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INFLUENCE OF CATIONIC SIZE ON THE TRANSITION TEMPERATURE OF THE $A^{II}B^{III}F_5$ COMPOUNDS OF $SrAlF_5$ TYPE

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The prediction that $SrAlF_5$ is ferroelectric with a Curie temperature of 685K, made on the basis of its previously published structure, was later confirmed with an experimental T_c = 715K as determined both by heat capacity and by dielectric measurement [1]. The present study reports a correlation between T_c and cation radius or electronic environment for members of the isomorphous $A^{II}B^{III}F_5$ family. T_c is found to increase with increasing $^{VIII}A^{2+}$ ionic radius and decrease with increasing $^{VI}B^{3+}$ ionic radius. Example is $BaFeF_5$ with T_c = 730K and $r(^{VIII}Ba^{2+})$ = 1.42 Å, $Ba_{0.5}Sr_{0.5}FeF_5$ with T_c = 620K and $r(^{VIII}Sr^{2+}$ = 1.26 Å) for $r(A^{2+})$ as the variable. It is possible to substitute Pb^{2+} for Sr^{2+} or Ba^{2+}, thereby introducing the influence of the Pb^{2+} lone pair into the structure. The effect of these substitutions on T_c have been determined and the results will be discussed.

1 S.C. Abrahams, J. Ravez, A. Simon and J.P. Chaminade, J. Appl. Phys. 52, 4740 (1981).