Lists of structure factors and anisotropic displacement parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71703 (4 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AL1067]

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A Precise Structure Redetermination of Nickel Ammonium Sulfate Hexahydrate, $Ni(H_2O)_6.2NH_4.2SO_4$

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Abstract

The $Ni(H_2O)_6$ ion is located at an inversion center. Six octahedral water molecules surround the Ni^{II} ion and form hydrogen bonds with the sulfate groups. Each ammonium group binds to the sulfate groups through hydrogen bonds.

Comment

This structure has been reported by Grimes, Kay & Webb (1963) and Montgomery & Lingafelter (1964), but the present structure is more precise in several respects.

The Ni^{II} ion is located at an inversion center. The six water molecules surrounding the Ni^{II} ion form octahedral geometry, with Ni—O(*W*) distances spanning the narrow range 2.041 (2)–2.067 (2) Å. The water molecules bind the sulfate groups through hydrogen bonds. Hydrogen bonds also exist between the ammonium and sulfate groups. In the sulfate ion, S—O(4) is *ca* 0.02 Å shorter than the other three S—O bonds. This is apparently due to differences in the number of hydrogen bonds accepted by these atoms; O(4) accepts only one hydrogen bond while O(1), O(2) and O(3) each accept three.

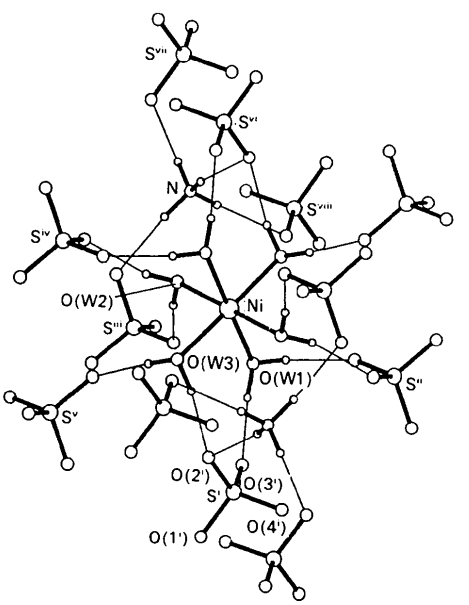

Fig. 1. A perspective view of the molecule with hydrogen bonds (thin lines) in the crystal structure. The Ni atom is situated at the inversion center. Symmetry codes: (i) $x, 0.5-y, -0.5+z$; (ii) $x, -1+y, -1+z$; (iii) $1-x, 1-y, 1-z$; (iv) $-x, 1-y, 1-z$; (v) $x, -1+y, z$; (vi) $-x, -0.5+y, 0.5-z$; (vii) $x, 1.5-y, -0.5+z$; (viii) $1-x, -0.5+y, 0.5-z$.

Experimental

Crystal data

$Ni(H_2O)_6.2NH_4.2SO_4$
M_r = 394.99
Monoclinic
$P2_1/c$
a = 6.244 (2) Å
b = 12.469 (4) Å
c = 9.195 (3) Å
β = 106.98 (3)°
D_x = 1.916 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.7107 Å
Cell parameters from 25 reflections
θ = 9.5–17.5°
μ = 1.81 mm^{-1}
T = 298 (3) K
Parallelepiped

V = 684.7 (4) Å^3
Z = 2

0.33 × 0.30 × 0.25 mm
Green

Data collection

Nicolet *R3m/V* diffractometer
$\theta/2\theta$ scans
Absorption correction: empirical (North, Phillips & Mathews, 1968)
T_{min} = 0.63, T_{max} = 1.00
1496 measured reflections
1496 independent reflections

1269 observed reflections [$I \geq \sigma(I)$]
θ_{max} = 25°
$h = 0 \rightarrow 7$
$k = 0 \rightarrow 14$
$l = -10 \rightarrow 10$
3 standard reflections
frequency: 60 min
intensity variation: ±0.5%

Refinement

Refinement on F
R = 0.029
wR = 0.044
S = 1.21
1269 reflections
89 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o) + 0.001(F_o)^2]$
$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.93 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}
Extinction correction: Zachariasen (1968)
Extinction coefficient: 1.1 (1)
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
Ni	0	0	0	1.370 (18)
S	0.26107 (9)	0.86330 (4)	0.59231 (6)	1.54 (2)
O(*W*1)	0.2993 (3)	−0.06667 (12)	0.00203 (17)	1.93 (6)
O(*W*2)	0.1621 (3)	0.10679 (13)	0.16814 (17)	2.06 (7)
O(*W*3)	−0.0343 (3)	−0.10970 (12)	0.16013 (17)	2.05 (7)
O(1)	0.3791 (3)	0.93309 (12)	0.72113 (17)	2.13 (7)
O(2)	0.0517 (3)	0.82243 (14)	0.6167 (2)	2.45 (8)
O(3)	0.4102 (3)	0.77224 (14)	0.5857 (2)	2.63 (8)
O(4)	0.2136 (4)	0.92460 (15)	0.45101 (19)	3.22 (9)
N	0.3559 (4)	0.34689 (16)	0.1349 (2)	2.37 (9)

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and bond distances and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71697 (6 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS1068]

Table 2. *Selected geometric parameters* (Å, °)

Ni—O(*W*1)	2.041 (2)	S—O(2)	1.480 (2)
Ni—O(*W*2)	2.067 (2)	S—O(3)	1.481 (2)
Ni—O(*W*3)	2.066 (2)	S—O(4)	1.461 (2)
S—O(1)	1.481 (2)		
O(*W*1)—Ni—O(*W*2)	90.48 (7)	O(1)—S—O(4)	109.2 (1)
O(*W*1)—Ni—O(*W*3)	90.52 (7)	O(2)—S—O(3)	109.6 (1)
O(*W*2)—Ni—O(*W*3)	91.35 (7)	O(2)—S—O(4)	110.9 (1)
O(1)—S—O(2)	109.7 (1)	O(3)—S—O(4)	109.3 (1)
O(1)—S—O(3)	108.2 (1)		

Non-H atoms were located by direct and Fourier methods and refined by anisotropic full-matrix least-squares techniques. H atoms were located by difference Fourier methods. *NRCVAX* (Gabe, Le Page, White & Lee, 1987) was used for all calculations.

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