SYNTHESIS AND CRYSTAL STRUCTURE OF LEAD PENTAFLUOROMANGANATE (III), PbMnF $_{\rm S}$

P. Bukovec, V. Kaučič, S. Gašperšič

Department of Chemistry and Chemical Technology, E. Kardelj University, Ljubljana (Yugoslavia)

and R. Hoppe Institute for Inorganic and Analytical Chemistry I, Justus-Liebig University, Giessen (F.R.G.)

Brown single crystals of $\rm PbMnF_5$ were obtained by tempering a mixture of $\rm PbF_2$ and $\rm MnF_3$ in sealed gold tubes at 550°C for ten days.

Crystal data: $M_r = 375.13$, monoclinic, $P2_{1/c}$, a = 5.008(3), b = 13.656(13), c = 5.640(3) Å, (3 = 93.04(4)°, V = 385.2 Å³, Z = 4, Dm = 5.96, $Dx = 6.16 \text{ Mgm}^{-3}$, $\mu(MoK_{\infty}) = 471.5 \text{ cm}^{-1}$, R = 0.156, Rw = 0.161.

Manganese is octahedrally coordinated by fluorine atoms. The octahedra share cis-fluorine atoms to give $\left[MnF_{4/1}F_{2/2}\right]$ infinite chains. The octahedra are Jahn-Teller distorted with the Mn-F bond distances of 2.10(3) and 2.16(4) Å in the direction of the distortion, the other Mn-F bond distances are in the range from 1.84(4) to 1.94(4) Å. The lead atoms are surrounded by eleven fluorine atoms, contact distances are in the range from 2.27(3) to 3.35(4) Å.

The Madelung Part of Lattice Energy, MAPLE, as well as Effective Coordination Numbers, ECoN, are calculated and discussed.