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catena-Poly[nickel(II)-bis(μ-2-aminoethanesulfonato-$\kappa^3N,O:O';\kappa^3O:N,O'$)]

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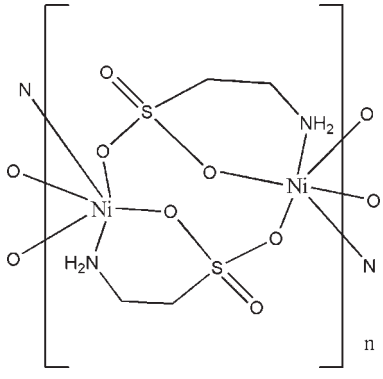
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.027; wR factor = 0.072; data-to-parameter ratio = 12.6.

In the title polymeric complex, $[Ni(C_2H_6NO_3S)_2]_n$, the Ni^{II} ion occupies a special position on an inversion centre and displays a slightly distorted octahedral coordination geometry, being linked to four sulfonate O atoms and to two N atoms of the taurine ligands. The sulfonate groups doubly bridge symmetry-related Ni^{II} centers, forming polymeric chains along the *a* axis.

Related literature

For general background to taurine complexes and their derivatives, see: Bottari & Festa (1998); Zhang & Jiang (2002); Zeng *et al.* (2003); Zhong *et al.* (2003). For our previous work on taurine complexes, see: Cai *et al.* (2004, 2006); Jiang *et al.* (2005).



Experimental

Crystal data

$[Ni(C_2H_6NO_3S)_2]$
M_r = 306.99
Monoclinic, $P2_1/n$
a = 5.1003 (17) Å
b = 8.231 (3) Å
c = 11.673 (4) Å
β = 97.492 (4)°
V = 485.9 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.44 mm^{-1}
T = 293 K
0.20 × 0.16 × 0.08 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.632, T_{max} = 0.829
2116 measured reflections
956 independent reflections
881 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.072
S = 1.06
954 reflections
76 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—N1^{i}	2.054 (2)	Ni1—O1^{i}	2.0916 (17)
Ni1—N1^{ii}	2.054 (2)	Ni1—O2	2.1185 (18)
Ni1—O1^{ii}	2.0916 (17)	Ni1—O2^{iii}	2.1185 (18)

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: BH2285).

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supporting information

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catena-Poly[nickel(II)-bis(*μ*-2-aminoethanesulfonato-$\kappa^3N,O:O';\kappa^3O:N,O'$)]

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S1. Comment

Taurine, an amino acid containing sulfur, is indispensable to human beings because of its applications in medicine and biochemistry (Bottari & Festa, 1998; Zhang & Jiang, 2002; Zeng *et al.*, 2003; Zhong *et al.*, 2003). Several taurine complexes and their derivatives have recently been prepared in our laboratory (Cai *et al.*, 2004; Jiang *et al.*, 2005; Cai *et al.*, 2006). As part of our ongoing investigation, the title polymeric Ni^{II} complex, (I), has been prepared and its structure determined.

A segment of the polymeric structure of (I) is illustrated in Fig. 1. The Ni^{II} ion is coordinated by four sulfonate O atoms and to two N atoms of the taurine ligands, displaying distorted octahedral coordination geometry. The sulfonate anions act as bridging ligands in (I). Neighbouring Ni atoms are bridged by two sulfonate anions, to form a zigzag polymeric chain along the *a* axis, as shown in Fig. 2. The polymeric chain has a repeat unit formed by two taurine and two Ni^{II} atoms related by an inversion centre, which coincides with the centre of the eight-membered $Ni_2S_2O_4$ ring formed by the atoms of two bridging ligands and the Ni atoms; the distance between the two Ni atoms is 5.100 (12) Å. In the structure of the title compound, there are two symmetry-independent "active" H atoms; both of them belong to the NH_2 group of the taurine ligand. They form intramolecular hydrogen bonds with sulfonate atom O3.

S2. Experimental

A solution of taurine (1.0 mmol) and KOH (1.0 mmol) in anhydrous methanol (10 ml) was added slowly to a solution of $Ni(CH_3COO)_2$ (1.0 mmol) in anhydrous methanol (10 ml). After stirring for 10 min, it was then dropped into a 25 ml Teflon-lined stainless steel reactor and heated at 393 K for five days. Thereafter, the reactor was slowly cooled to room temperature and green block-shaped crystals suitable for X-ray diffraction were collected.

S3. Refinement

H atoms were positioned geometrically (C—H = 0.97 Å and N—H = 0.80 Å) and included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}$(carrier atom).

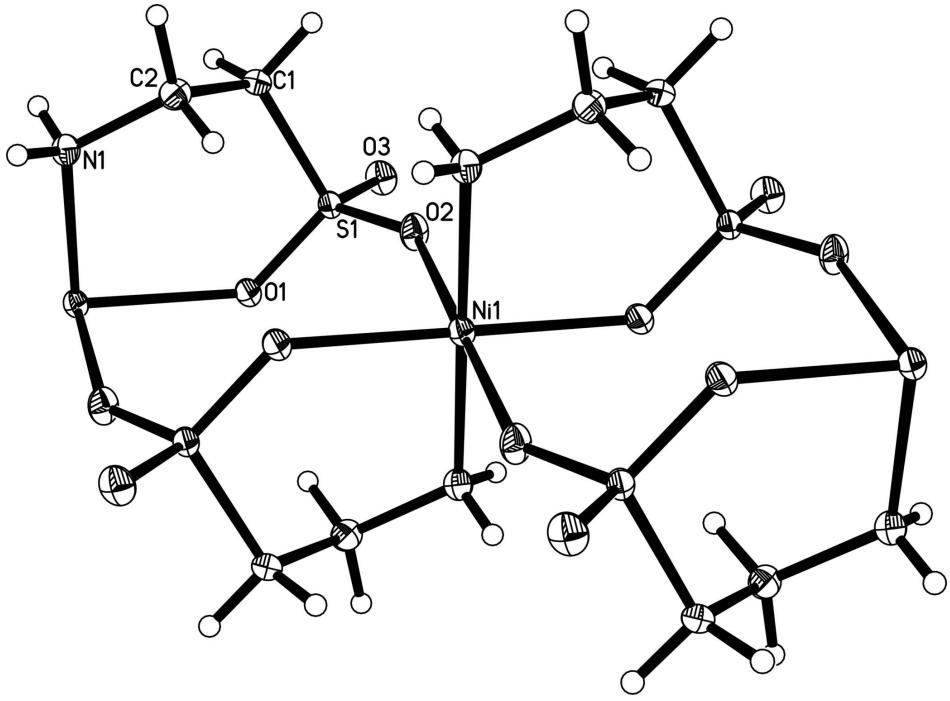

Figure 1

A segment of the polymeric structure of (I) with 30% probability displacement ellipsoids (arbitrary spheres for H atoms)

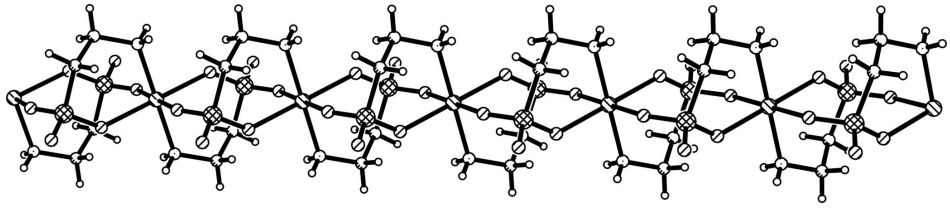

Figure 2

The one-dimensional polymeric chain of the title complex.

***catena*-Poly[nickel(II)-bis(*μ*-2-aminoethanesulfonato-$\kappa^3N,O:O';\kappa^3O:N,O'$)]**

Crystal data

$[Ni(C_2H_6NO_3S)_2]$
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Hall symbol: -P 2yn
a = 5.1003 (17) Å
b = 8.231 (3) Å
c = 11.673 (4) Å
β = 97.492 (4)°
V = 485.9 (3) Å^3
Z = 2
$F(000)$ = 316
D_x = 2.098 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 783 reflections
θ = 3.0–27.6°
μ = 2.44 mm^{-1}
T = 293 K
Block, green
0.20 × 0.16 × 0.08 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans

Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.632, T_{max} = 0.829
2116 measured reflections
956 independent reflections
881 reflections with $I > 2\sigma(I)$

R_{int} = 0.026
θ_{max} = 26.0°, θ_{min} = 3.0°
h = −5→6
k = −6→10
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.072
S = 1.06
954 reflections
76 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.044P)^2 + 0.1P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.0000	1.0000	1.0000	0.01738 (17)
S1	0.46761 (11)	0.95864 (7)	0.81432 (5)	0.01601 (18)
O1	0.6637 (3)	1.0584 (2)	0.88498 (15)	0.0213 (4)
O2	0.2125 (3)	0.9622 (2)	0.85798 (16)	0.0241 (4)
O3	0.4412 (4)	1.0004 (2)	0.69297 (16)	0.0255 (4)
C1	0.5831 (5)	0.7569 (3)	0.8243 (2)	0.0228 (5)
H1A	0.4468	0.6865	0.7857	0.027*
H1B	0.7363	0.7484	0.7833	0.027*
C2	0.6583 (4)	0.6964 (3)	0.9465 (2)	0.0222 (5)
H2A	0.5292	0.7340	0.9946	0.027*
H2B	0.6568	0.5785	0.9469	0.027*
N1	0.9230 (4)	0.7550 (3)	0.99449 (19)	0.0196 (4)
H1C	0.963 (6)	0.719 (4)	1.058 (3)	0.024*
H1D	1.023 (6)	0.715 (4)	0.956 (3)	0.024*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0148 (2)	0.0200 (3)	0.0172 (3)	−0.00114 (15)	0.00144 (18)	−0.00013 (16)
S1	0.0137 (3)	0.0212 (3)	0.0132 (3)	0.0001 (2)	0.0022 (2)	−0.0009 (2)
O1	0.0194 (8)	0.0201 (9)	0.0230 (9)	−0.0006 (7)	−0.0025 (7)	−0.0012 (7)
O2	0.0156 (8)	0.0361 (10)	0.0216 (10)	−0.0001 (7)	0.0062 (7)	0.0006 (7)
O3	0.0274 (10)	0.0341 (11)	0.0153 (10)	−0.0008 (7)	0.0038 (8)	0.0021 (7)
C1	0.0224 (12)	0.0205 (12)	0.0243 (13)	0.0017 (10)	−0.0015 (10)	−0.0071 (10)
C2	0.0196 (11)	0.0190 (11)	0.0287 (13)	−0.0028 (9)	0.0060 (10)	0.0014 (10)
N1	0.0204 (10)	0.0213 (10)	0.0171 (10)	0.0001 (9)	0.0018 (8)	0.0032 (9)

Geometric parameters (Å, º)

Ni1—N1^{i}	2.054 (2)	O1—Ni1^{iv}	2.0916 (17)
Ni1—N1^{ii}	2.054 (2)	C1—C2	1.513 (3)
Ni1—O1^{ii}	2.0916 (17)	C1—H1A	0.9700
Ni1—O1^{i}	2.0916 (17)	C1—H1B	0.9700
Ni1—O2	2.1185 (18)	C2—N1	1.474 (3)
Ni1—O2^{iii}	2.1185 (18)	C2—H2A	0.9700
S1—O3	1.447 (2)	C2—H2B	0.9700
S1—O2	1.4584 (18)	N1—Ni1^{iv}	2.054 (2)
S1—O1	1.4630 (18)	N1—H1C	0.80 (3)
S1—C1	1.760 (2)	N1—H1D	0.80 (3)
N1^{i}—Ni1—N1^{ii}	180.000 (1)	S1—O1—Ni1^{iv}	132.53 (11)
N1^{i}—Ni1—O1^{ii}	86.09 (8)	S1—O2—Ni1	147.91 (12)
N1^{ii}—Ni1—O1^{ii}	93.91 (8)	C2—C1—S1	114.49 (17)
N1^{i}—Ni1—O1^{i}	93.91 (8)	C2—C1—H1A	108.6
N1^{ii}—Ni1—O1^{i}	86.09 (8)	S1—C1—H1A	108.6
O1^{ii}—Ni1—O1^{i}	180.000 (1)	C2—C1—H1B	108.6
N1^{i}—Ni1—O2	93.06 (8)	S1—C1—H1B	108.6
N1^{ii}—Ni1—O2	86.94 (8)	H1A—C1—H1B	107.6
O1^{ii}—Ni1—O2	89.52 (7)	N1—C2—C1	110.97 (19)
O1^{i}—Ni1—O2	90.48 (7)	N1—C2—H2A	109.4
N1^{i}—Ni1—O2^{iii}	86.94 (8)	C1—C2—H2A	109.4
N1^{ii}—Ni1—O2^{iii}	93.06 (8)	N1—C2—H2B	109.4
O1^{ii}—Ni1—O2^{iii}	90.48 (7)	C1—C2—H2B	109.4
O1^{i}—Ni1—O2^{iii}	89.52 (7)	H2A—C2—H2B	108.0
O2—Ni1—O2^{iii}	180.000 (1)	C2—N1—Ni1^{iv}	119.67 (16)
O3—S1—O2	111.34 (11)	C2—N1—H1C	110 (2)
O3—S1—O1	112.85 (11)	Ni1^{iv}—N1—H1C	108 (2)
O2—S1—O1	111.54 (11)	C2—N1—H1D	106 (2)
O3—S1—C1	106.05 (11)	Ni1^{iv}—N1—H1D	107 (2)
O2—S1—C1	107.59 (12)	H1C—N1—H1D	106 (3)
O1—S1—C1	107.09 (11)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*D*···O3^{v}	0.80 (3)	2.50 (3)	3.171 (3)	143 (3)
N1—H1*C*···O3^{vi}	0.80 (3)	2.41 (3)	3.121 (3)	149 (3)

Symmetry codes: (v) −*x*+3/2, *y*−1/2, −*z*+3/2; (vi) *x*+1/2, −*y*+3/2, *z*+1/2.