

Yong-Rong Xie,* Yan-Chao Yang,
Xiao-Yong Yuan and Rui-Qing
YangCollege of Chemistry and Life Science, Gannan
Normal University, Ganzhou 341000, People's
Republic of ChinaCorrespondence e-mail:
yongrongxie@yahoo.com.cn

Key indicators

Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(C-C) = 0.003$ Å
 R factor = 0.030
 wR factor = 0.086
Data-to-parameter ratio = 17.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Hexaaquanickel(II) 2-methyl-5-nitrobenzene-
sulfonate tetrahydrate

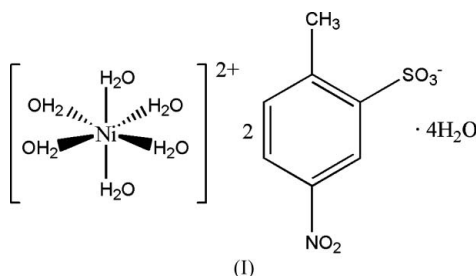
In the title complex, $[\text{Ni}(\text{H}_2\text{O})_6](\text{C}_7\text{H}_6\text{NO}_5\text{S})_2 \cdot 4\text{H}_2\text{O}$, each Ni^{II} cation lies on an inversion center and is octahedrally coordinated by six water molecules. The anions do not coordinate to the nickel, but act as counter-ions. The crystal structure is composed of alternating layers of $[\text{Ni}(\text{H}_2\text{O})_6]^{2+}$ cations and anions. The $[\text{Ni}(\text{H}_2\text{O})_6]^{2+}$ cations, water molecules and anions are connected through a complex pattern of hydrogen-bonding interactions, resulting in a three-dimensional supramolecular network.

Received 13 September 2006

Accepted 14 September 2006

Comment

The crystal structure of potassium 2-methyl-5-nitrobenzenesulfonate (X^-) (Xie *et al.*, 2006) has been reported previously. We present here the structure of the nickel complex, $[\text{Ni}(\text{H}_2\text{O})_6]X_2 \cdot 4\text{H}_2\text{O}$, (I). The analysis indicates that the crystal structure is built up of $[\text{Ni}(\text{H}_2\text{O})_6]^{2+}$ cations, two uncoordinated X^- anions and four uncoordinated water molecules. The Ni^{II} atom is located on a crystallographic inversion center and is coordinated by the six water molecules in an octahedral environment. The Ni—O bond distances range from 2.0441 (12) to 2.0618 (13) Å. The average Ni—O bond distance of 2.053 Å is similar to the values in other nickel complexes (Ma *et al.*, 2003; Batsanov *et al.*, 2001; Zhang *et al.*, 2004). The crystal structure comprises alternating layers of $[\text{Ni}(\text{H}_2\text{O})_6]^{2+}$ cations and sulfonate anions furnishing a three-dimensional supramolecular network.



Experimental

A mixture of $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ (1.185 g, 5.0 mmol), 2-methyl-5-nitrobenzenesulfonic acid (2.17 g, 10.0 mmol) and 70% ethanol solution (20 ml) was stirred at room temperature for 30 min. Green single crystals of complex (I) were obtained from the filtered solution at room temperature over a period of 3 d. The product was isolated, washed three times with 70% ethanol solution and dried in a vacuum desiccator using CaCl_2 (yield: 65%). Analysis calculated for $[\text{Ni}(\text{H}_2\text{O})_6](\text{C}_7\text{H}_6\text{NO}_5\text{S})_2 \cdot 4\text{H}_2\text{O}$: C 25.05, H 4.81, N 4.17%; found: C 24.95, H 4.93, N 4.04%.

Crystal data

[Ni(H₂O)₆](C₇H₆NO₅)₂·4H₂O
M_r = 671.25
 Triclinic, *P*1̄
a = 7.2421 (4) Å
b = 7.6642 (4) Å
c = 13.7999 (7) Å
 α = 74.077 (1)°
 β = 76.324 (1)°
 γ = 68.212 (1)°

V = 676.14 (6) Å³
Z = 1
D_x = 1.648 Mg m⁻³
 Mo *K*α radiation
 μ = 0.96 mm⁻¹
T = 292 (2) K
 Plate, green
 0.55 × 0.25 × 0.09 mm

Data collection

Bruker SMART APEXII CCD
 area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
T_{min} = 0.750, *T_{max}* = 0.910

3911 measured reflections
 3086 independent reflections
 2653 reflections with *I* > 2σ(*I*)
R_{int} = 0.012
 θ_{max} = 27.7°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.030
wR (*F*²) = 0.086
S = 1.09
 3086 reflections
 180 parameters
 H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.0507*P*)²
 + 0.2656*P*]
 where *P* = (*F_o*² + 2*F_c*²)/3
 (Δ/*σ*)_{max} < 0.001
 Δρ_{max} = 0.41 e Å⁻³
 Δρ_{min} = -0.34 e Å⁻³
 Extinction correction: SHELXL97
 Extinction coefficient: 0.0149 (8)

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O4—H4A...O7 ⁱ	0.85	1.94	2.779 (2)	169
O4—H4B...O2	0.85	2.00	2.777 (2)	151
O5—H5A...O8 ⁱⁱ	0.85	1.97	2.768 (2)	156
O5—H5B...O3 ⁱⁱⁱ	0.85	2.02	2.821 (2)	156
O6—H6A...O7 ⁱⁱⁱ	0.85	1.89	2.742 (2)	178
O6—H6B...O3	0.85	2.31	3.118 (3)	158
O7—H7A...O1 ^{iv}	0.85	1.96	2.777 (2)	160
O7—H7B...O8	0.85	2.15	2.957 (2)	157
O8—H8A...O1	0.85	2.12	2.953 (2)	167
O8—H8B...O3 ^v	0.85	2.23	2.914 (2)	137

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

H atoms bonded to C atoms were placed in calculated positions, with C—H = 0.93 or 0.96 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C), and were included in the refinement in the riding-model approximation. The H atoms of water molecules were located in difference Fourier maps

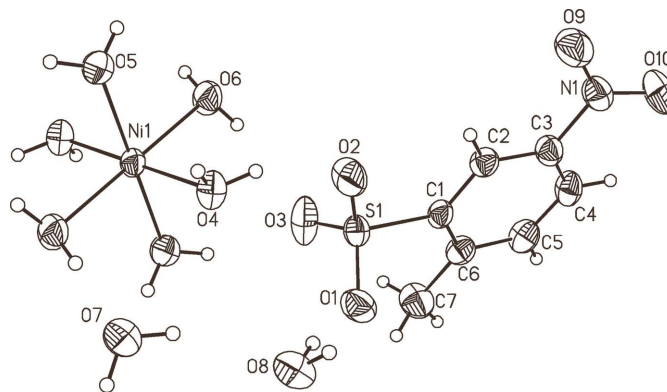


Figure 1

View of the asymmetric unit, expanded to show the complete coordination of Ni^{II}, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabeled atoms in the cation are related to labeled atoms by -*x*, 1 - *y*, 1 - *z*.

and then idealized and treated as riding, with O—H = 0.85 Å and *U*_{iso}(H) = 1.5*U*_{eq}(O).

Data collection: SMART (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2004); software used to prepare material for publication: SHELXTL.

The authors thank the Jiangxi Provincial Educational Foundation of the People's Republic of China (Nos. 20040729 and 20060237), the Natural Science Foundation of Jiangxi Province of the People's Republic of China (No. 0620007) and the Gannan Normal University Foundation (No. 200409).

References

Batsanov, A. S., Howard, J. A. K., Moore, N. S. & Kilner, M. (2001). *Acta Cryst.* E57, m485–m487.
 Bruker (2004). SMART (Version 6.0), SAINT (Version 6.0) and SHELXTL (Version 5.1). Bruker AXS Inc., Madison, Wisconsin, USA.
 Ma, J.-F., Yang, J. & Liu, J.-F. (2003). *Acta Cryst.* E59, m483–m484.
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
 Xie, Y.-R., Lui, G.-R. & Yuan, X.-Y. (2006). *Acta Cryst.* E62, m1016–m1017.
 Zhang, Z.-Y., Gao, S., Huo, L.-H., Zhao, H., Zhao, J.-G. & Ng, S. W. (2004). *Acta Cryst.* E60, m544–m545