Crystal structure of tetraaquabis(perrhenato)nickel(II), $\text{Ni}(\text{ReO}_4)_2(\text{H}_2\text{O})_4$

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Received December 20, 1996, transferred to 1st update of database ICSD in 1998, CSD-No. 402773

$\text{H}_8\text{NiO}_{12}\text{Re}_2$, triclinic, $P\bar{1}$ (No. 2), $a = 6.658(1) \text{ \AA}$, $b = 6.763(1) \text{ \AA}$, $c = 7.161(1) \text{ \AA}$, $\alpha = 65.38(1)^\circ$, $\beta = 70.27(1)^\circ$, $\gamma = 71.65(1)^\circ$, $V = 270.1 \text{ \AA}^3$, $Z = 1$, $R(F) = 0.056$, $R_w(F) = 0.053$.

Table 1. Parameters used for the X-ray data collection

Crystal:	pale green prism, size 0.15 x 0.2 x 0.65 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	241.20 cm ⁻¹
Diffraction:	Siemens P4
Scan mode:	ω
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	55°
$N(hkl)_{\text{unique}}$:	1230
Criterion for F_o :	$F_o > 3 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	71
Program:	SHELXTL-plus

Source of material: Perrhenic acid was added dropwise to a suspension of $\text{NiCO}_3/\text{Ni}(\text{OH})_2$ in water. The mixture was stirred and warmed up to 323 K until a clear green solution was formed. Green crystals of the title compound were obtained by slow evaporation of water.

The title compound crystallizes isotypically with $\text{Cu}(\text{ReO}_4)_2(\text{H}_2\text{O})_4$ (see ref. 1). The tetrahedra around the rhenium atoms are slightly distorted. The distance of rhenium to the oxygen atom bound to nickel (176(1) pm) is marginally longer than the average Re—O distance (171(2) pm). The octahedron around nickel is almost regular with distances ranging from 203.8(9) pm to 206.1(11) pm with a mean value of 204.8(15) pm.

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Re(1)	2i	0.08474(8)	0.32084(8)	0.29095(7)	0.0241(4)	0.0182(4)	0.0175(3)	0.0023(3)	-0.0030(2)	-0.0093(3)
Ni(1)	1d	1/2	0	0	0.021(1)	0.016(1)	0.017(1)	0.005(1)	-0.0043(9)	-0.0095(9)
O(1)	2i	-0.189(2)	0.325(2)	0.383(2)	0.029(6)	0.029(6)	0.029(5)	0.015(5)	0.002(4)	-0.009(4)
O(2)	2i	0.188(2)	0.272(2)	0.494(2)	0.062(8)	0.033(7)	0.038(6)	0.003(6)	-0.020(6)	-0.012(5)
O(3)	2i	0.125(2)	0.568(2)	0.103(2)	0.065(8)	0.040(7)	0.028(5)	-0.025(7)	-0.009(5)	-0.003(5)
O(4)	2i	0.204(2)	0.111(2)	0.179(2)	0.040(6)	0.033(6)	0.043(6)	0.011(5)	-0.018(5)	-0.029(5)
O(5)	2i	0.348(2)	-0.075(2)	-0.160(2)	0.043(7)	0.042(7)	0.045(6)	-0.008(6)	-0.012(5)	-0.027(5)
O(6)	2i	0.514(2)	0.305(2)	-0.229(1)	0.030(5)	0.026(6)	0.023(4)	0.009(4)	-0.004(4)	-0.011(4)

Acknowledgment. C. Mujica thanks the Max-Planck-Gesellschaft for supporting a sabbatical stay at the Max-Planck-Institut für Festkörperforschung, Stuttgart.

References

- Mujica, C.; Peters, K.; Peters, E.-M.; v. Schnering, H. G.: Crystal structure of tetraaquabis(perrhenato)copper (II), $\text{Cu}(\text{ReO}_4)_2(\text{H}_2\text{O})_4$. *Z. Kristallogr. NCS* **212** (1997) 294.
- Sheldrick, G. M.: Program Package SHELXTL-plus. Release 4.1. Siemens Analytical X-Ray Instruments Inc., Madison (WI 53719), USA 1990.