Access to metastable complex ion conductors via mechanosynthesis: Preparation, microstructure and conductivity of (Ba,Sr)LiF_3 with inverse perovskite structure

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S1

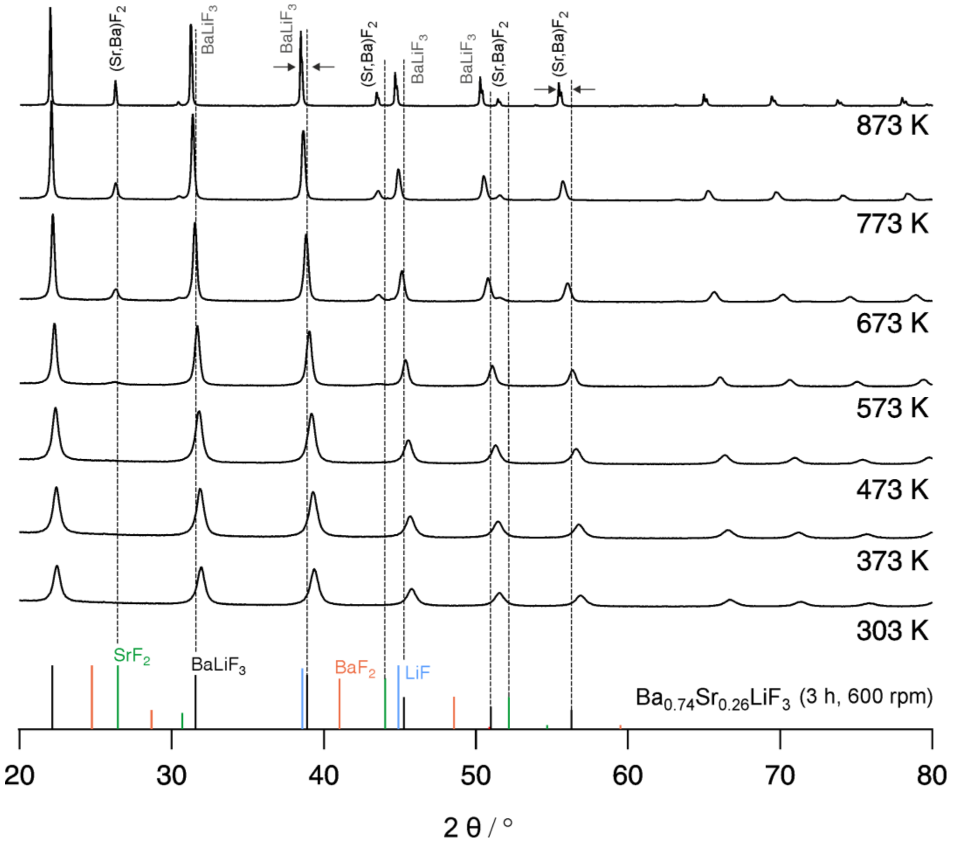

Fig. S1: In situ XRPD showing the decomposition of $Ba_{0.74}Sr_{0.26}F_2$ prepared by high-energy ball milling. The equilibration time before each scan was 60 min. Heating and cooling rates were set to 12 K/min. With increasing temperature Sr-rich (Ba,Sr)F_2 is formed. Interestingly, $BaLiF_3$ rather than BaF_2 is reformed. Dashed lines shall help to compare with literature values for pure SrF_2 and $BaLiF_3$ (indicated by vertical lines). Note that the peaks of $BaLiF_3$ shift towards smaller diffraction angles due to lattice expansion when the perovskite is exposed to elevated temperatures. See main text for further details.

S2

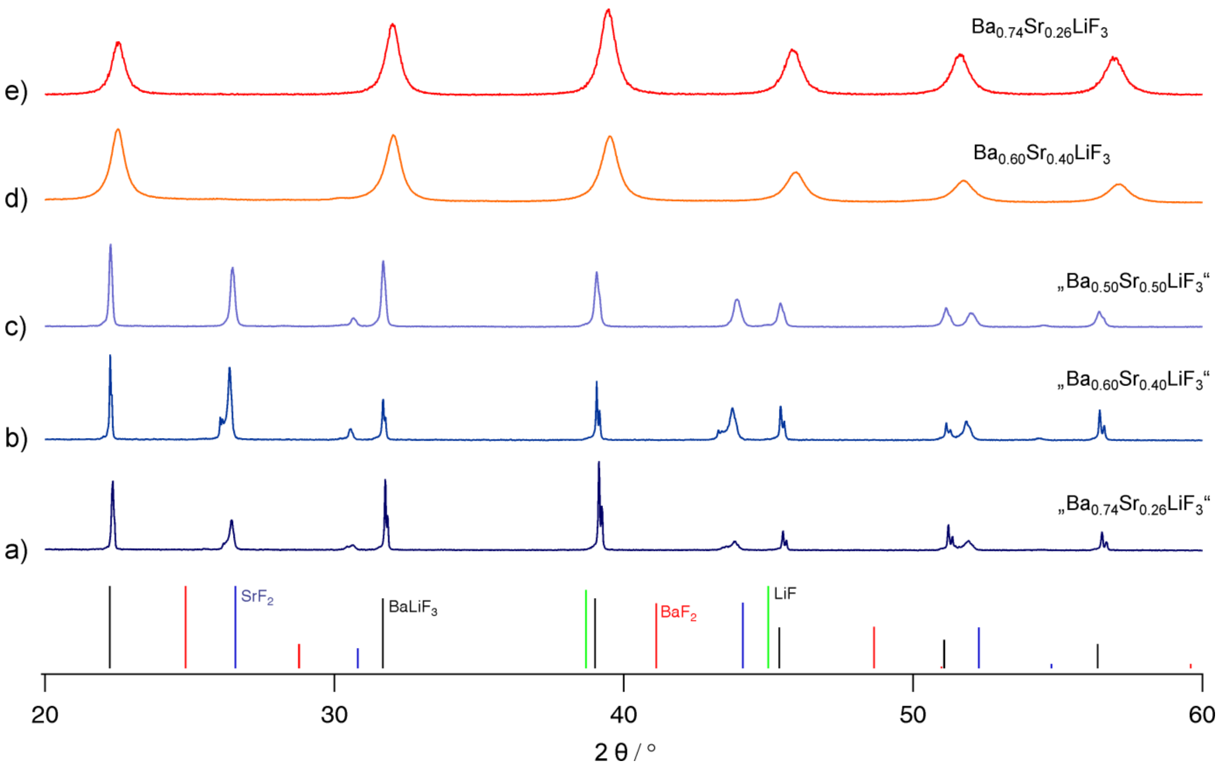

Fig. S2: a) to b) XRPD of stoichiometric mixtures of BaF_2, SrF_2 and LiF which were ground, heated at 973 K and then air-quenched. c) XRPD of an equimolar mixture of BaF_2 and SrF_2 which was mixed with LiF, milled for 48 h in the Fritsch planetary mill, heated at 1023 K (5 h) and then air-quenched. In each case a mixture of different phases is formed. The peaks belonging to SrF_2 are clearly visible proving the failure of the synthesis route. The amount of Sr incorporated into $BaLiF_3$ turns out to be rather small not exceeding more than 10 %. d) and e) XRPD of $Ba_{0.60}Sr_{0.40}F_2$ and $Ba_{0.74}Sr_{0.26}F_2$ which were prepared using a mechanochemical route, i. e., the source materials were treated for several hours in a planetary mill.