
$V = 581.60$ (8) Å^3	

Data collection

Bruker SMART APEX area-detector diffractometer	2236 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.015$
ω and φ scans	$\theta_{max} = 27.5°$
Absorption correction: none	$h = -8 \rightarrow 9$
5004 measured reflections	$k = -11 \rightarrow 11$
2564 independent reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2 + 0.0934P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.038$	
$wR(F^2) = 0.112$	
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
2564 reflections	$\Delta\rho_{max} = 0.22$ e Å^{-3}
207 parameters	$\Delta\rho_{min} = -0.33$ e Å^{-3}
All H-atom parameters refined	

Table 1
Selected geometric parameters (Å, °).

S1—O1	1.444 (1)	N3—C8	1.317 (2)
S1—O2	1.456 (1)	C1—C2	1.376 (2)
S1—O3	1.463 (1)	C1—C6	1.397 (2)
S1—C1	1.762 (2)	C2—C3	1.389 (2)
O4—C7	1.315 (2)	C3—C4	1.400 (2)
O5—C7	1.212 (2)	C3—C7	1.482 (2)
O6—C4	1.357 (2)	C4—C5	1.393 (2)
N1—C8	1.313 (2)	C5—C6	1.369 (3)
N2—C8	1.326 (2)		
O1—S1—O2	113.2 (1)	C4—C3—C7	119.5 (2)
O1—S1—O3	112.3 (1)	O6—C4—C5	118.1 (2)
O2—S1—O3	111.8 (1)	O6—C4—C3	122.1 (2)
O1—S1—C1	106.6 (1)	C5—C4—C3	119.9 (2)
O2—S1—C1	106.4 (1)	C6—C5—C4	120.3 (2)
O3—S1—C1	105.9 (1)	C5—C6—C1	120.1 (1)
C2—C1—C6	120.0 (1)	O5—C7—O4	123.9 (2)
C2—C1—S1	120.3 (1)	O5—C7—C3	123.3 (2)
C6—C1—S1	119.7 (1)	O4—C7—C3	112.8 (2)
C1—C2—C3	120.6 (1)	N1—C8—N3	120.4 (2)
C2—C3—C4	119.2 (1)	N1—C8—N2	119.8 (2)
C2—C3—C7	121.3 (1)	N3—C8—N2	119.8 (2)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4*o*···O3^{i}	0.84 (1)	1.78 (1)	2.611 (2)	171 (3)
O6—H6*o*···O5	0.85 (1)	1.80 (2)	2.601 (2)	155 (3)
N1—H1*n*2···O1	0.84 (1)	2.01 (1)	2.851 (2)	177 (2)
N1—H1*n*1···O3^{ii}	0.84 (1)	2.05 (1)	2.885 (2)	172 (2)
N2—H2*n*1···O2	0.85 (1)	2.16 (1)	2.988 (2)	166 (2)
N2—H2*n*2···O6^{iii}	0.85 (1)	2.52 (2)	3.246 (2)	143 (2)
N3—H3*n*1···O6^{iii}	0.86 (1)	2.19 (1)	3.006 (2)	159 (2)
N3—H3*n*2···O2^{ii}	0.86 (1)	2.13 (1)	2.949 (2)	160 (2)

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

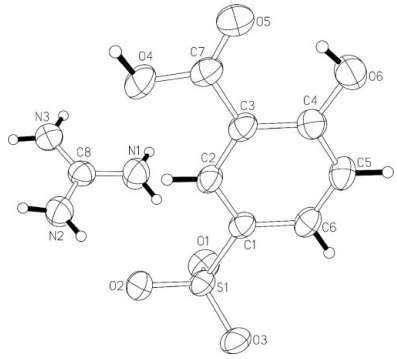


Figure 1
*ORTEP*II (Johnson, 1976) plot of $CH_6N_3^+\cdot C_7H_5O_6S^-$, with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

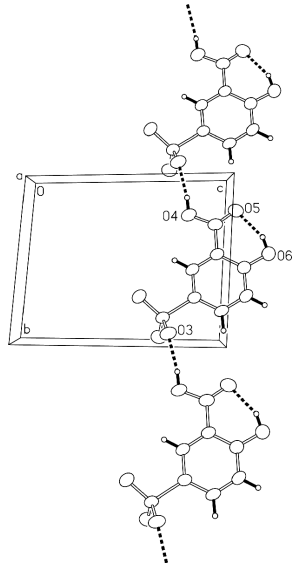


Figure 2
*ORTEP*II (Johnson, 1976) plot of the the hydrogen-bonded $[C_7H_5O_6S]^-$ chain.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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