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AGRELLITE, A NEW ROCK-FORMING MINERAL IN REGIONALLY METAMORPHOSED AGPAITIC ALKALIC ROCKS

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ABSTRACT

Agrellite ($NaCa_2Si_4O_{10}F$) occurs in a regionally metamorphosed agpaitic rock complex in Villedieu Township, Témiscaming County, Québec, Canada. It is found in pegmatitic lenses and pods and in mafic gneisses composed principally of albite, microcline, alkalic amphibole (kataphorite-arfvedsonite), aegirine-augite with or without eudialyte and nepheline. In addition, the following minerals are found in small but widely varying amounts: hiortdahlite, other members of the wöhlerite group, mosandrite, miserite, britholite, vlasovite, calcite, fluorite, clinohumite, norbergite, zircon, biotite, phlogopite, galena and a new unnamed mineral ($CaZrSi_2O_7$). The commonest occurrence is in the pegmatitic pods which have probably resulted from partial melting of the agpaitic rocks during amphibolite-facies metamorphism. Agrellite forms white crystals from a few mm up to 100 mm in length; color white to greyish or greenish white, lustre pearly on cleavages, H. 5.5, cleavages $\{110\}$ and $\{1\bar{1}0\}$ excellent, $\{010\}$ poor, biaxial negative, $2V$ 47°, n_α 1.567, n_β 1.579, n_γ 1.581, optic axial plane approximately (010). The chemical composition (in wt. %) is SiO_2 58.83, TiO_2 0.01, Al_2O_3 0.10, Fe_2O_3 0.11, MnO 0.25, CaO 25.70, SrO 0.16, BaO 0.06, MgO 0.02, ZrO_2 0.18, *RE* 3.84, Na_2O 7.90, K_2O 0.22, H_2O+ 0.4, F 4.45, sum 102.23 − (O = F) 1.87, total 100.36. Rare earths are CeO_2 1.13, Y_2O_3 1.07, La_2O_3 0.54, Pr_2O_3 0.10, Nd_2O_3 0.41, Sm_2O_3 0.12, Eu_2O_3 0.02, Gd_2O_3 0.15, Dy_2O_3 0.14, Ho_2O_3 0.03, Er_2O_3 0.07, Tm_2O_3 0.01, Yb_2O_3 0.04, Lu_2O_3 0.01. The calculated formula is $(Na_{4.06}K_{0.07})(Ca_{7.30}RE_{0.47})(Mn, Fe, Sr, Ba, Mg, Zr)_{0.14}(Si_{15.61}Al_{0.03})O_{39.70}(F_{3.73}OH_{0.71})$ or $(Na,K)_{1.03}(Ca, RE, etc.)_{1.94}Si_{3.91}O_{9.93}(F, OH)_{1.11}$, $Z = 4$, S.G. calc. 2.887, measured 2.902. Single crystal X-ray study indicates that the mineral is triclinic; the true cell has *a* 7.773, *b* 18.942, *c* 6.984Å, *α* 90.148°, *β* 116.84°, *γ* 94.145°, *V* 914.5Å³, lattice *P*. An alternative double-volume unit cell has almost perfect monoclinic geometry, and the strongest reflections show nearly perfect monoclinic symmetry. The strongesy powder lines measured are 3.44(s) (200, $\bar{1}50$), 3.33(s) ($\bar{2}20$), 3.19(vs) (150, 051), 3.14(vs) (220, 060, $\bar{2}02$, 002), 2.58(s) ($\bar{2}\bar{5}1$, $\bar{1}70$). The name is for Dr. Stuart O. Agrell, Department of Mineralogy and Petrology, University of Cambridge, England. Pronunciation is a-grell'ĭte.

SOMMAIRE

L'agrellite ($NaCa_2Si_4O_{10}F$) se rencontre dans un complexe de roches agpaitiques, à métamorphisme régional, dans le canton de Villedieux, comté de Témiscamingue, Québec, Canada. Elle se trouve dans des lentilles pegmatitiques et dans des gneiss mafiques composés principalement d'albite, de microcline, d'amphibole alcaline (kataphorite-arfvedsonite), d'aegirine-augite avec ou sans eudialyte et néphéline. De plus, les minéraux suivants se trouvent en petites quantités, d'ailleurs très variables: hiortdahlite, d'autres membres du groupe wöhlérite, mosandrite, misérite, britholite, vlasovite, calcite, fluorine, clinohumite, norbergite, zircon, biotite, phlogopite, galène et un nouveau minéral sans non ($CaZrSi_2O_7$). L'agrellite se présente le plus fréquemment dans les lentilles pegmatitiques qui proviennent probablement de la fusion partielle des roches agpaitiques au cours du métamorphisme du faciès amphibolite.

Elle form des cristaux de dureté 5½ de quelques mm à 100mm de long, qui passent du blanc au gris ou au blanc verdâtre, ont un éclat nacré sur les clivages: $\{110\}$ et $\{1\bar{1}0\}$, excellents; $\{010\}$, indistint. Optiquement elle est biaxe négative, $2V$ 47°, n_α 1.567, n_β 1.579, n_γ 1.581, plan des axes optiques voisin de (010). La composition chimique pourcentages en poids est SiO_2 58.83, TiO_2 0.01, Al_2O_3 0.10, Fe_2O_3 0.11, MnO 0.25, CaO 25.70, SrO 0.16, BaO 0.06, MgO 0.02, ZrO_2 0.18, *TR* 3.84, Na_2O 7.90, K_2O 0.22, H_2O + 0.4, F 4.45, total 102.23 − (O = F) 1.87, total 100.36. Les terres rares sont: CeO_2 1.13, Y_2O_3 1.07, La_2O_3 0.54, Pr_2O_3 0.10, Nd_2O_3 0.41, Sm_2O_3 0.12, Eu_2O_3 0.02, Gd_2O_3 0.15, Dy_2O_3 0.14, Ho_2O_3 0.03, Er_2O_3 0.07, Tm_2O_3 0.01, Yb_2O_3 0.04, Lu_2O_3 0.01. Formule calculée: $(Na_{4.06}K_{0.07})$ $(Ca_{7.30}TR_{0.47})$ $(Mn, Fe, Sr, Ba, Mg, Zr)_{0.14}$ $(Si_{15.61}Al_{0.03})$ $O_{39.70}$ $(F_{3.73}OH_{0.71})$ ou $(Na, K)_{1.03}$ $(Ca, TR, etc.)_{1.94}Si_{3.91}$ $O_{9.93}$ $(F, OH)_{1.11}$, $Z = 4$, densité calculée 2.887, mesurée 2.902. L'étude par rayons X d'un cristal unique indique un minéral triclinique; la maille vraie possède les dimensions *a* 7.773, *b* 18.942, *c* 6.984Å, α 90.148°, β 116.84°, γ 94.145°, *V* 914.5Å³, avec réseau *P*. Il existe une maille double quasi monoclinique, et les réflexions les plus fortes soulignent cette pseudosymétrique presque parfaite. Les raies de poudre les plus fortes ont été mesurées aux espacements suivants: 3.44(F) $(200, \bar{1}50)$, 3.33(F) $(\bar{2}20)$, 3.19 (FF) (150, 051), 3.14 (FF) $(220, 060, \bar{2}02, 002)$, 2.57 (F) $(\bar{2}\bar{5}1, \bar{1}70)$. Le nom honore le Dr Stuart O. Agrell du Département de minéralogie et de pétrologie de l'Université de Cambridge, en Angleterre.

(Traduit par le journal)

INTRODUCTION

Agpaitic alkalic rocks are relatively uncommon and in every case they are characterized by a wealth of unusual minerals. Among the better known occurrences are the plutonic intrutions of Ilimaussaq in Greenland and Lovozero in the U.S.S.R. All the examples described until recently have been unmetamorphosed igneous rocks but two examples are now known in Canada where such rocks have undergone regional metamorphism in the amphibolite facies. The first of these is a group called the Red Wine Complexes centred at Lat. 62°30′W, Long. 54°10′N, in central Labrador (Currie *et al.* 1975), where the rocks have been largely transformed into gneisses characterized by an abundance of arfvedsonite, jadeitic pyroxene (up to 70 percent jadeite), titanian ferro-omphacite, titanian aegirine, aenigmatite and varying amounts of albite, microcline and nepheline. The second occurrence is the Kipawa Complex on the Kipawa River, Villedieu Township, Témiscaming County, Québec, at Lat. 78°29′31″ W, Long. 45°47′49″ N, and it is in this complex that agrellite occurs. Type specimens of agrellite are preserved in the collections of the University of Toronto, Department of Geology (Petrology Collection); Royal Ontario Museum; Smithsonian Institution; Department of Mineralogy and Petrology, University of Cambridge; British Museum of Natural History; National Museum of Canada; Geological Survey of Canada; Institute for the Mineralogy, Geochemistry and Crystal Chemistry of the Rare Elements, Moscow, USSR.

GENERAL GEOLOGY

The complex is poorly exposed in forested country. The commonest rocks are banded gneisses composed of albite, microcline, alkalic amphibole (arfvedsonite and kataphorite), aegirine-augite, nepheline and eudialyte. Eudialyte is concentrated in thin layers up to 10 mm thick. Calcite and fluorite are ubiquitous accessories and locally assume essential proportions. Within the gneisses are minor carbonate rocks of uncertain character composed of calcite, diopside, phlogopite, clinohumite, norbergite and zircon. Other gneisses are rich in biotite. Most of the gneisses contain the rarer minerals hiortdahlite, other members of the wöhlerite group, mosandrite, miserite, britholite, vlasovite, the new unnamed mineral $CaZrSi_2O_7$, accessory galena, and several other as yet unidentified minerals. Some gneisses are composed of more than seventy percent of agrellite. Pegmatitic pods and lenses within the gneisses are composed of these minerals and agrellite, but their proportions vary considerably. A common type of pegmatitic lens consists of agrellite in interlocking crystals up to 100 mm in length together with eudialyte up to 50 mm across, microcline, mosandrite and a small amount of amphibole. Other types are primarily eudialyte with amphibole and mosandrite, or eudialyte with mosandrite and vlasovite, the latter in crystals up to 100 mm in size. Accounts of vlasovite, the new mineral $CaZrSi_2O_7$, and hiortdahlite from Kipawa are given by Gittins *et al.* (1973) and Aarden & Gittins (1974). The gneisses are complexly folded but the pegmatitic pods show no evidence of deformation and frequently contain minerals displaying euhedral character. It seems very likely that partial melting has occurred during regional metamorphism and that the pegmatitic rocks represent the crystallization of the resultant liquid. Intergrowths of calcite and fluorite have

TABLE 1. ANALYSES OF AGRELLITE

	1	2	3	4		5
SiO_2	57.79	57.90	58.83	58.83		
TiO_2	0.01			0.01	CeO_2	1.13
Al_2O_3	1.32	0.80	0.10	0.10	Y_2O_3	1.07
Fe_2O_3	0.11 *	0.42 *		0.11 *	La_2O_3	0.54
MnO	0.25	0.20		0.25	Pr_2O_3	0.10
CaO	25.70	26.43	35.94	25.70	Nd_2O_3	0.41
SrO	0.16 * *			0.16 * *	Sm_2O_3	0.12
BaO	0.06 * *			0.06 * *	Eu_2O_3	0.02
MgO	0.02			0.02	Gd_2O_3	0.15
ZrO_2	0.18			0.18	Dy_2O_3	0.14
RE	2.57	3.84	3.61	3.84	Ho_2O_3	0.03
Na_2O	7.90	7.13		7.90	Er_2O_3	0.07
K_2O	0.22	0.20		0.22	Tm_2O_3	0.01
H_2O +	0.4	0.17		0.4	Yb_2O_3	0.04
F	4.45 +	4.60		4.45	Lu_2O_3	0.01
	101.14	101.69	98.48	102.23		
O=F	1.87	1.93		1.87		
	99.27	99.76		100.36		

1. Classical wet chemical analysis; analyst J. Gittins (except for SrO and BaO as noted below)
2. Classical wet chemical analysis; analyst A.W. Bykova, IMGRE, Moscow, U.S.S.R. (Except for rare earths by spectrographic methods)
3. Electron microprobe analysis by E.L. Gasparrini, University of Toronto
4. Most probable composition (combined sources)
5. Rare earths by spectrographic analysis; analyst L. Loginova, IMGRE, Moscow, U.S.S.R.

* Total iron expressed as Fe_2O_3

* * Analyst: C.O. Ingamells, preliminary figure only

\+ Analyst: J. Gittins 4.28, 4.61, Schwarzkopf Microanalytical Laboratory 4.30, 4.60

a texture identical to that which results from eutectic crystallization in the system calcite-fluorite (Gittins & Tuttle 1964) and probably result from the crystallization of anatectic melts. Whether agrellite is a mineral of primary igneous crystallization that has undergone subsequent metamorphic recrystallization, or has formed during regional metamorphism, is not known.

CHEMICAL COMPOSITION

Chemical analyses of agrellite are tabulated in Table 1. Because of the large size of the crystals, concentrates of very high purity are readily prepared for analysis. Classical wet chemical methods were employed for SiO_2, ΣRE, CaO, SrO, BaO and MgO; spectrophotometry for TiO_2, MnO and total Fe as Fe_2O_3; the Penfield method for H_2O+, and flame photometry for Na_2O and K_2O. Particular difficulties were encountered with SiO_2, Al_2O_3 and the rare earths. Because of high F content, silica tends to volatilize as SiF_4 during the initial fusion of the mineral in Na_2CO_3, and low values always result. Accordingly, the SiO_2 value determined by electron microprobe analysis has been accepted as the most reliable. The classical ammonia precipitation of the R_2O_3 group is complicated in the case of agrellite by the presence of the rare earths. These are precipitated to varying degrees according to the pH of the solution and no adequate control is possible. To overcome this difficulty, the rare earths were determined as a group by the oxalate precipitation method. They were also determined individually by emission spectroscopy. Al_2O_3, was determined by electron microprobe analysis. ZrO_2 was determined by the mandelic acid method. Fluorine was determined by the method of steam distillation and thorium nitrate titration. H_2O+ is quoted to only one decimal place because it is so much less abundant than fluorine that the latter causes interference in the Penfield method.

An independent analysis by A. W. Bykova was kindly arranged by E. I. Semenov of IMGRE, Moscow, U.S.S.R. Spectrographic analysis of the rare earths was also carried out in the same institute and the results are given in Table I. A different specimen was used for the Russian analysis. The calculated mineral formula is

$$(Na_{4.06}K_{0.07})(Ca_{7.30}RE_{0.47})(Mn,Fe,Sr,Ba,Mg,Zr)_{0.14}(Si_{15.61}Al_{0.03})O_{39.70}(F_{3.73}OH_{0.71}).$$

This may be simplified to

$$(Na,K)_{1.03}(Ca,RE,\ etc.)_{1.94}Si_{3.91}O_{9.93}(F,OH)_{1.11}$$

and the general formula taken as

$$NaCa_2Si_4O_{10}F.$$

X-RAY DIFFRACTION STUDY

Unit cell and symmetry

Single crystals of agrellite were examined initially by standard photographic methods on oscillation, Weissenberg and precession cameras. The symmetry was established as triclinic, and approximate unit cell dimensions were obtained. The cell dimensions were refined by least-squares analysis of 2θ values obtained for 20 reflections on a Picker automatic single-crystal diffractometer, with the results and estimated standard deviations shown in Table 2. The elongation of the crystals is taken as the c_o axis.

TABLE 2. CRYSTALLOGRAPHY OF AGRELLITE

Triclinic true* cell	Pseudo-monoclinic true cell	Pseudo-monoclinic sub-cell
$a_0 = 7.773(1)\text{Å}$	$a_1 = [201]_0 = 13.871\text{Å}$	$a_2 = \frac{1}{2}a_1$
$b_0 = 18.942(1)$	$b_1 = c_0 = 6.984$	$b_2 = \frac{1}{2}b_1$
$c_0 = 6.984(1)$	$c_1 = b_0 = 18.942$	$c_2 = c_1$
$\alpha_0 = 90.148(5)°$	$\alpha_1 = \alpha_0 = 90.148°$	$\alpha_2 = \alpha_1$
$\beta_0 = 116.84(1)°$	$\beta_1 = 94.795°$	$\beta_2 = \beta_1$
$\gamma_0 = 94.145(7)°$	$\gamma_1 = 90.145°$	$\gamma_2 = \gamma_1$
Lattice *P*	Lattice *C*	Lattice *I*
$V_0 = 914.5(1)\text{Å}^3$	$V_1 = 2V_0$	$V_2 = \frac{1}{2}V_0$
$Z_0^{**} = 4$	$Z_1 = 8$	$Z_2 = 2$

* This unit cell was chosen at the start of the investigation as (apparently) the reduced cell. After the parameters were refined it turned out not to be the reduced cell, but it was retained for convenience nevertheless. The reduced cell has $a = [101]_0 = 7.757$, $b = [0\bar{1}0]_0 = 18.942$, $c = [00\bar{1}]_0 = 6.984\text{Å}$, $\alpha = 90.148°$, $\beta = 116.61°$, $\gamma = 85.71°$.

Figures in parentheses represent the standard deviation, in terms of least units cited to their immediate left, as given by the least-squares refinement.

**Z = number of units of $NaCa_2Si_4O_{10}F$ per cell.

TABLE 3. *X*-RAY POWDER DATA FOR AGRELLITE

d(obs)	*I**	$(hkl)_0$	*d*(calc)**
9.45	W	020	9.439
6.66	W	110	6.671
4.71	W	040	4.719
3.83	M	101	3.842
		$\bar{2}11$	3.824
3.73	VW	$\bar{2}\bar{1}1$	3.725
3.44	S	200	3.456
		$\bar{1}50$	3.435
3.33	S	$\bar{2}20$	3.335
3.19	VS	$\bar{1}50$	3.204
		051	3.173
3.14	VS	220	3.162
		060	3.146
		$\bar{2}02$	3.120
		002	3.114
3.05	W	$\bar{1}\bar{3}2$	3.059
		$\bar{1}32$	3.054
2.99	VW	$\bar{2}22$	2.994
		$0\bar{2}2$	2.992
2.92	VW	$\bar{2}\bar{2}2$	2.933
		022	2.923
2.78	VW	251	2.792
		$\bar{1}\bar{6}1$	2.771
2.68	VW	240	2.685
2.65	W	$0\bar{4}2$	2.648
		$\bar{2}42$	2.645
2.58	S	$\bar{2}\bar{5}1$	2.610
		$\bar{1}70$	2.585
2.53	VW	$\bar{2}\bar{4}2$	2.562
		$\bar{1}52$	2.560
		042	2.553
2.43	W		
2.36	VW		
2.31	S		
2.26	M		
2.14	VW		
2.11	W		
2.04	MS		
2.00	VW		

d-values in Å. Photographic data, 114.6 mm diameter Philips camera. Filtered Cu radiation. Many more reflections with *d* less than 2.0Å were observed.

* Visually estimated intensities. VW = very weak, W = weak, M = medium, S = strong, V = very strong.

***d*- values calculated from cell dimensions in first column of Table 2.

An alternative double-volume unit cell can be chosen which has almost perfect monoclinic geometry; dimensions are also given in Table 2.

Oscillation photographs taken with c_0 as rotation axis showed that l_0 = even layer lines were much stronger than the l_0 = odd ones, and also that spots on the strong layer lines (but not those on the weak ones) appeared to be related by a mirror plane of symmetry perpendicular to c_0. These features, strongly reminiscent of the situation with wollastonite and pectolite crystals, were confirmed by Weissenberg and precession photographs, and these also revealed that the agrellite triclinic cell has not only pseudo-halving of the c_0-axis, but also shows a pseudo-*I* lattice type. The subcell which would result if only the strongest reflections were considered is very nearly monoclinic in symmetry as well as in geometry; the parameters are included in Table 2.

Full intensity data have been collected and the crystal structure is under investigation by Bown & Gibbs.

Powder data

Interplanar spacings measured from standard powder photographs are given in Table 3, together with visual estimates of line intensities. The photographs showed some preferred orientation. In assigning indices to some of these lines, account has been taken of the intensities of the reflections as seen on single-crystal photographs.

INFRARED SPECTRUM

The infrared spectrum of agrellite is given in Figure 1.

PHYSICAL AND OPTICAL PROPERTIES

Agrellite forms crystals from a few mm up to 100 mm in length. Color is white to greyish or greenish white; lustre pearly on cleavages. Cleavage {110} and {1$\bar{1}$0} excellent, {010} poor. Hardness 5.5, specific gravity (measured by heavy liquid suspension and subsequent determination of the liquid specific gravity) 2.902, calculated 2.887.

All measurements of optical properties were made in sodium light. As with the single crystal X-ray study the *c*-axis was chosen to coincide with the elongation of the crystals. Properties

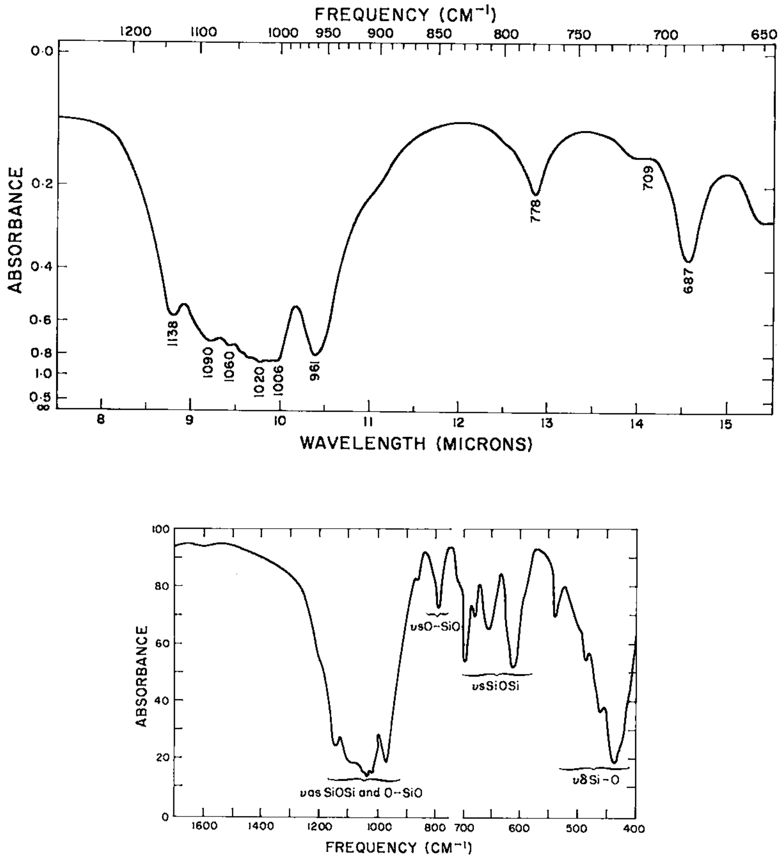

FIG. 1. Infrared spectra of agrellite.
(a) Schwarzkopf Microanalytical Laboratory, Woodside, N.Y., U.S.A.
(b) Department of Mineralogy, University of Kiev, U.S.S.R.
Absorption bands:
νas— **1145**, 1090, 1033, 1012, **967**, 860;
νs O-SiO – 786; γs SiOSi – **698**, 677, **653**, **613**;
νs Si-O – **538**, 497, 485, 460, 436, 420 sh.

are:
$n\alpha$ 1.567, $n\beta$ 1.579, $n\gamma$ 1.581, $n\gamma$–$n\alpha$ 0.014, $2V\alpha$ negative 47°, OAP≈(010), colorless in thin section.

Orientation of the principal vibration directions is shown in Figure 2 and is defined by the following angles:

	ϕ	φ
$\perp$ (010)	0°	90°
$\perp$ (110)	66°	90°
$\perp$ $(\bar{1}10)$	106°	90°
X	274°	88
Y	184°	84°
Z	23°	6°

Extinction angles for fragments lying on

(010)	$c \wedge z'$	=	2°
(110)	$c \wedge z'$	=	0.5°
$(1\bar{1}0)$	$c \wedge z'$	=	5°

STABILITY

No systematic study of the stability has yet been attempted. Attempts to synthesize agrellite from oxide mixes have so far failed. Preliminary study of the system Na$_2$O-CaO-SiO$_2$-F suggests that agrellite has a primary phase volume adjacent to that of wollastonite and that its crys-

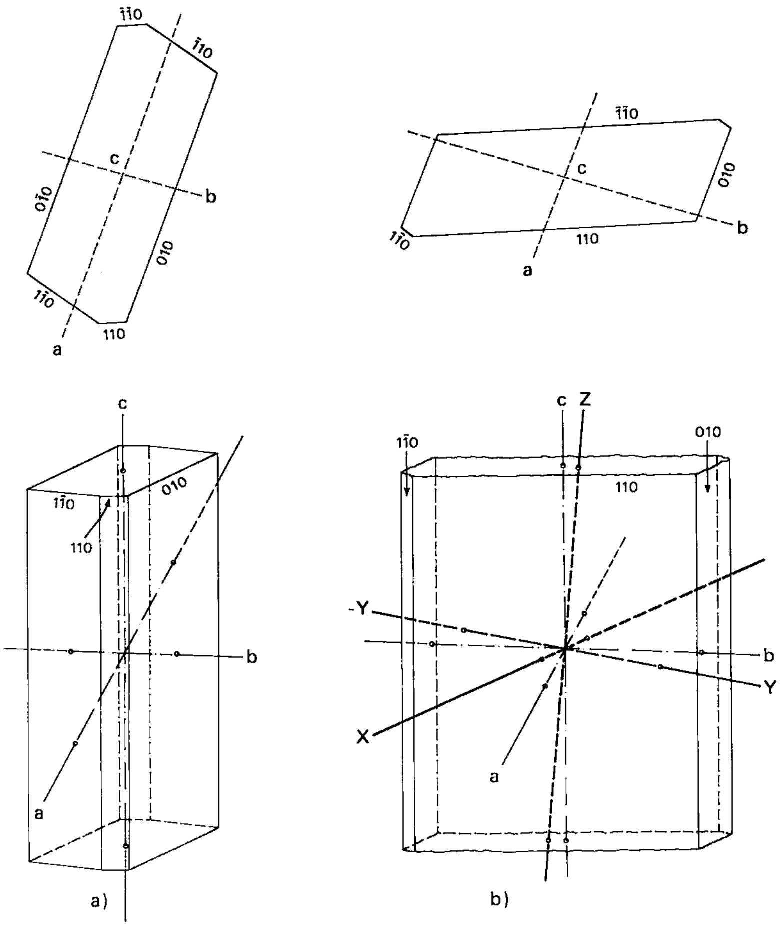

FIG. 2. The two most common habits of agrellite crystals: a) dominant form (010), and b) dominant form (110). The position of thte principal vibration directions X,Y,Z is shown in 2b.

tallization in preference to wollastonite is favoured by high a_F.

DERIVATION OF THE NAME

The mineral is named after Dr. Stuart O. Agrell, Department of Mineralogy and Petrology, University of Cambridge, England, and was approved by the Commission on New Mineral Names in June, 1973. Pronunciation is a-grell′īte.

ACKNOWLEDGMENTS

This study has been financed by research grants from the National Research Council of Canada which are gratefully acknowledged. The chemical analytical work was done largely in the Department of Mineralogy and Petrology, University of Cambridge, while J. G. was on leave from the University of Toronto, and he is indebted to Professor W. A. Deer and to Mr. J. H. Scoon for the use of the Cambridge rock-analysis laboratory. J. G. is further indebted to the Nuffield Foundation for a Fellowship during this period. We are indebted to Mr. M. Haslop for the preparation of mineral concentrates and to Mr. K. Rickson for assistance in the X-ray laboratories. The University of Toronto electron microprobe is partly supported by National Research Council grants to Professor J. C. Rucklidge to whom we are indebted for the supervision of the facility and for the data reduction programs employed in the

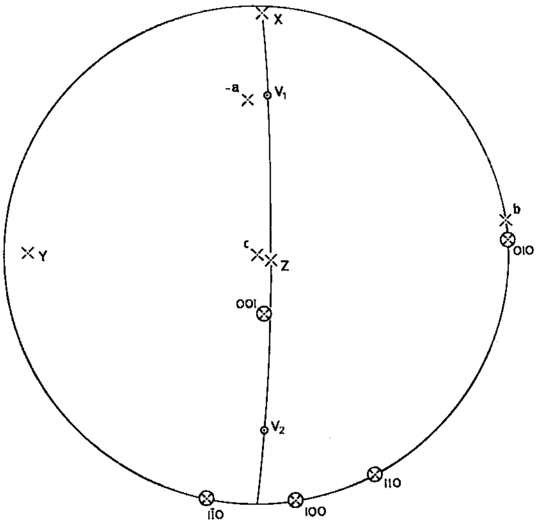

FIG. 3. Stereographic projection of optical and crystallographic elements of agrellite.

analytical procedures. It is a particular pleasure to record our gratitude to Dr. E. I. Semenov of the Institute for the Mineralogy, Geochemistry and Crystal Chemistry of the Rare Elements for his cooperation and exchange of specimen material. Part of the crystallographic work was done at Virginia Polytechnic Institute and State University, and M. G. B. is grateful to Professor G. V. Gibbs for his valuable advice and the use of his facilities.

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