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Potassium tris(2-aminoethanesulfonato-κ^2N,O)nickelate(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.041
wR factor = 0.085
Data-to-parameter ratio = 12.8

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

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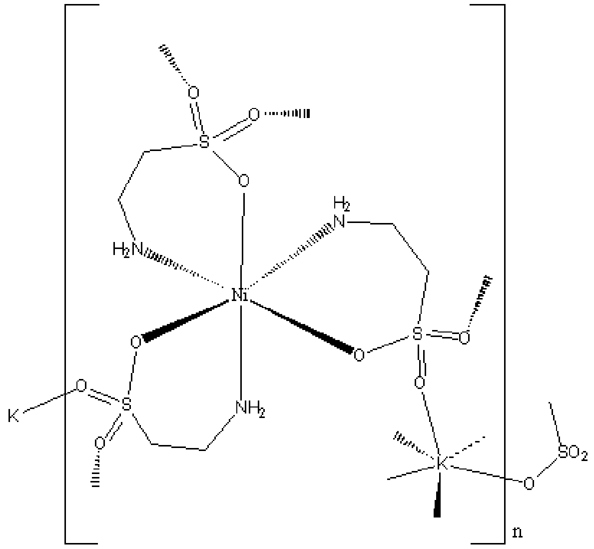
The hydrothermal reaction of $Ni(NO_3)_2{\cdot}2H_2O$, KOH and taurine produced the title compound, $K[Ni(C_2H_6NSO_3)_3]$. The Ni^{II} atom is chelated by the three taurinate ligands in a deformed octahedral geometry and in a facial manner. Each taurinate ligand bridges two K^+ ions via its sulfonate group, forming a three-dimensional framework.

Comment

The design and synthesis of novel coordination complexes have attracted considerable attention (Subramanian & Zaworotko, 1995), due to applications in many areas (Zhao *et al.*, 2001). Taurine, an amino acid containing sulfur, is indispensable to human beings and has important physiological functions. Recently, many Schiff base complexes derived from taurine have been reported (Zhang & Jiang, 2002; Zeng *et al.*, 2003; Jiang *et al.*, 2004; Zhang *et al.*, 2005). On the other hand, few taurinate complexes have been reported, because organosulfonates, $(RSO_3)^-$, are typically employed as 'non-coordinating' anions. This has prompted us to search for such complexes. We report here the synthesis and crystal structure of the title compound, (I).



(I)

The asymmetric unit of (I) consists of one Ni^{II} atom, three taurinate ligands and one K^+ ion. The Ni atom is bonded to three O and three N atoms in a slightly deformed octahedral geometry (Fig. 1 and Table 1). The Ni atom forms six-membered chelate rings ($NiNC_2SO$) with each taurinate ligand. This is a facial isomer. Each sulfonate group of the taurinate ligand takes part in the formation of a hydrogen

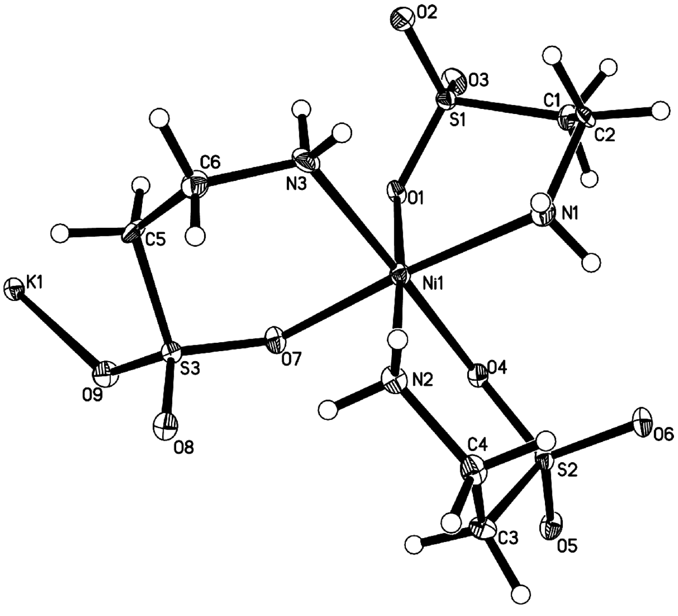


Figure 1

The asymmetric unit of the complex anion in (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

bond (Table 2) with the amino group of a neighbouring ligand in the complex.

The coordination modes of the sulfonate group have been much less well studied. The sulfonate group, as a tetrahedral oxygen-donating building block, may bridge sites of a coordination polymer chain to dictate the interchain geometry. The most common coordination modes of the sulfonate group are monodentate and μ_2-bridging, while μ_3-bridging is very rare. The coordination mode of the sulfonate group in (I) is μ_3-bridging, which makes the S—O(—Ni) bonds [1.485 (4)–1.496 (4) Å] much longer than those previously reported [S—O(—Cu) 1.453 (3) and 1.456 (3) Å; Zhong *et al.*, 2003; Cai *et al.*, 2004]. The S═O(···K) bonds [1.458 (4)–1.470 (4) Å] are slightly longer than the uncoordinated S═O bond in taurine [1.446 (12)–1.457 (13) Å; Zhang & Jiang, 2002].

The K atom is surrounded by six O atoms from different taurinate ligands in a triangular prismatic geometry (Fig. 2). Atoms O2$^{\rm iii}$, O8$^{\rm iv}$ and O9 are in the upper plane, while atoms O3$^{\rm i}$, O5$^{\rm ii}$ and O6$^{\rm v}$ are located in the lower plane [symmetry codes: (i) $-\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} + z$; (ii) $-\frac{1}{2} - x, \frac{1}{2} + y, z - \frac{1}{2}$; (iii) $-x, 2 - y, \frac{1}{2} + z$; (iv) $-x, 2 - y, z - \frac{1}{2}$; (v) $x - \frac{1}{2}, \frac{3}{2} - y, z$.] The title complex forms a three-dimensional structure through the K···O linkage. The K···O distances are in the range 2.693 (4)–2.866 (4) Å, suggesting weak electrostatic interactions.

Experimental

A solution of taurine (1.5 mmol) and KOH (2.0 mmol) in anhydrous methanol (10 ml) was added slowly to a solution of $Ni(NO_3)_2 \cdot 2H_2O$ (0.5 mmol) in anhydrous methanol (10 ml). After stirring for 10 min, dimethylformamide (5 ml) was added slowly to the mixture. The mixture was then placed in a 25 ml Teflon-lined stainless steel reactor and heated at 370 K for 6 d. Thereafter, the reactor was slowly cooled to room temperature and green prism-shaped crystals of (I) suitable for X-ray diffraction were obtained in a yield of 65%. Analysis found (%): C 15.34, H 1.68, N 8.95, S 20.43; required (%): C 15.31, H 1.71, N 8.93, S 20.46. IR (KBr, ν, cm^{-1}): 1032.7, 1164.2, 1233.3 ($-SO_3$), 3263.8, 3305.0 (N—H).

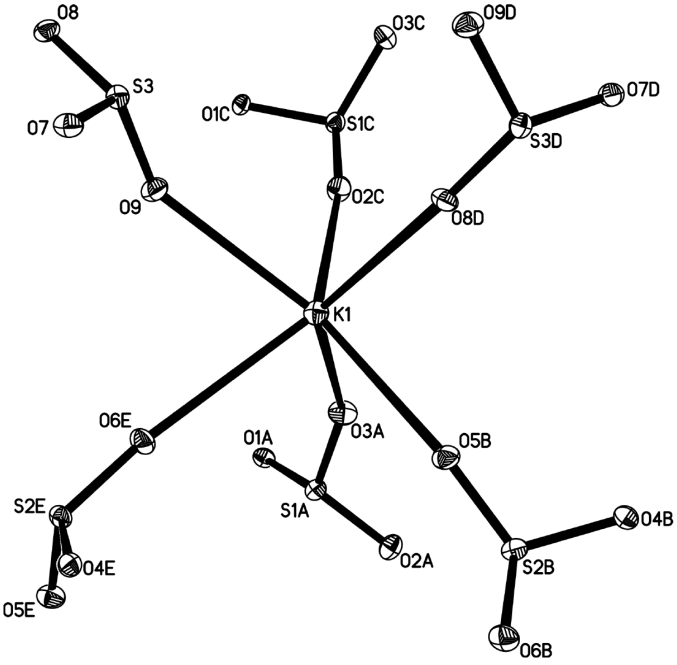


Figure 2

The coordination environment of the K$^+$ ion in (I), with displacement ellipsoids at the 30% probability level. [Symmetry codes: (A) $-\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} + z$; (B) $-\frac{1}{2} - x, \frac{1}{2} + y, z - \frac{1}{2}$; (C) $-x, 2 - y, \frac{1}{2} + z$; (D) $-x, 2 - y, z - \frac{1}{2}$; (E) $x - \frac{1}{2}, \frac{3}{2} - y, z$.]

Crystal data

$K[Ni(C_2H_6NSO_3)_3]$
$M_r = 470.22$
Orthorhombic, $Pna2_1$
$a = 10.712$ (9) Å
$b = 15.593$ (13) Å
$c = 9.556$ (8) Å
$V = 1596$ (2) Å^3
$Z = 4$
$D_x = 1.957$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 4244 reflections
$\theta = 2.1$–25.0°
$\mu = 1.92$ mm^{-1}
$T = 293$ (2) K
Prism, blue
0.14 × 0.10 × 0.06 mm

Data collection

Rigaku Mercury CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\rm min} = 0.674$, $T_{\rm max} = 0.891$
9501 measured reflections

2663 independent reflections
2455 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.057$
$\theta_{\rm max} = 25.0°$
$h = -12 \rightarrow 12$
$k = -18 \rightarrow 17$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.085$
$S = 1.07$
2663 reflections
208 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0388P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.50$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.41$ e Å^{-3}
Extinction correction: none
Absolute structure: Flack (1983), with 1156 Friedel pairs
Flack parameter: 0.01 (2)

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Table 1
Selected geometric parameters (Å, °).

Ni1—N1	2.110 (4)	K1—O2^{i}	2.806 (4)
Ni1—N2	2.108 (4)	K1—O3^{ii}	2.693 (4)
Ni1—N3	2.120 (5)	K1—O5^{iii}	2.791 (4)
Ni1—O1	2.126 (4)	K1—O6^{iv}	2.866 (4)
Ni1—O4	2.130 (4)	K1—O8^{v}	2.826 (4)
Ni1—O7	2.105 (4)	K1—O9	2.702 (4)
O7—Ni1—N2	92.05 (17)	N1—Ni1—O1	95.74 (16)
O7—Ni1—N1	174.01 (16)	N3—Ni1—O1	90.10 (17)
N2—Ni1—N1	89.62 (17)	O7—Ni1—O4	83.85 (15)
O7—Ni1—N3	91.56 (17)	N2—Ni1—O4	93.88 (16)
N2—Ni1—N3	92.13 (18)	N1—Ni1—O4	90.30 (16)
N1—Ni1—N3	94.12 (18)	N3—Ni1—O4	172.56 (16)
O7—Ni1—O1	82.36 (14)	O1—Ni1—O4	83.50 (14)
N2—Ni1—O1	174.03 (15)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*D*···O6	0.90	2.36	3.190 (6)	154
N2—H2*D*···O8	0.90	2.24	3.076 (6)	154
N3—H3*D*···O2	0.90	2.41	3.161 (6)	140

H atoms were positioned geometrically (C—H = 0.97 Å and N—H = 0.90 Å) and included in the refinement in the riding model approximation, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(carrier atom).

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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