The crystal structure of a Li,Be-rich brittle mica: a dioctahedral–trioctahedral intermediate

Jiunn-Chorng Lin and Stephen Guggenheim

Department of Geological Sciences
University of Illinois at Chicago
Chicago, Illinois 60680

Abstract

The crystal structure of a Li,Be-rich mica from Zimbabwe, intermediate in composition between the trioctahedral mica bityite-$2M_1$ [$Ca(LiAl_2)(AlBeSi_2)O_{10}(OH)_2$] and the dioctahedral mica margarite-$2M_1$ [$CaAl_2(Al_2Si_2)O_{10}(OH)_2$], has been studied by single crystal X-ray analysis ($R_1 = 0.030$, $R_2 = 0.031$) in space group Cc. On a statistical basis, the M(1) site (mean M(1)–O = 2.14Å) contains 0.55 Li and 0.45 vacancy, whereas the M(2) and M(3) sites (mean M(2)–O, = 1.902, M(3)–O = 1.903Å) are fully occupied by Al. In the tetrahedral sites, the ordering of Al,Be relative to Si is nearly complete (mean T–O: 1.723, 1.721, 1.632, 1.628Å) with a similar pattern to that found in margarite. This pattern violates the center of symmetry of the ideal space group $C2/c$. Such ordering is not environmentally induced and is a consequence of a more stable cation charge distribution. Hydrogen positions at ρ values of 22° and 58° are associated at each hydroxyl and indicate the effect on the O—H vector of vacancy and lithium substitutions in M(1), respectively. Apparent thermal parameters are explained by positional deviations of atoms between dioctahedral and trioctahedral regions. Generally, for all micas, the counter rotation of octahedral upper and lower oxygen triads in M(2) is related linearly to the difference in size of neighboring octahedra, and causes a small reduction in the lateral dimensions of the octahedral sheet. Octahedral flattening is most greatly affected by the field strength of neighboring octahedral cations, and less affected by either tetrahedral/octahedral misfit or the octahedral cation size.

Introduction

Bityite, $Ca(LiAl_2)(AlBeSi_2)O_{10}(OH)_2$, was described by Lacroix (1908) using material from Mt. Bity, Madagascar and again in 1947 by Rowledge and Hayton using impure material from Londonderry, Western Australia. Strunz (1956) gave X-ray powder and optical data of the Mt. Bity material. He found the structure to be a two layer modification and illustrated also the complex nature of the twinning found in this material. More recently, reported occurrences of bityite or micas of intermediate compositions between bityite and the dioctahedral mica, margarite-$2M_1$, $Ca(Al_2)(Al_2Si_2)O_{10}(OH)_2$, have been noted from the Middle Urals (Kutukova, 1959), three pegmatites in Zimbabwe (Gallagher and Hawkes, 1966), and a tin vein in Uganda (Gallagher and Hawkes, 1966). Unpublished data (Lin and Guggenheim) confirm that material from Pizzo Marcio, Val Vigezzo, Piemonte, Italy is lithium and beryllium rich also. Infrared data of material from Salisbury, Zimbabwe and Bikita, Zimbabwe have been presented by Farmer and Velde (1973).

Although early workers (*e.g.*, Holzner, 1936) have suggested that certain micas intermediate in composition may be composed of varying proportions of interleaved dioctahedral and trioctahedral layers, no such examples have been found. It is generally agreed that a complete simple solid solution series between dioctahedral and trioctahedral micas (where an octahedral cation substitutes for a vacancy) does not appear to exist in nature, although it has been documented in synthetic systems (Toraya *et al.*, 1978a). Cases do exist in nature when the vacancy is ordered in the M(1) site (for example, lepidolite-$2M_2$ as refined by Takeda *et al.*, 1971) but cations are disordered over the other octahedral sites, thereby discounting a simple solid solution relationship between two end members. However, bityite represents a special case for sev-

APPENDIX 1   OBSERVED AND CALCULATED STRUCTURE AMPLITUDES

K	L	10FO	10FC

H = 0

H = 1

H = 2

H = 3

Read across →

K L 10FO 10FC

H= 6

H= 4

H= 7

H= 5

H= 8

K	L	10FO	10FC	K	L	10FO	10FC
		H = 9		0	-2	250	239
				0	0	162	166
1	-11	82	81				
1	-10	73	68				
1	-7	131	124				
1	-5	155	145				
1	1	91	83				
1	2	152	160				
1	9	111	108				
1	12	96	87				
1	13	89	104				
3	-17	122	101				
3	-11	169	154				
3	-9	149	134				
3	-7	99	98				
3	-3	251	238				
3	-1	90	86				
3	5	218	232				
3	7	120	135				
3	11	224	241				
5	-15	82	83				
5	-11	79	69				
5	-7	111	109				
5	-5	179	175				
5	-4	79	80				
5	0	92	89				
5	2	179	168				
5	5	90	85				
5	9	81	89				
7	-8	77	71				
7	-7	91	101				
7	-6	75	67				
7	1	104	98				
7	2	96	91				
		H = 10					
0	-6	117	108				
0	-4	104	99				