S_{18}

ON THE KNOWLEDGE OF CUBIC Rb_2MnF_6

P. Bukovec* and R. Hoppe
Department of Chemistry and Chemical Technology, 'E. Kardelj', University Ljubljana (Yugoslavia) and Institut für Anorganische und Analytische Chemie der Justus Liebig-Universität, Giessen (F.R.G.)

Rb_2MnF_6 has been prepared by the fluorination of the mixture NH_4MnF_3 + 2RbCl at 350°C. About 500 mg of the sample has been dissolved in 10 ml 40% HF and allowed to crystallize slowly at room temperature. In a few days, light yellow, octahedral single crystals appeared, which were stable when exposed to air. Before the crystal structure analysis, the single crystals have been tempered in fluorine at 320°C for two days. Cubic crystals (Fm3m) with a=8.527(1) Å remained unchanged during treatment.

The structure has been refined from four circle diffractometer data (Philips PW 1100, MoKα, 69 I_o(hkl), R=5.8 and R_w=3.3%). The distance d(Mn-F) of 1.782(6) Å (6x) is in accordance with the newly obtained data on K_2MnF_6. The Madelung Part of Lattice Energy, MAPLE, for Rb_2MnF_6 and MnF_4 has been calculated. MAPLE for the latter compound (2573 kcal/mol) is in good agreement with the one from K_2MnF_6 (2563 kcal/mol). Calculated Effective Coordination Numbers, ECoN, agree with the naif counted values only for Mn^{4+}(ECoN=6.0). For Rb^+ and F^- the ECoN values are 13.2 and 8.9 respectively.