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Potassium 2-(1*H*-tetrazol-1-yl)ethanesulfonate

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Key indicators

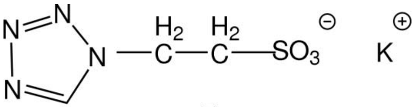
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.035
wR factor = 0.104
Data-to-parameter ratio = 21.2

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

In the title salt, $K^+\cdot C_3H_5N_4SO_3^-$, the potassium cation is surrounded by five O and two N atoms to form a KO_5N_2 irregular polyhedron. By sharing the edges and corners, the polyhedra are linked together giving polymeric layers parallel to the *bc* plane. The layers are additionally stabilized by C—H···O hydrogen bonds.

Comment

Taurine, 2-aminoethanesulfonic acid, and its derivatives are of great interest because of their importance for the medicine and food industries. To date, analogues of taurine formed by replacing the amino group by tetrazole derivatives have not been synthesized. In the present paper, we report the synthesis and crystal structure of a potassium salt of 2-(1*H*-tetrazol-1-yl)ethanesulfonic acid, (I). The asymmetric unit of (I) is shown in Fig. 1.



(I)

In (I), the tetrazole ring geometry is typical of 1-substituted tetrazoles with alkyl or aryl substituents (Cambridge Structural Database; Version 5.26 of November 2004; Allen, 2002). Formal double bonds N2═N3 and N4═C5 are the shortest in the ring, while the lengths of the three other ring bonds lie in the rather narrow range 1.326 (3)–1.350 (2) Å (Table 1). The tetrazole ring is essentially planar, the mean deviation of the

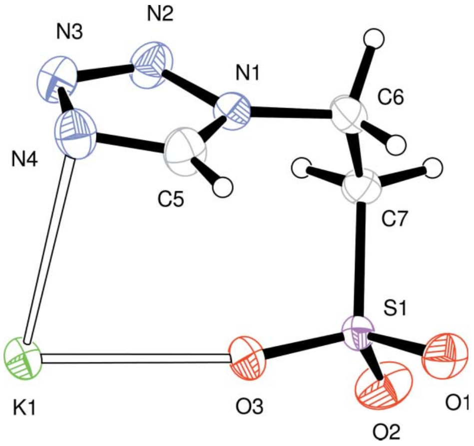


Figure 1
ORTEP-3 plot (Farrugia, 1997) of the asymmetric unit of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as spheres of arbitrary radius.

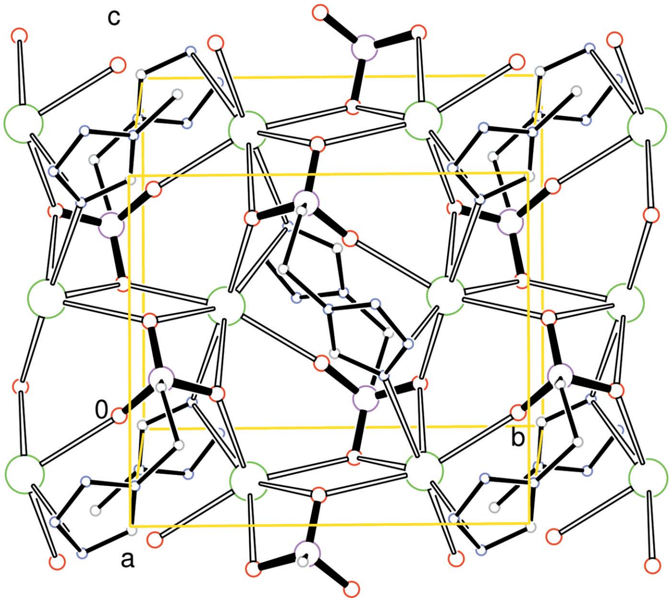


Figure 2
A fragment of a polymeric layer in the structure of (I). H atoms are omitted for clarity.

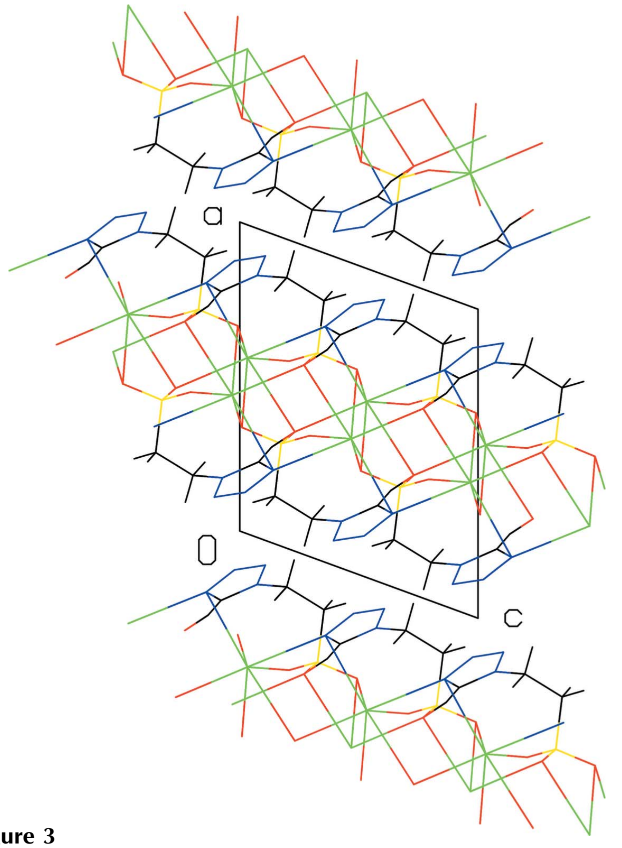


Figure 3
Layered structure of (I), viewed along the *b* axis.

tetrazole ring atoms from their least-squares plane being 0.0024 (13) Å. The geometry of the ethanesulfonate group is also normal.

Within a range of 3.2 Å the potassium cation is surrounded by five O and two N atoms (Table 1) belonging to five anions, to form a rather irregular KO_5N_2 polyhedron. Two anions are bonded to K^+ in monodentate fashion *via* O atoms, one anion is connected only through the N atom [K—N distance 2.9458 (19) Å], and the two remaining anions show bidentate linking *via* either two O atoms or an N and an O atom. Only atom N4 of the tetrazole ring is involved in the coordination of the K^+ cation; this is similar to transition metal complexes, because N4 is the best electron donor atom in the ring. By sharing edges and corners, the potassium polyhedra are linked together giving polymeric layers parallel to the *bc* plane (Figs. 2, 3). Within a layer, there are C—H···O hydrogen bonds (Table 2). Only van der Waals interactions exist between the layers.

Experimental

Compound (I) was prepared by neutralizing 2-(1-*H*-tetrazole-1-yl)ethanesulfonic acid with potassium hydroxide. The above acid was obtained by heterocyclization of 2-aminoethanesulfonic acid with ethyl orthoformate and sodium azide in acetic acid (molar ratio 1:3:1.1:8) using a method similar to that described previously (Gaponik *et al.*, 1985). Single crystals were grown by slow evaporation of an ethanol solution.

Crystal data

$K^+\cdot C_3H_5N_4O_3S^-$
$M_r = 216.27$
Monoclinic, $P2_1/c$
$a = 10.328$ (3) Å
$b = 9.593$ (3) Å
$c = 8.480$ (2) Å
$\beta = 110.08$ (2)°
$V = 789.1$ (4) Å^3
$Z = 4$
$D_x = 1.820$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.91$ mm^{-1}
$T = 294$ (2) K
Plate, colourless
0.44 × 0.42 × 0.08 mm

Data collection

Nicolet R3m four-circle diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.690$, $T_{max} = 0.931$
2460 measured reflections
2314 independent reflections
2027 reflections with $I > 2\sigma(I)$
$R_{int} = 0.013$
$\theta_{max} = 30.1°$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.104$
$S = 1.05$
2314 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 0.3192P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}

Table 1
Selected bond lengths (Å).

K1—O3	2.6835 (17)	N1—C5	1.326 (3)
K1—O1^{i}	2.6984 (17)	N1—N2	1.345 (2)
K1—O2^{ii}	2.737 (2)	N1—C6	1.458 (2)
K1—O2^{iii}	2.9123 (18)	N2—N3	1.292 (2)
K1—O1^{iii}	2.9359 (17)	N3—N4	1.350 (2)
K1—N4^{iv}	2.9458 (19)	N4—C5	1.313 (3)
K1—N4	3.199 (2)		

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

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C5—H5⋯O1^{v}	0.93	2.41	3.282 (3)	156

Symmetry code: (v) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

The H atoms were included in geometrically calculated positions (C—H = 0.97 Å for the methylene groups and C—H = 0.93 Å for the CH group of the tetrazole ring) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *R3m Software* (Nicolet, 1980); cell refinement: *R3m Software*; data reduction: *R3m Software*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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