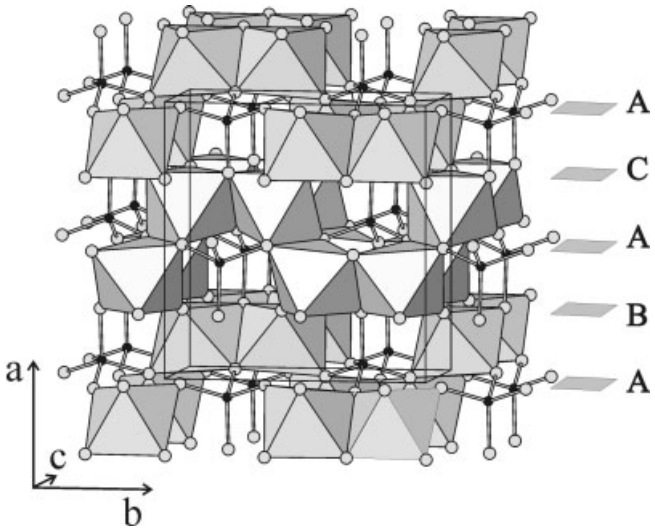
Crystal structure of dialuminum difluorotetraoxogermanate, $Al_2GeO_4F_2$

M. D. Mathews[I], A. K. Tyagi[I] and J. Köhler*,[II]

[I] Applied Chemistry Division, Bhabha Atomic Research Centre, Mumbai - 400 085, India
[II] Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany

Received June 23, 2003, accepted and available on-line August 22, 2003; CSD-No. 409714



Abstract

$Al_2F_2GeO_4$, orthorhombic, *Pnma* (No. 62), $a = 8.985(1)$ Å, $b = 8.521(1)$ Å, $c = 4.755(1)$ Å, $V = 364.0$ Å^3, $Z = 4$, $R(P) = 0.095$, $R(I) = 0.061$, $T = 295$ K.

Source of material

The white colored title compound was obtained by heating intimate mixtures of appropriate amounts of predried AlF_3(99.9%; ALPHA), Al_2O_3 (99.9%; ALPHA) and GeO_2 (99.9%; ALPHA) at 973 K for 24 h in an argon filled sealed platinum tube, followed by a slow cooling to room temperature.

Discussion

A new oxidefluoride $Al_2GeO_4F_2$ which is isotypic to topaz [1] and $V_2GeO_4F_2$ [2] has been prepared.

The refinements have been performed with an ordering of O and F on the anion sites as found in topaz and $V_2GeO_4F_2$. There are three types of oxygen atoms in the structure of $Al_2GeO_4F_2$ which are arranged in a close packing (cf. figure). One third of the octahedral holes are occupied by Al and one-twelfth of tetrahedral holes by Ge. The Ge—O bond distances within the GeO_4 tetrahedra are ranging from 1.732(5) Å to 1.773(3) Å. It is remarkable that in the AlO_4F_2 octahedra the Al—F bond distances of 1.791(3) Å and 1.844(4) Å are shorter than the Al—O bond distances which range from 1.865(4) Å to 1.902(4) Å. A similar situation is found for $Al_2GeO_4(OH)_2$ [3] where the Al—O(4) distances are short (1.863 Å and 1.866 Å) compared to the distances of Al to O(1), O(2) and O(3) which belong to the GeO_4 tetrahedra. The GeO_4 tetrahedra and AlO_4F_2 octahedra are connected via two common edges to give zigzag chains along *b* axis. These chains are linked via corners to form a three dimensional network. It may be noted that the occurrence of such oxidefluorides or oxidehydroxide is quite limited [3,4].

Table 1. Data collection and handling.

Powder:	white
Wavelength:	Cu K_α radiation (1.54051 Å)
μ:	172.76 cm^{-1}
Diffractometer, scan mode:	Scintag XDS2000, ω/θ
$2\theta_{max}$, stepwidth:	99.69°, 0.02°
$N(points)_{measured}$:	4484
$N(hkl)_{measured}$:	225
$N(param)_{refined}$:	22
Programs:	CSD [5], DIAMOND [6]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	B_{iso}
Al(1)	8*d*	0.1326(2)	0.0817(2)	0.5920(4)	0.74(4)
Ge(1)	4*c*	0.4389(1)	1/4	0.4009(3)	1.68(3)
F(1)	8*d*	0.7532(3)	0.0540(3)	0.5981(7)	1.00
O(1)	4*c*	0.2480(5)	1/4	0.4517(9)	1.00
O(2)	4*c*	0.0373(5)	1/4	0.7772(9)	1.00
O(3)	8*d*	0.9918(3)	0.0814(4)	0.2933(7)	1.00

Acknowledgment. The authors thank BMBF for financial support.

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* Correspondence author (e-mail: j.koehler@fkf.mpg.de)