Crystal structure of lead yttrium fluoride, $Pb_8Y_6F_{34}$, *a new fluorite-related anion-rich fluoride*

J. Köhler*[I], A. K. Tyagi[II] and S. N. Achary[II]

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

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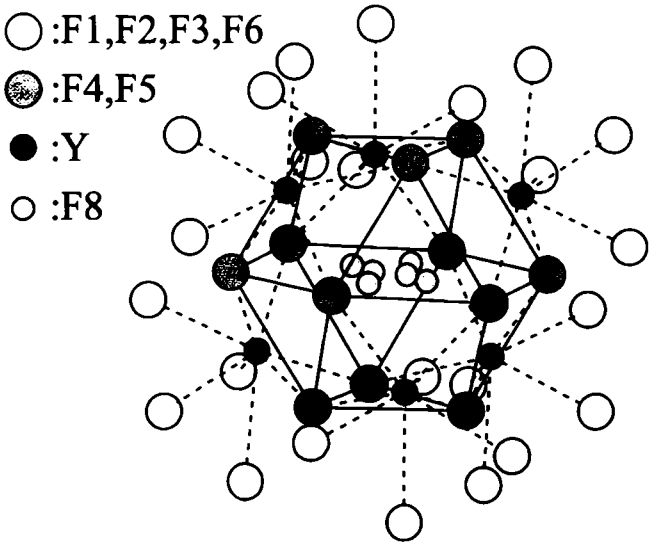

Abstract

$F_{34}Pb_8Y_6$, trigonal, $R\bar{3}$ (No. 148), a = 10.81871(1) Å, c = 19.9564(3) Å, V = 2022.9 Å^3, Z = 3, $R(P)$ = 0.122, $R(I)$ = 0.078, T = 295 K

Source of material

The white colored title compound was obtained by heating intimate mixtures of appropriate amounts of PbF_2 (99.9% Alfa), YF_3 (99.9% Alfa) at 973 K for 24 h in an argon filled sealed platinum tube, followed by a slow cooling to room temperature.

Discussion

A new fluoride $Pb_4Y_3F_{17}$ which is isotypic to $Ba_4Er_3F_{17}$ [1] has been prepared. The structure of $Pb_4Y_3F_{17}$ can be described as an ordered anion-rich fluorite structure. The higher anion/cation ratio 34/14, instead of 28/14 in CaF_2, is formally obtained by a transformation of an empty F_8 cube into a F_{12} cuboctahedra which is filled by one additional F atom on a six fold split postion [2]. Together with six surrounding YF_9 polyhedra, the Y_6F_{37} clusters are formed (cf. figure). The trivalent Y are antiprismatically surrounded by 8 F (d(Y—F) = 214 pm to 247 pm) with an additional F(6) capping one of the square faces (d(Y—F(6)) = 252 pm). Pb(1) is 10-fold coordinated (d(Pb—F) = 226 to 279 pm) whereas Pb(2) is surrounded by 11 (10+1) F atoms (d(Pb—F) = 246 pm to 340 pm). Based on the structural analysis it has been shown that this mixed fluoride can be understood as a member of the series M_xF_{2x+6} (x = 14) considering the double of the formula $Pb_4Y_3F_{17}$.

Table 1. Data collection and handling.

Powder:	white
Wavelength:	Cu $K_{\alpha 1}$ radiation (1.54051 Å)
μ:	115.29 cm^{-1}
Diffractometer, scan mode:	Stoe PSD, tramsmission, $\omega/2\theta$
$2\theta_{max}$, stepwith:	106.0°, 0.02°
$N(points)_{measured}$:	5100
$N(hkl)_{measured}$:	495
$N(param)_{refined}$:	38
Programs:	CSD [3], ATOMS [4]

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

Atom	Site	Occ.	x	y	z	U_{iso}
Pb(1)	6*c*		0	0	0.2586(2)	0.021(2)
Pb(2)	18*f*		0.2292(3)	0.0369(3)	0.0836(2)	0.0274(8)
Y	18*f*		0.0900(7)	0.6127(7)	0.0835(3)	0.010(1)
F(1)	18*f*		0.036(3)	0.767(3)	0.038(1)	0.019
F(2)	18*f*		0.426(3)	0.291(3)	0.110(1)	0.019
F(3)	18*f*		0.475(3)	0.082(3)	0.032(1)	0.019
F(4)	18*f*		0.203(2)	0.485(3)	0.034(1)	0.019
F(5)	18*f*		0.267(3)	0.392(2)	0.174(1)	0.019
F(6)	6*c*		0	0	0.145(2)	0.019
F(7)	3*a*		0	0	0	0.019
F(8)	18*f*	0.167	0.02(2)	0.06(1)	0.502(6)	0.019

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* Correspondence author (e-mail: J.Koehler@fkf.mpg.de)