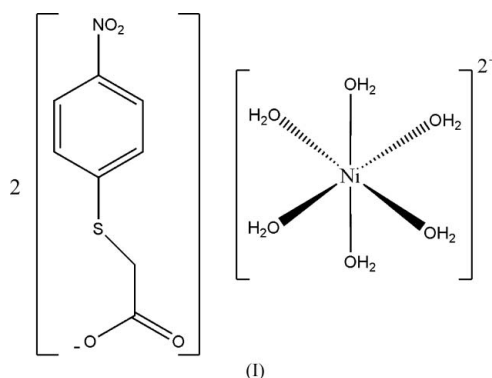


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Key indicatorsSingle-crystal X-ray study
 $T = 291$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.032
 wR factor = 0.116
Data-to-parameter ratio = 16.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**Hexaaquanickel(II) bis[(4-nitrophenyl-
sulfanyl)acetate]**In the title compound, $[\text{Ni}(\text{H}_2\text{O})_6](\text{C}_8\text{H}_6\text{NO}_4\text{S})_2$, the Ni^{II} atom lies on an inversion center and is six-coordinated in an octahedral environment. Cations and anions are linked by $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds into a three-dimensional network.Received 6 November 2006
Accepted 20 November 2006**Comment**Simple carboxylic acids containing the 4-nitrophenyl group exhibit a variety of supramolecular aggregation patterns (Glidewell *et al.*, 2002). We have previously reported the structure of hexaaquacobalt(II) bis(4-nitrophenoxyacetate) pentahydrate (Gao *et al.*, 2006). Recently, our attention has been focused on (4-nitrophenylsulfanyl)acetic acid, whose crystal structure has been reported previously (Glidewell *et al.*, 2002). In this paper, we report a new complex, (I), synthesized by the reaction of (4-nitrophenylsulfanyl)acetic acid and nickel(II) dinitrate hexahydrate in an aqueous solution.The Ni^{II} atom lies on an inversion center and is coordinated by six water molecules in an octahedral environment (Fig. 1). The anion is almost planar, the largest deviation being 0.220 (2) Å for atom O2; however, the sulfanylacetate group is slightly twisted with a C1–S1–C7–C8 torsion angle of 10.24 (17)°. Cations and anions are linked through $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds, resulting in a three-dimensional supramolecular network (Table 1).**Experimental**

(4-Nitrophenylsulfanyl)acetic acid was prepared by nucleophilic reaction of chloroacetic acid and 4-nitrothiophenol under basic conditions. (Nobles & Thompson, 1965). Nickel dinitrate hexahydrate (0.582 g, 2 mmol) and (4-nitrophenylsulfanyl)acetic acid (0.394 g, 2 mmol) were dissolved in hot water (10 ml) and the pH was adjusted to 6 with 0.01 M sodium hydroxide. Yellow crystals separated from the filtered solution after several days.

Crystal data

[Ni(H₂O)₆](C₈H₆NO₄S)₂
M_r = 591.20
 Triclinic, *P* $\bar{1}$
a = 7.365 (6) Å
b = 7.368 (7) Å
c = 11.755 (10) Å
 α = 98.33 (3)°
 β = 99.61 (3)°
 γ = 109.29 (3)°

V = 579.8 (9) Å³
Z = 1
D_x = 1.693 Mg m⁻³
 Mo *K*α radiation
 μ = 1.09 mm⁻¹
T = 291 (2) K
 Block, yellow
 0.48 × 0.18 × 0.07 mm

Data collection

Rigaku R-Axis RAPID
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
T_{min} = 0.625, *T_{max}* = 0.925

5748 measured reflections
 2634 independent reflections
 2208 reflections with *I* > 2σ(*I*)
R_{int} = 0.021
 θ_{max} = 27.5°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.032
wR (*F*²) = 0.116
S = 1.16
 2634 reflections
 160 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 0.196P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.47 \text{ e \AA}^{-3}$
 $\Delta\rho_{min} = -0.44 \text{ e \AA}^{-3}$

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> |
|----------------------------|-------------|---------------|-----------------------|-------------------------|
| O6—H61···O3 ⁱ | 0.85 | 1.98 | 2.821 (3) | 168 |
| O6—H62···O2 | 0.86 | 1.85 | 2.641 (4) | 154 |
| O5—H51···O2 ⁱⁱ | 0.86 | 1.90 | 2.749 (3) | 171 |
| O5—H52···O1 ⁱⁱⁱ | 0.85 | 1.96 | 2.794 (3) | 167 |
| O7—H72···O1 ⁱⁱ | 0.85 | 1.83 | 2.676 (3) | 176 |

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

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 (aromatic) or 0.97 Å (methylene), and with *U*_{iso}(H) = 1.2*U*_{eq}(C). Water H atoms were initially located in a difference Fourier map, but they were treated as riding on their parent atoms, with O—H = 0.85 Å, H···H = 1.39 Å and *U*_{iso}(H) = 1.5*U*_{eq}(O).

Data collection: RAPID-AUTO (Rigaku, 1998); cell refinement: RAPID-AUTO; data reduction: CrystalStructure (Rigaku/MS,

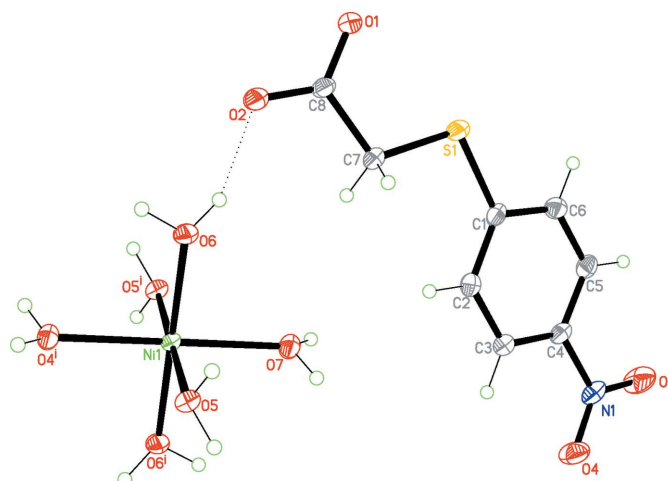


Figure 1

The molecular structure of (I) with the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii. A dashed line indicates the intermolecular O—H···O hydrogen-bonding interaction. [Symmetry code: (i) 2 - *x*, 1 - *y*, 1 - *z*.

2002); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXL97.

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