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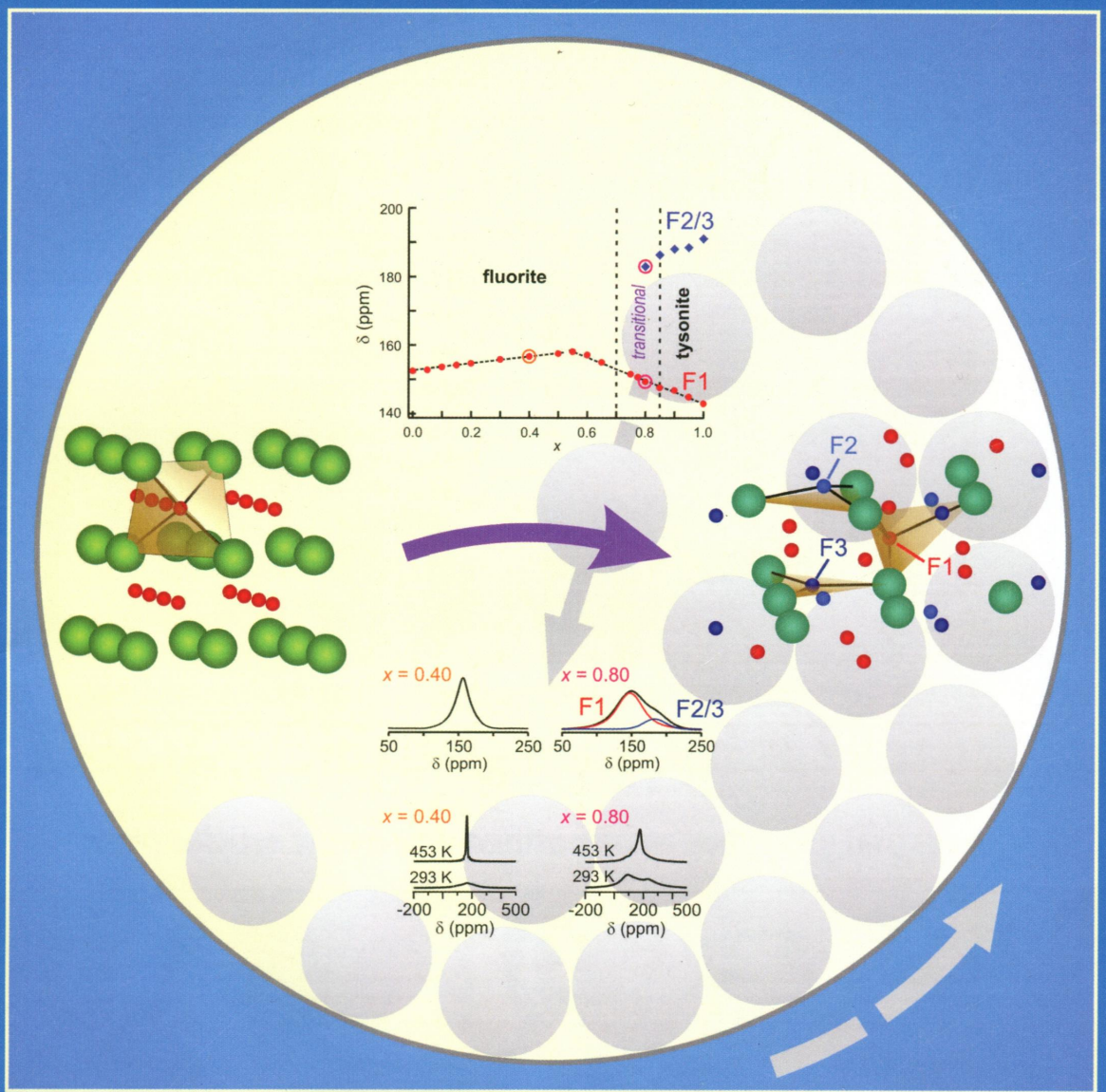

Continuous Structural Transition of Mechanosynthesized $Ba_{1-x}La_xF_{2+x}$ and F^- Mobility Revealed by ^{19}F NMR
(see page 7117)

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ON THE COVER: Continuous structural transition of mechanosynthesized $Ba_{1-x}La_xF_{2+x}$ and F^- mobility revealed by ^{19}F NMR. The system $Ba_{1-x}La_xF_{2+x}$ was mechanosynthesized for $0 \leq x \leq 1$ by high-energy ball-milling mixtures of BaF_2 and LaF_3. Thus the miscibility gap $x \approx 0.55-0.85$, open until now, was closed. As revealed by ^{19}F MAS NMR chemical shift values for the fluorite lattice and for the F1 site in the tysonite lattice, the structure of $Ba_{1-x}La_xF_{2+x}$ continuously changes from fluorite to tysonite in the range $x \approx 0.70-0.85$. Moreover, the ^{19}F chemical shifts for the F2 and F3 sites in the tysonite lattice, which could not be discriminated here, tend towards those for the F1 site with decreasing x. Complete motional narrowing of the static ^{19}F NMR lines of the samples with $0.10 \leq x \leq 0.50$ at $T \geq 453$ K indicates that the corresponding fluoride ions are highly mobile. In the samples with $0.60 \leq x \leq 0.85$, the number ratio of slow (or non-mobile) to highly mobile fluoride ions increases with increasing x. Furthermore, a change of the fluoride ion conduction mechanism can be observed by analyzing the shape of the NMR lines. See page 7117.

Articles

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Additions and Corrections

(S) Supporting Information available via online article