X-Ray Crystal Structure of $Er_6Pb_3(SiO_4)_6$, a Second Phase in the Lead–Erbium–Silicate System

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Summary A study of the three-component systems Er_2O_3–PbO–SiO_2 has revealed the existence of two new phrases, $Er_6Pb_3(SiO_4)_6$ and $Er_4PbSi_5O_{17}$, and these have been prepared as single crystals; the crystal structure of $Er_6Pb_3(SiO_4)_6$ is described.

THE preparation and crystallization of the $Er_6Pb_3(SiO_4)_6$ and $Er_4PbSi_5O_{17}$ phases have been described previously,[1] and the crystal structure of $Er_4PbSi_5O_{17}$ has been reported.[2] We now report the crystal structure of $Er_6Pb_3(SiO_4)_6$.

Crystal data: pink crystals, hexagonal, $a = b = 9{\cdot}642$, $c = 6{\cdot}780$ Å. Systematic absences for $00l$ are $l = 2n + 1$. The subsequent structure determination has shown the space-group to be $P6_3/m$ with one $Er_6Pb_3(SiO_4)_6$ unit per unit cell. *X*-Ray intensity data were collected on an automated diffractometer using *Mo*-$K\alpha$ radiation and a

scintillation counter. Full-matrix least-squares structure factor refinement using 364 absorption corrected reflections gives an R value of 0·044. The atomic co-ordinates with Er and SiO_4 tetrahedra occupy the 6*h* positions and the 4*f* positions are partially occupied by three Pb atoms. The Figure shows the packing of the metals and SiO_4 tetrahedra.

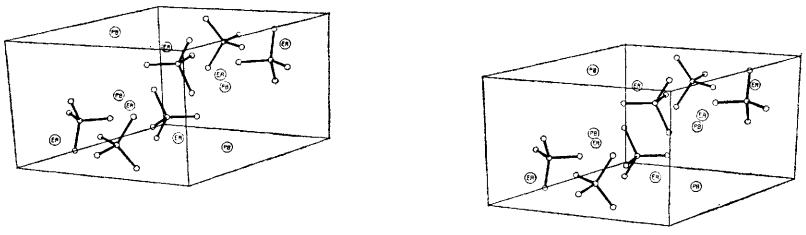

FIGURE. The arrangement of Pb, Er, and SiO_4 tetrahedra with the unit cell in $Er_6Pb_3(SiO_4)_6$.

e.s.d.'s are given in the Table. The structure is 'apatite-like' but differs in structure and constitution from the other known 'apatite- and oxyapatite-like' lead silicate compounds.[3]

TABLE

Atomic fractional co-ordinates ($\times 10^4$) with e.s.d.'s in parentheses.

	x	*y*	*z*	Site symmetry
Er	2349(1)	2486(1)	7500	6*h*
Pb	6667	3333	−44(3)	4*f*
Si	4175(8)	3883(9)	25	6*h*
O(1)	3580(23)	5156(24)	25	6*h*
O(2)	6125(23)	4338(23)	25	6*h*
O(3)	3703(19)	2779(19)	499(28)	12*i*

The six-fold Er occupancy and partial Pb occupancy correspond to Gd(1) and Gd(2) in the 'apatite-like' compound, $7Gd_2O_3{\cdot}9SiO_2$.[4] In $Er_6Pb_3(SiO_4)_6$ there is no evidence for the 'free O' being distributed at the two-fold positions on the 6_3 axis as occurs in $7Gd_2O_3{\cdot}9SiO_2$. The Er ions are surrounded by five O atoms from neighbouring SiO_4 tetrahedra with Er–O distances ranging from 2·34 to 2·62 ± 0·01Å, while the Pb ions are surrounded by nine O atoms with distances ranging from 2·30 to 2·66 ±0·01 Å. Within the SiO_4 tetrahedra Si–O distances range from 1·59 to 1·64 ± 0·01 Å.

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