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ONEILLITE: A NEW Ca-DEFICIENT AND *REE*-RICH MEMBER OF THE EUDIALYTE GROUP FROM MONT SAINT-HILAIRE, QUEBEC, CANADA

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ABSTRACT

Oneillite, ideally $Na_{15}Ca_3\ Mn_3Fe_3\ Zr_3Nb\ (Si_{25}O_{73})\ (O,OH,H_2O)_3(OH,Cl)_2$, is a new member of the eudialyte group from Mont Saint-Hilaire, Quebec. It occurs as yellowish brown anhedral grains up to 2 mm in diameter. Associated minerals include albite, sodalite, pyrite and aegirine. It is transparent to translucent, with a vitreous luster and white streak. It is brittle, with a hardness of 5–6 (Mohs scale). It has no cleavage, no parting, and an uneven fracture. It is uniaxial negative with ω 1.6450(3) and ε 1.6406(3). It is trigonal, space group $R3$, a 14.192(1) and c 29.983(3) Å, V 5230(1) Å^3, $Z = 3$. The strongest X-ray powder-diffraction lines [d in Å $(I)(hkl)$] are: 11.348(44.2)(101), 7.100(33)(110), 6.021(36.1)(021), 5.683(30.8)(202), 4.291(36.5)(205), 3.389(42.9)($\bar{1}41$), 3.199(30.8)(208), 3.150(34.9)($\bar{2}37$), 2.964(100)($\bar{3}45$) and 2.844(89.1)(404). The infrared spectrum is given. An electron-microprobe analysis of the grain of oneillite chosen for refinement of the structure gave Na_2O 13.60, K_2O 0.28, CaO 2.90, MnO 7.70, FeO 3.00, SrO 0.09, Al_2O_3 0.18, Y_2O_3 0.78, La_2O_3 2.88, Ce_2O_3 5.14, Pr_2O_3 0.48, Nd_2O_3 1.45, Gd_2O_3 0.20, SiO_2 43.46, ZrO_2 11.44, HfO_2 0.16, Nb_2O_5 3.48, Ta_2O_5 0.14, Cl 0.76, H_2O 0.63, $O \equiv Cl$ 0.17, total 98.58 wt.%. The proportion of H_2O was calculated from stoichiometry on the basis of the crystal-structure analysis. The empirical formula of oneillite, based on 78.09 anions as determined in the crystal-structure analysis is: $(Na_{14.37}\mathit{REE}_{1.53}K_{0.20}Sr_{0.03})_{\Sigma 16.13}$ $(Ca_{1.77}\mathit{REE}_{0.59}Na_{0.66})_{\Sigma 3.02}$ $(Mn_{2.76}Y_{0.24})_{\Sigma 3.00}$ $(Fe_{1.43}Mn_{0.96}Zr_{0.25})_{\Sigma 2.64}$ $(Zr_{2.93}Nb_{0.05}Hf_{0.03})_{\Sigma 3.01}$ $(Nb_{0.85}Ta_{0.02})_{\Sigma 0.87}$ $(Si_{24.77}Al_{0.12})_{\Sigma 24.89}$ $O_{73}(O,OH,H_2O)_{3.09}$ $(OH_{1.27}Cl_{0.73})_{\Sigma 2.00}$. $D_{meas.} = 3.20(3)$, $D_{calc.} = 3.22(3)$ g/cm^3. Compared to the eudialyte structure, the unique feature in oneillite is the ordering of Mn and Ca + *REE* at the *M*1 site, which lowers the symmetry from $R3m$ to $R3$. Determination of the crystal structure was dependent on the recognition of a merohedral twin. The *REE* content is the highest hitherto reported, with *REE* occupying almost 50% of *Na*(4).

Keywords: oneillite, eudialyte, new mineral species, crystal structure, merohedral twin, Mont Saint- Hilaire, Quebec, Canada.

SOMMAIRE

L'oneillite, dont la composition idéale est $Na_{15}Ca_3\ Mn_3Fe_3\ Zr_3Nb\ (Si_{25}O_{73})\ (O,OH,H_2O)_3(OH,Cl)_2$, est une nouvelle espèce minérale, membre du groupe de l'eudialyte, provenant du mont Saint-Hilaire, Québec. On la trouve en cristaux brun jaunâtre atteignant un diamètre de 2 mm. Lui sont associés albite, sodalite, pyrite et aegyrine. Elle est transparente à translucide, avec un éclat vitreux et une rayure blanche. Elle est cassante, et sa dureté est 5–6 (échelle de Mohs). Elle est sans clivage, sans plan de séparation, et se casse avec une fracture inégale. L'oneillite est uniaxe négative, avec ω 1.6450(3) et ε 1.6406(3). Elle est trigonale, groupe spatial $R3$, a 14.192(1) et c 29.983(3) Å, V 5230(1) Å^3, $Z = 3$. Les raies les plus intenses du spectre de diffraction X, méthode des poudres [d en Å $(I)(hkl)$] sont: 11.348(44.2)(101), 7.100(33)(110), 6.021(36.1)(021), 5.683(30.8)(202), 4.291(36.5)(205), 3.389(42.9)($\bar{1}41$), 3.199(30.8)(208), 3.150(34.9)($\bar{2}37$), 2.964(100)($\bar{3}45$) et 2.844(89.1)(404). Nous présentons le spectre d'absorption dans l'infra-rouge. Une analyse à la microsonde électronique du cristal choisi pour l'ébauche de la structure cristalline a donné (en %, poids) Na_2O 13.60, K_2O 0.28, CaO 2.90, MnO 7.70, FeO 3.00, SrO 0.09, Al_2O_3 0.18, Y_2O_3 0.78, La_2O_3 2.88, Ce_2O_3 5.14, Pr_2O_3 0.48, Nd_2O_3 1.45, Gd_2O_3 0.20, SiO_2 43.46, ZrO_2 11.44, HfO_2 0.16, Nb_2O_5 3.48, Ta_2O_5 0.14, Cl 0.76, H_2O 0.63, $O \equiv Cl$ 0.17, pour un total de 98.58. La proportion de H_2O a été calculée à partir de la stoechiométrie, telle que confirmée par l'analyse de la structure cristalline. La formule empirique de l'oneillite, sur une base de 78.09 anions aussi déterminée par l'analyse de la structure, est: $(Na_{14.37}\mathit{TR}_{1.53}K_{0.20}Sr_{0.03})_{\Sigma 16.13}$ $(Ca_{1.77}\mathit{TR}_{0.59}Na_{0.66})_{\Sigma 3.02}$ $(Mn_{2.76}Y_{0.24})_{\Sigma 3.00}$ $(Fe_{1.43}Mn_{0.96}Zr_{0.25})_{\Sigma 2.64}$ $(Zr_{2.93}Nb_{0.05}Hf_{0.03})_{\Sigma 3.01}$ $(Nb_{0.85}Ta_{0.02})_{\Sigma 0.87}$ $(Si_{24.77}Al_{0.12})_{\Sigma 24.89}$ $O_{73}(O,OH,H_2O)_{3.09}(OH_{1.27}Cl_{0.73})_{\Sigma 2.00}$. $D_{mes.} = 3.20(3)$, $D_{calc.} = 3.22(3)$ g/cm^3. Par rapport à la structure de l'eudialyte, l'aspect distinctif de l'oneillite est la mise en ordre de Mn et de Ca + *TR* (terres rares) sur le site *M*1. C'est ce qui abaisse la symétrie de $R3m$ à $R3$. L'ébauche de la structure cristalline

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n'a été réussie que par prise en compte d'une macle méroédrique. La teneur en terres rares est la plus élevée qui soit connue; en fait, les terres rares occupent presque 50% du site *Na*(4).

Mots-clés: oneillite, eudialyte, nouvelle espèce minérale, structure cristalline, macle méroédrique, Mont Saint-Hilaire, Québec, Canada.

INTRODUCTION

During a systematic study of the chemistry of the Na-rich zirconosilicate eudialyte (Johnsen & Gault 1997), several private collectors contributed specimens that enabled us to sample a broad spectrum of eudialyte-group minerals from various occurrences. One of these specimens, sent to us by Colonel (Ret.) Quintin Wight of Ottawa, Ontario, was shown to be a unique, Ca-deficient, rare-earth-element-rich member of the eudialyte group. This sample, which is the holotype specimen of the new species described here, oneillite, was collected from the Poudrette Quarry, Mont Saint-Hilaire, Quebec in 1994. The purpose of this paper is to describe this new member of the eudialyte group, its structure and occurrence.

Oneillite is named in honor of John Johnston O'Neill (1886–1966), a geologist with the Geological Survey of Canada and later a professor of geology at McGill University, Montreal, Quebec. He was the first to describe the geology of Mont Saint-Hilaire and the first to report eudialyte and other rare, peralkaline minerals at this locality (O'Neill 1914). A graduate of McGill, Yale and the University of Wisconsin, Dr. O'Neill was a member of the famous Stefansson Arctic Expedition of 1913–1918 and later went on to become Dean of Science and Dean of Engineering at McGill University.

The new mineral species and its name have been approved by the Commission on New Minerals and Mineral Names, IMA. The holotype specimen of oneillite (catalogue no. CMNMC 81565) is housed in the collection of the Canadian Museum of Nature in Ottawa.

OCCURRENCE

Mont Saint-Hilaire is an alkaline intrusive complex and one of the ten Monteregian Hills, a series of genetically related plutons aligned along the St. Lawrence Valley for almost 150 km eastward from Oka to Megantic in the province of Quebec. It has become well-known for its diversity of mineral species (Horváth & Gault 1990); indeed, this diversity is also exhibited in the wide variation in chemistry in the eudialyte-group minerals from this locality (Johnsen & Gault 1997). In addition to oneillite, two other members of the eudialyte group, khomyakovite and manganokhomyakovite, have recently been described from Mont Saint-Hilaire (Johnsen *et al.* 1999).

The holotype specimen was collected in the Poudrette quarry at the contact between a vein of fine-grained albite and the host rock, nepheline syenite. Associated species are albite and sodalite, with minor pyrite and aegirine. Only one specimen was collected containing approximately 100 mg of oneillite; to date no further similar material has been found.

PHYSICAL AND OPTICAL PROPERTIES

Oneillite occurs as yellowish brown, anhedral grains up to 2 mm in diameter in a fine-grained albite matrix. It is vitreous, transparent to translucent, with a white streak. It is nonfluorescent in short- and long-wave ultraviolet light. It is brittle, with no cleavage, no parting and an uneven fracture. It has a Mohs hardness of 5–6. The density of oneillite, measured by suspension in methylene iodide, is 3.20(3) g/cm^3, which compares well with the calculated density, 3.22 g/cm^3.

Oneillite is uniaxial negative, $\omega = 1.6450(3)$ and $\varepsilon = 1.6406(3)$ ($\lambda = 589$ nm); some grains show an anomalous $2V$ up to $15 \pm 2°$ (sample 9 in Johnsen *et al.* 1997). The mineral shows no pleochroism. A Gladstone–Dale calculation gives a compatibility index of –0.004, which is rated as superior (Mandarino 1981).

CHEMICAL COMPOSITION

Chemical analyses were done in wavelength-dispersion (WD) mode on a JEOL 733 electron microprobe using Tracor Northern 5500 and 5600 automation. Data reduction was done with a PAP routine in XMAQNT (pers. commun., C. Davidson, CSIRO). The operating voltage was 15 kV, and the beam current was 20 nA. Data for all elements in the samples were collected for 25 s or 0.50% precision, whichever was attained first. Forty-six elements were sought, but only those detected are reported here. The presence of H_2O in oneillite was confirmed by infrared spectroscopy and crystal-structure analysis. Standards used in the electron-microprobe analyses were: vlasovite (Na$K\alpha$, Si$K\alpha$, Zr$L\alpha$), sanidine (K$K\alpha$), diopside (Ca$K\alpha$), celestine (Sr$L\alpha$), tephroite (Mn$K\alpha$), almandine (Fe$K\alpha$), chrysoberyl (Al$K\alpha$), a set of synthetic *REE* phosphates (La$L\alpha$, Ce$L\alpha$, Pr$L\beta$, Nd$L\alpha$, Gd$L\alpha$), synthetic yttrium iron garnet (YIG) (Y$L\alpha$), synthetic hafnon (Hf$L\alpha$), synthetic $MnNb_2O_6$ (Nb$L\alpha$), synthetic $NiTa_2O_6$ (Ta$L\alpha$), and marialite (Cl$K\alpha$). Data for the standards were collected for 50 s or 0.25% precision, whichever was attained first. For oneillite, two analyses were performed on two separate grains taken from the unique specimen. The composition of the grain selected for structure analysis is reported here along with the range of the results: Na_2O 13.60 (13.60–13.62), K_2O 0.28 (0.23–0.28), CaO 2.90 (2.90–3.13), MnO 7.70 (6.98–7.70), FeO 3.00 (3.00–3.01), SrO 0.09 (0.00–0.09), Al_2O_3 0.18 (0.11–0.18), Y_2O_3 0.78 (0.74–0.78), La_2O_3 2.88 (2.87–2.88), Ce_2O_3 5.14 (5.11–5.14), Pr_2O_3 0.48 (0.42–0.48), Nd_2O_3 1.45 (1.38–1.45), Gd_2O_3 0.20 (0.00–0.20), SiO_2 43.46 (43.46–44.35), ZrO_2 11.44 (11.44–11.48), HfO_2 0.16 (0.00–0.16), Nb_2O_5 3.48 (2.91–3.48), Ta_2O_5 0.14 (0.00–0.14), Cl 0.76 (0.76–0.82), H_2O 0.63, $O \equiv Cl$ 0.17, total 98.58 wt.%. The proportion of H_2O was calculated by stoichiometry from the crystal-structure analysis. The empirical formula of oneillite, based on 78.09 anions, as determined in the crystal-structure analysis, is $(Na_{14.37}\mathit{REE}_{1.53}K_{0.20}Sr_{0.03})_{\Sigma 16.13}$ $(Ca_{1.77}\mathit{REE}_{0.59}Na_{0.66})_{\Sigma 3.02}$ $(Mn_{2.76}Y_{0.24})_{\Sigma 3}$ $(Fe_{1.43}Mn_{0.96}Zr_{0.25})_{\Sigma 2.64}$ $(Zr_{2.93}Nb_{0.05}Hf_{0.03})_{\Sigma 3.01}$ $(Nb_{0.85}Ta_{0.02})_{\Sigma 0.87}$ $(Si_{24.77}Al_{0.12})_{\Sigma 24.89}O_{73}$ $(O,OH,H_2O)_{\Sigma 3.09}$ $(OH_{1.27}Cl_{0.73})_{\Sigma 2}$ or, ideally, $Na_{15}Ca_3Mn_3Fe_3Zr_3Nb(Si_{25}O_{73})(O,OH,H_2O)_3(OH)_2$.

INFRARED ANALYSIS

The infrared spectrum of oneillite (Fig. 1) was obtained using a Bomem Michelson MB–120 Fourier transform infrared (IR) spectrometer with a diamond anvil cell as a microsampling device. The broad absorption bands at 3309 and 1647 cm^{-1} are assigned to the [OH] stretching mode and the $[H_2O]$ bending mode, respectively. The two small bands at 1455 and 1474 cm^{-1} are attributed to the stretching mode of a $[CO_3]$ group. Although the amount of (CO_3) is small, it is sufficient to register on the IR spectrum, which is extremely sensitive to the presence of any molecular vibration modes of a crystal. These two bands are also noted in manganokhomyakovite (Johnsen *et al.* 1999) and kentbrooksite (Johnsen *et al.* 1998). The (CO_3) group can be accommodated within the crystal structure at the *F*1 site. Note that the disordered *F*1 site has bond lengths F1a – F1b of 1.26(2) Å in a trigonal array (bond angle 117.9[6]°), much like that of a (CO_3) group. The bands at 927, 978, and 1013 cm^{-1} are assigned to the symmetric stretching of $[SiO_4]$ and indicate considerable split-

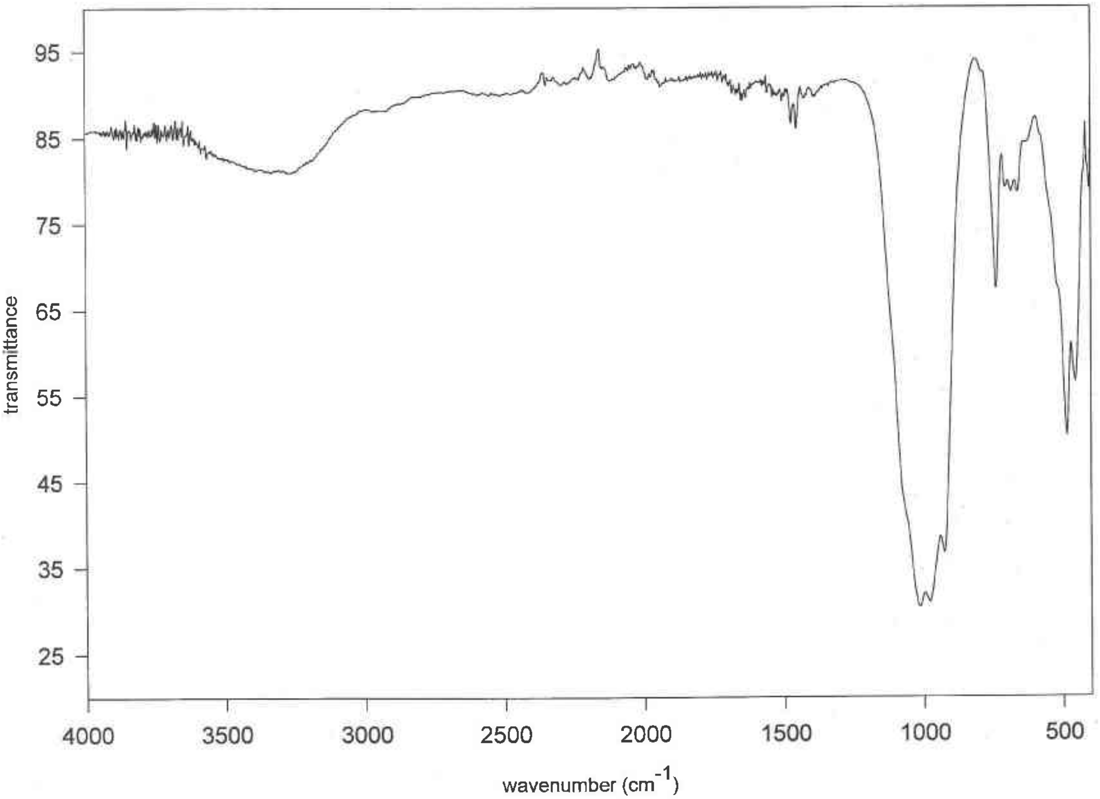

FIG. 1. Infrared spectrum of oneillite.

ting of the [SiO_4] vibration modes, attributable to a structure with crystallographically distinct [SiO_4] groups. Bands at 662, 684, 706 and 741 cm^{-1} are assigned to bending of [SiO_4]. Bands at 406, 455 and 485 cm^{-1} could not be unequivocally assigned, but are likely due to vibrations involving the larger polyhedra, with bond distances greater than 2 Å.

X-RAY CRYSTALLOGRAPHY AND CRYSTAL-STRUCTURE DETERMINATION

X-ray powder-diffraction data collected on a Stoe transmission-type diffractometer are shown in Table 1. Cu$K\alpha_1$ radiation was selected, with a curved Ge monochromator, and data were collected in transmission scan mode on a flat sample. Intensities were measured with a linear position-sensitive detector with an aperture covering a range of 6° in 2θ, a step scan of 0.01°, and a 2θ range 5–90°; the total time of data collection was 65 h. Least-squares refinements based on 81 reflections gave the unit-cell parameters: *a* 14.192(1), *c* 29.983(3) Å.

The crystal-structure analysis of oneillite was done on two different crystals with concordant results. The single crystal of oneillite used for the collection of X-ray-diffraction intensity data presented in this paper is a ground sphere 0.12 mm in diameter. Intensity data were collected on a fully automated Siemens four-circle diffractometer operated at 50 kV and 40 mA with graphite-monochromatized Mo$K\alpha$ radiation. A set of 50 reflections was used to center the crystal and refine the

TABLE 1. ONEILLITE: X-RAY POWDER-DIFFRACTION DATA

I/I_0	d_{obs}	d_{calc}(Å)	*h*	*k*	*l*
44.2	11.348	11.372	1	0	1
19.9	9.997	9.994	0	0	3
28.9	9.480	9.505	0	1	2
33.0	7.100	7.096	1	1	0
16.9	6.387	6.399	1	0	4
36.1	6.021	6.020	0	2	1
5.6	5.789	5.786	$\bar{1}$	2	3
30.8	5.683	5.686	2	0	2
6.0	5.377	5.389	0	1	5
7.0	4.998	4.997	0	0	6
36.5	4.291	4.292	2	0	5
21.9	4.086	4.086	$\bar{1}$	2	6
28.2	3.948	3.948	$\bar{2}$	3	4
5.8	3.670	3.672	$\bar{1}$	3	5
8.0	3.581	3.585	0	1	8
18.5	3.549	3.548	2	2	0
21.4	3.512	3.514	0	2	7
42.9	3.389	3.387	$\bar{1}$	4	1
13.3	3.324	3.324	$\bar{3}$	4	2
30.8	3.199	3.200	2	0	8
34.9	3.150	3.149	$\bar{2}$	3	7
4.1	3.107	3.103	$\bar{1}$	4	4
4.8	3.058	3.057	4	0	1
29.9	3.013	3.016	$\bar{1}$	2	9
		3.010	0	4	2
100.0	2.964	2.963	$\bar{3}$	4	5
14.3	2.892	2.893	$\bar{2}$	4	6
89.1	2.844	2.843	4	0	4
5.5	2.808	2.807	$\bar{3}$	5	1
7.4	2.770	2.771	$\bar{2}$	5	2
10.2	2.694	2.695	0	2	10
12.4	2.667	2.667	$\bar{1}$	4	7
10.6	2.641	2.639	$\bar{3}$	5	4
29.4	2.585	2.585	0	3	9
12.8	2.521	2.522	$\bar{3}$	4	8
		2.519	$\bar{2}$	3	10
4.4	2.498	2.498	0	0	12
		2.497	4	0	7
11.0	2.375	2.376	0	4	8
13.3	2.366	2.365	3	3	0
11.0	2.317	2.316	$\bar{2}$	6	1
4.5	2.267	2.267	1	0	13
7.4	2.253	2.253	$\bar{2}$	5	8
		2.251	$\bar{1}$	4	10
4.2	2.216	2.218	$\bar{2}$	6	4
8.8	2.184	2.184	$\bar{1}$	6	2
8.9	2.167	2.166	$\bar{4}$	6	5
15.2	2.146	2.146	4	0	10
11.9	2.130	2.132	0	5	7
		2.129	$\bar{3}$	4	11
5.9	2.048	2.048	6	0	0
6.1	2.042	2.043	$\bar{2}$	4	12
		2.042	$\bar{2}$	6	7
6.9	2.016	2.016	$\bar{4}$	7	1
8.6	2.006	2.006	0	6	3
11.8	1.975	1.974	$\bar{4}$	6	8
6.8	1.932	1.931	$\bar{5}$	7	3
4.0	1.909	1.910	$\bar{1}$	4	13
7.6	1.901	1.902	$\bar{1}$	6	8
		1.901	0	5	10
9.6	1.897	1.895	0	6	6
6.5	1.792	1.792	0	2	16
10.6	1.756	1.757	0	4	14
6.0	1.744	1.745	0	6	9
		1.744	$\bar{5}$	8	2
5.8	1.710	1.709	$\bar{3}$	8	4
8.2	1.696	1.695	2	0	17
8.4	1.694	1.694	$\bar{5}$	7	9
		1.693	$\bar{2}$	8	2
6.6	1.641	1.642	$\bar{1}$	4	16
5.6	1.622	1.622	$\bar{1}$	2	18
7.9	1.600	1.600	4	0	16
8.7	1.590	1.590	$\bar{5}$	8	8
		1.589	$\bar{1}$	7	10
4.0	1.574	1.574	$\bar{4}$	6	14
5.7	1.562	1.561	$\bar{3}$	5	16
5.8	1.545	1.546	$\bar{5}$	7	12
5.4	1.536	1.537	$\bar{1}$	6	14
4.2	1.494	1.494	$\bar{2}$	3	19
		1.494	$\bar{7}$	9	2
7.8	1.477	1.477	$\bar{5}$	9	7
5.2	1.431	1.430	0	6	15
5.2	1.427	1.427	$\bar{1}$	3	20
6.2	1.408	1.408	$\bar{4}$	10	1

Stoe diffractometer data, transmission mode on flat sample; Cu$K\alpha_1$ radiation.
Indexing based on cell: $a = 14.192(1)$, $c = 29.983(3)$ Å, $V = 5230(1)$ A^3.

TABLE 2. ONEILLITE: CRYSTAL DATA AND STRUCTURE REFINEMENT

Sample identification	oneillite (sample 5 in Johnsen & Grice [1999])
Wavelength	0.71073 Å
Crystal system; space group	Trigonal; *R*3
Unit-cell dimensions, 4-circle data	$a = 14.2084(8)$ Å, $c = 29.959(3)$ Å
Volume	5237.8(7) Å^3
Crystal size	sphere diameter 0.12 mm
θ range for data collection	2.04 to 30.06°
Index ranges	$0 \leq h \leq 17, 0 \leq k \leq 17, -42 \leq l \leq 42$
Reflections collected	3815
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3803 / 0 / 426
Goodness-of-fit on F^2	1.043
Final *R* indices [$I > 2\sigma(I)$]	$R1 = 0.032$, $wR2 = 0.072$
R indices (all data)	$R1 = 0.036$, $wR2 = 0.074$
Isotropic refinement	$R1$ / $wR2$: 0.070 / 0.133
Largest diff. peak and hole	1.01 and -0.84 e·A^{-3}
ψ merge before/after	1.16 / 0.87
$\lvert E^2 - 1 \rvert$	0.702
effect of TWIN command	$R1$: 0.107 → 0.032

cell parameters. Assuming a non-centrosymmetric rhombohedral cell, one asymmetric unit of intensity data was collected (*i.e.*, $+h+k \pm l$) up to 2θ = 60° using a θ:2θ scan-mode, with scan speeds inversely proportional to intensity, varying from 3 to 29.3°/minute. The data collection consisted of 3815 reflections with more than 85% observed (*i.e.*, $F_o > 4\sigma F_o$). Information relevant to the data collection and structure determination is given in Table 2.

For the ellipsoidal absorption correction, 15 intense diffraction-maxima in the range 12 to 60° 2θ were chosen for Ψ diffraction-vector scans after the method of North *et al.* (1968). The converging *R* for the Ψ-scan dataset decreased from 1.16% before the absorption correction to 0.87% after the absorption correction. The excellent convergence attests to the near-spherical shape of the crystal. The minimum and maximum transmission factors for the linear-absorption corrections are 0.604 and 0.585, respectively. Assigning phases to a set of normalized structure-factors gave a mean value $\mid E^2 - 1 \mid$ of 0.702, strongly indicative of a non-centrosymmetric space-group. The $\mid E^2 - 1 \mid$ value is significantly lower than for other samples of eudialyte, which have values in the range of 0.79–1.04 (Johnsen & Grice 1999). The incongruously low value of $\mid E^2 - 1 \mid$ for oneillite is a result of merohedral twinning (Herbst-Irmer & Sheldrick 1998). The structure was solved and refined in space group *R*3. The structure refined to $R1 = 0.107$ both in *R*3*m* and *R*3 until it was recognized that the *m*-plane in ordinary eudialyte is a twin plane in oneillite. After the introduction of the twin operator, the *R*1 index dropped to 0.032. Reduction of the intensity data, structure determination and initial refinement of the structure were done with the SHELXTL (Sheldrick 1990) package of computer programs. The final refinements were done with the SHELXL–93 program (Sheldrick 1993). The strategy applied to the final stages of the refinement as well as the site-assignment procedure were described in detail by Johnsen & Grice (1999).

The final atomic coordinates, isotropic displacement parameters and selected bond-lengths for the oneillite structure are presented by Johnsen & Grice (1999, sample 5). Lists of observed and calculated structure-factors and of anisotropic displacement factors have been submitted to the Depository of Unpublished Data, CISTI, National Research Council of Canada, Ottawa, Ontario K1A 0S2, Canada.

DESCRIPTION AND DISCUSSION OF THE STRUCTURE

Oneillite is a member of the eudialyte group. As described by Johnsen & Grice (1999), the structure of eudialyte-group minerals consists of layers of six-membered rings of [$M(1)O_6$] octahedra (mainly Ca) joined by [$M(2)O_n$] polyhedra (Fe or Mn) and sandwiched between two pseudo-centrosymmetrically related layers of three-membered and nine-membered silicate rings forming a 2:1 composite layer. The 2:1 composite layers are cross-linked by Zr in octahedral coordination and are related to one another in accordance with the rhombohedral symmetry. Voids in the open structure are filled with five distinct [$Na\Phi_n$] polyhedra, of which the [$Na(4)\Phi_n$] polyhedron is particularly suitable as a host of relatively heavy elements such as *REE* and Sr. *M*(3) and *Si*(7) are two central sites of the two crystallographically distinct nine-membered silicate rings, and related by the substitution $^{[6]}M(3) + {}^{[4]}Si(7) \Leftrightarrow 2^{[4]}Si(7)$, in which *M*(3) typically is occupied by Nb.

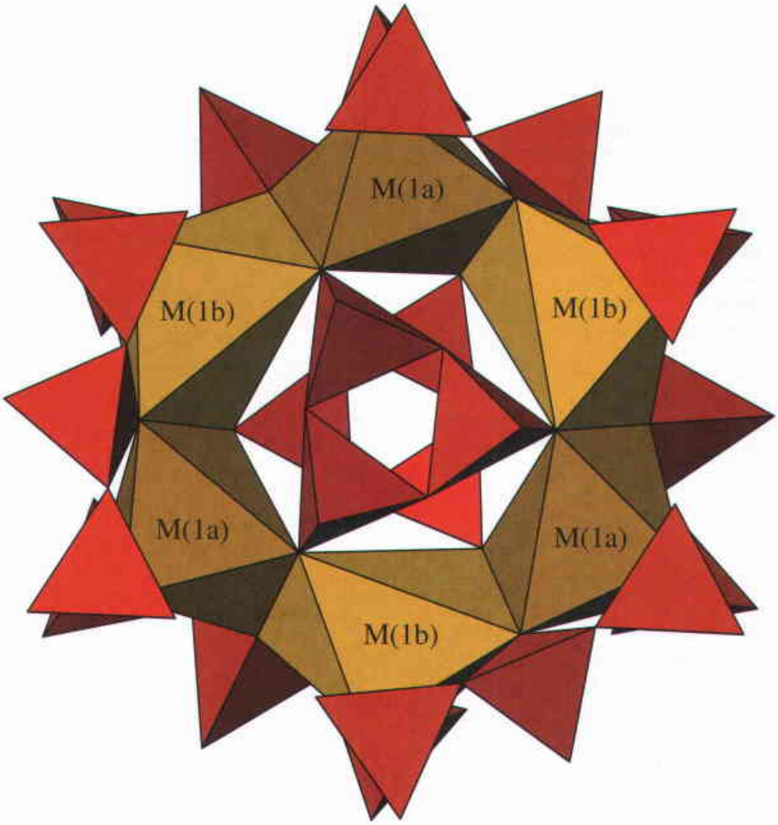

FIG. 2. A six-fold ring of alternating [$M(1a)O_6$] and [$M(1b)O_6$] octahedra with attached [SiO_4] tetrahedra in oneillite viewed along [001].

The principal property that distinguishes oneillite from other members of the eudialyte group is the cation ordering of $M(1)$ into two distinct sites $M(1a)$ and $M(1b)$ alternating in the six-fold ring, which destroys the mirror planes (Fig. 2). Ca is normally the primary element in $M(1)$ with Mn, *REE* and Y as the common substituents. As the ratio Ca/(Ca + Mn + *REE* + Y) in $M(1)$ decreases, the [$M(1)O_6$] octahedron, with an average bond-length equal to 2.35(2) Å, becomes more distorted until it splits into a relatively small and a relatively large octahedron. The smaller [$M(1a)O_6$] octahedron, with an average bond-length of 2.227 Å, accommodates mostly Mn, whereas the larger [$M(1b)O_6$] octahedron, with an average bond-length of 2.431 Å, accommodates Ca and the *REE* (Johnsen & Grice 1999).

In oneillite, *REE* are also accommodated in two of the Na sites, primarily in *Na*(4), where *REE* constitute close to 50% of the population. In total, the *REE* content (10.15 wt% REE_2O_3, ~2.12 atoms per formula unit (*apfu*) *REE*, Y_2O_3 not included) is the highest content hitherto reported in the literature. Oneillite is further characterized by an exceptionally low content of Ca, only 1.77 *apfu*, and contents of Mn and Nb that are among the highest reported. The concept of a solid-solution series between the classic eudialyte, rich in Si, Ca, Fe and Cl, and kentbrooksite (Johnsen *et al.* 1998), rich in Nb, *REE*, Mn and F, as presented by Johnsen & Gault (1997), was modified by Johnsen & Grice (1999), who proposed that the series extends beyond kentbrooksite to the eudialyte-group mineral now described as oneillite.

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REFERENCES

HERBST-IRMER, R. & SHELDRICK, G.M. (1998): Refinement of twinned structures with SHELXL97. *Acta Crystallogr.* **B54**, 443-449.

HORVÁTH, L. & GAULT, R.A. (1990): The mineralogy of Mont Saint-Hilaire, Quebec. *Mineral. Rec.* **21**, 284-360.

JOHNSEN, O. & GAULT, R.A. (1997): Chemical variation in eudialyte. *Neues Jahrb. Mineral., Abh.* **171**, 215-237.

________, ________, GRICE, J.D. & ERCIT, T.S. (1999): Khomyakovite and manganokhomyakovite, two new members of the eudialyte group from Mont Saint-Hilaire, Quebec, Canada. *Can. Mineral.* **37**, 893-899.

________ & GRICE, J.D. (1999): The crystal chemistry of the eudialyte group. *Can. Mineral.* **37**, 865-891.

________, ________ & GAULT, R.A. (1998): Kentbrooksite from the Kangerdlugssuaq intrusion, East Greenland, a new Mn–REE–Nb–F end-member in a series within the eudialyte group: description and crystal structure. *Eur. J. Mineral.* **10**, 207-219.

________, PETERSEN, O.V. & GAULT, R.A. (1997): Optical data on minerals of the eudialyte group: discussion of the eucolite – mesodialyte – eudialyte terminology. *Neues Jahrb. Mineral., Monatsh.*, 371-383.

MANDARINO J.A. (1981): The Gladstone–Dale relationship. IV. The compatibility concept and its application. *Can. Mineral.* **19**, 441-450.

NORTH, A.T.C., PHILLIPS, D.C. & MATHEWS, F.S. (1968): A semi-empirical method of absorption correction. *Acta Crystallogr.* **A24**, 351-359.

O'NEILL, J.J. (1914): St. Hilaire (Beloeil) and Rougemont Mountains, Quebec. *Geol. Surv. Can., Mem.* **43**.

SHELDRICK, G.M. (1990): *SHELXTL, a Crystallographic Computing Package* (revision 4.1). Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin.

________ (1993): *SHELXL–93. Program for the Refinement of Crystal Structures.* University of Göttingen, Göttingen, Germany.

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