The Crystal Structure of the New Rare-earth Silicate $Er_4PbSi_5O_{17}$

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Summary An *X*-ray crystallographic structure determination of a previously unidentified silicate type with an empirical formula $Er_4PbSi_5O_{17}$ is described.

THE crystallization of $Er_4PbSi_5O_{17}$ from the $PbO–SiO_2Er_2O_3$ system at temperatures between 750 °C and 1250 °C has been described.[1] The compound is of particular interest because a spectral analysis in the $4s_{3/2}$ region of the spectrum shows there are eight absorption lines. *Crystal data:* pink crystals, monoclinic, $a = 5{\cdot}534$, $b = 10{\cdot}58$, $c = 6{\cdot}960$ Å, $\beta = 107{\cdot}2°$. Systematic absences for $0k0$ are $k = 2n + 1$. The subsequent structure determination has shown the space group to be $P2_1/m$ with $Z = 4$ for the $1/2[Er_4Pb(Si_2O_7)(Si_3O_{10})]$ unit. *X*-ray intensity data were collected on an automated diffractometer using Mo–K_α radiation and a scintillation counter. The structure was solved by Patterson and Fourier methods. The full-matrix least-squares structure-factor refinement using 864 absorption corrected reflections gives an *R* value of 0·091.

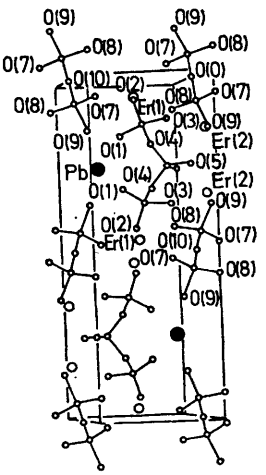

FIGURE 1

The structure is most unusual since it possesses a combination of both $Si_3O_{10}^{8-}$ and $Si_2O_7^{6-}$ anions. The packing of these around the erbium and lead is shown in Figure 1. A space group requirement is that these anions have mirror and centrosymmetric symmetry, respectively. The centrosymmetric $Si_2O_7^{6-}$ anion with a linear bridging Si–O–Si angle has been reported in $Sc_2Si_2O_7$,[2] $Yb_2Si_2O_7$,[3] and $Er_2Si_2O_7$.[3] The $Si_3O_{10}^{8-}$ anion is quite rare in silicates and has only previously been described in $Ho_4(Si_3O_{10})SiO$,[4] ardenite,[5] kilchoanite[6] and $(Ca_8Si_5O_{18})$ natrolite.[7] The two noncrystallographically equivalent erbium ions are in highly distorted octahedral co-ordination with their six nearest oxygen neighbours. Lead has a distorted five-fold pyramidal co-ordination with its nearest oxygen neighbours.

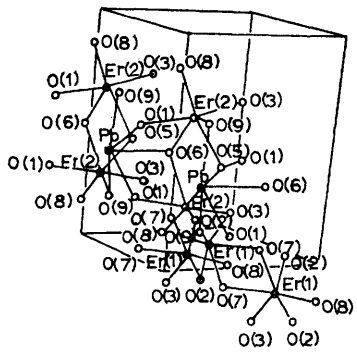

FIGURE 2

These metal–oxygen groups are building units for the complicated three-dimensional Er–O–Pb–O clusters shown in Figure 2. Si–O distances range from 1·57 to 1·79 (0·06) (av. 1·64) Å within the $Si_2O_7^{6-}$ anions and 1·59 to 1·69 (0·06) (av. 1·67) Å within the $Si_3O_{10}^{8-}$ anions. Er(1)–O distances range from 2·18 to 2·28 (0·04) Å, Er(2)–O from 2·22 to 2·46 (0·04) Å, and Pb–O from 2·40 to 2·51 (0·04) Å.

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