

Crystal structure and phase transitions of layered perovskite CsScF₄ crystal Supplementary Material (ESI) for CrystEngComm

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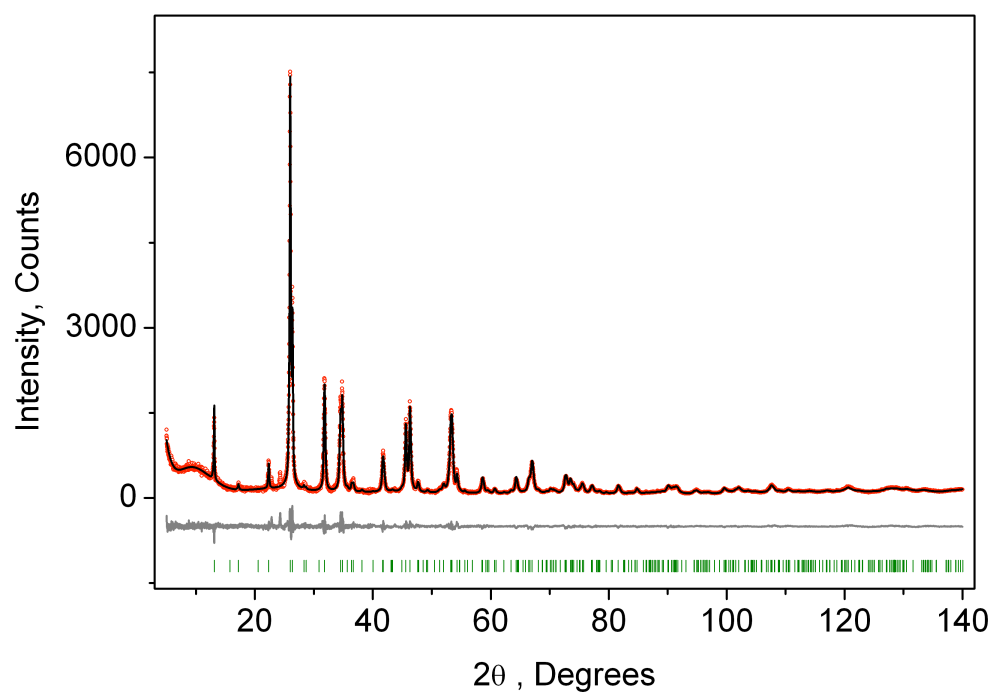
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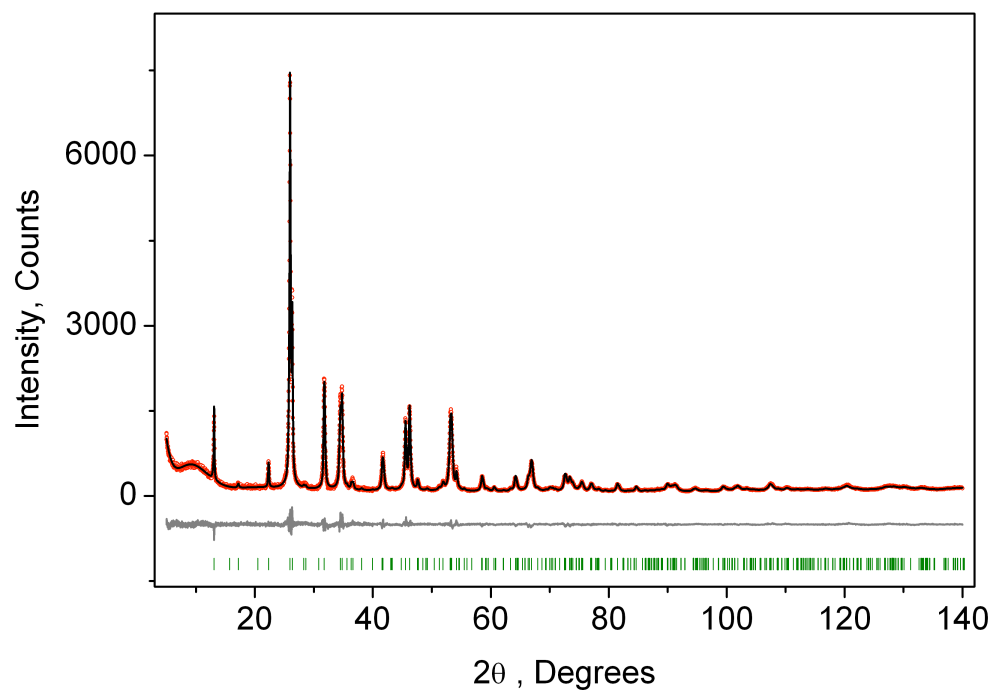
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This work is devoted to the complex research of temperature phase transitions in CsScF₄ crystal. Crystal structure was solved and refined at different temperatures by Rietveld method. Structural phase transitions have been investigated by spectroscopic methods some of them for the first time: Brillouin spectroscopy, Raman spectroscopy, IR absorption spectroscopy and NMR. The symmetry analysis of the center Brillouin zone of all phases is presented. The vibrational spectra of the crystal in three phases have been calculated. The structural phase transitions mechanism was determined. The transitions at $T_1 = 475$ K and $T_2 = 317.5$ K are of displacement type. The Raman soft modes have been associated with rotations of ScF₆ octahedral group.

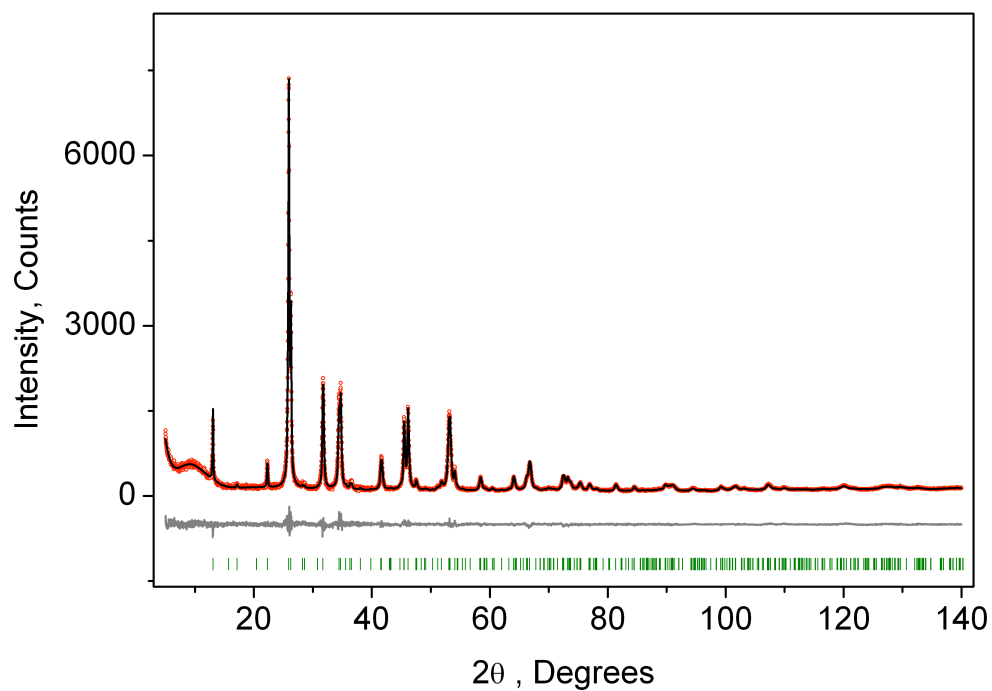
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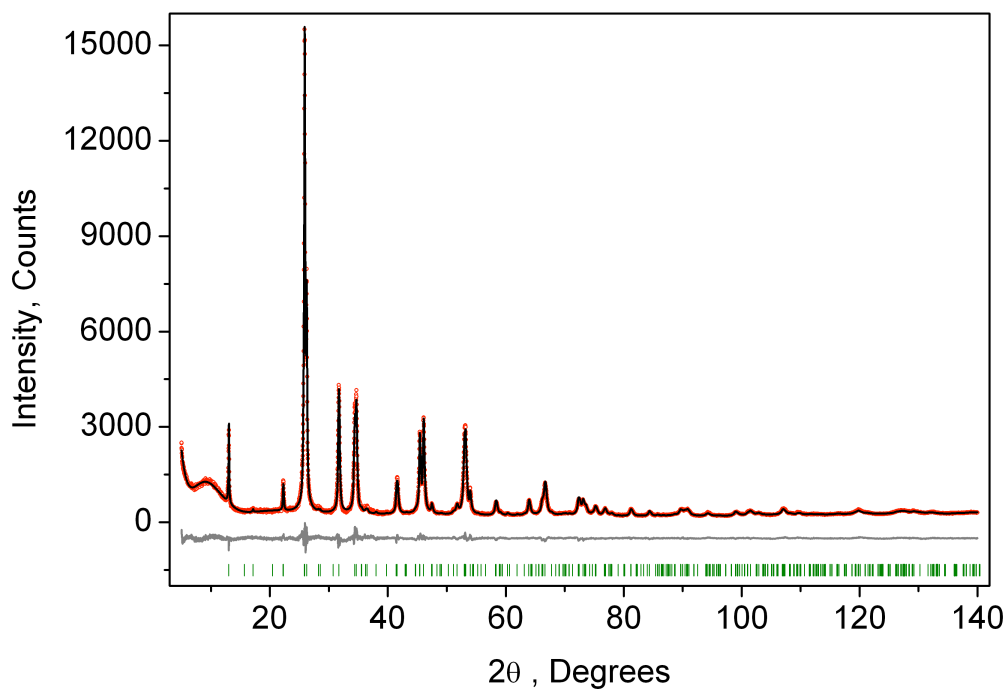
Supplementary Fig. 1. Rietveld difference plot of CsScF4 at 133 K (*Pmmn* phase).



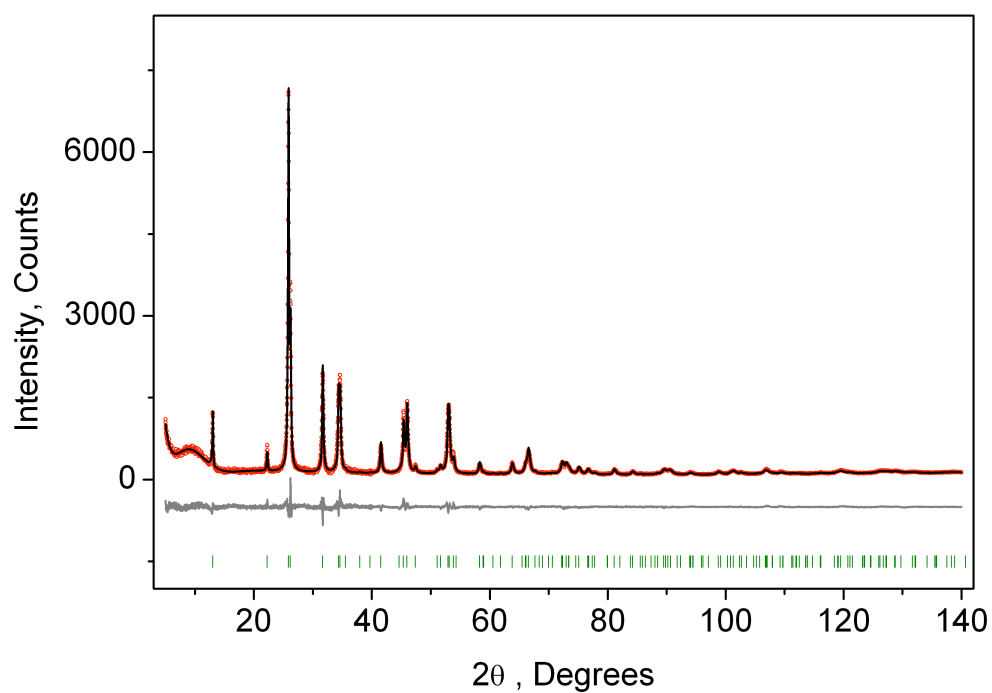
Supplementary Fig. 2. Rietveld difference plot of CsScF4 at 193 K (*Pmmn* phase).



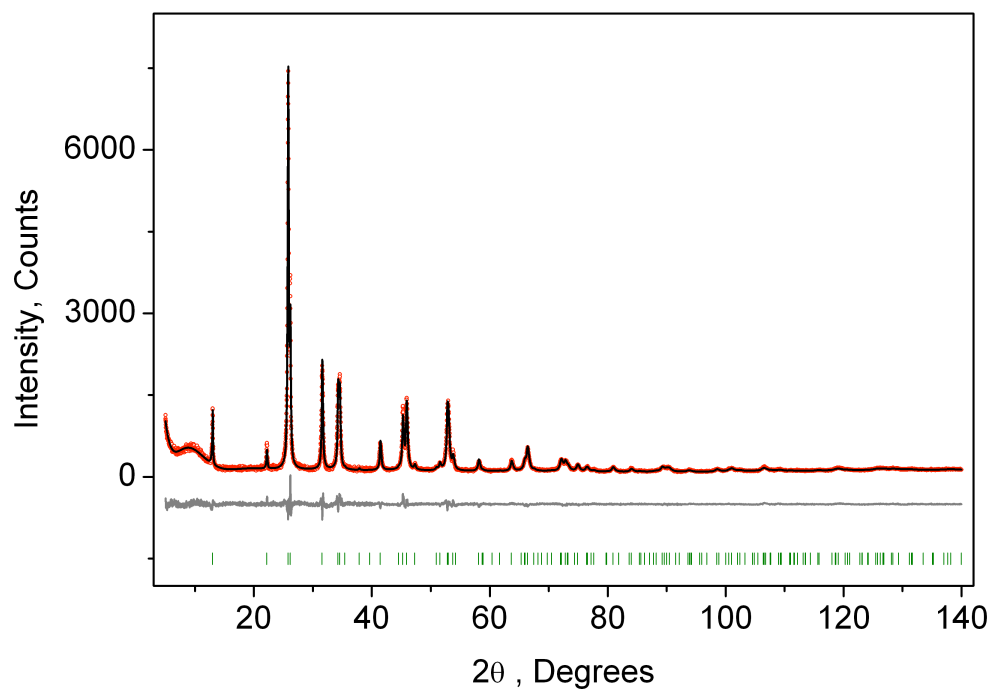
Supplementary Fig. 3. Rietveld difference plot of CsScF4 at 253 K (*Pmmn* phase).



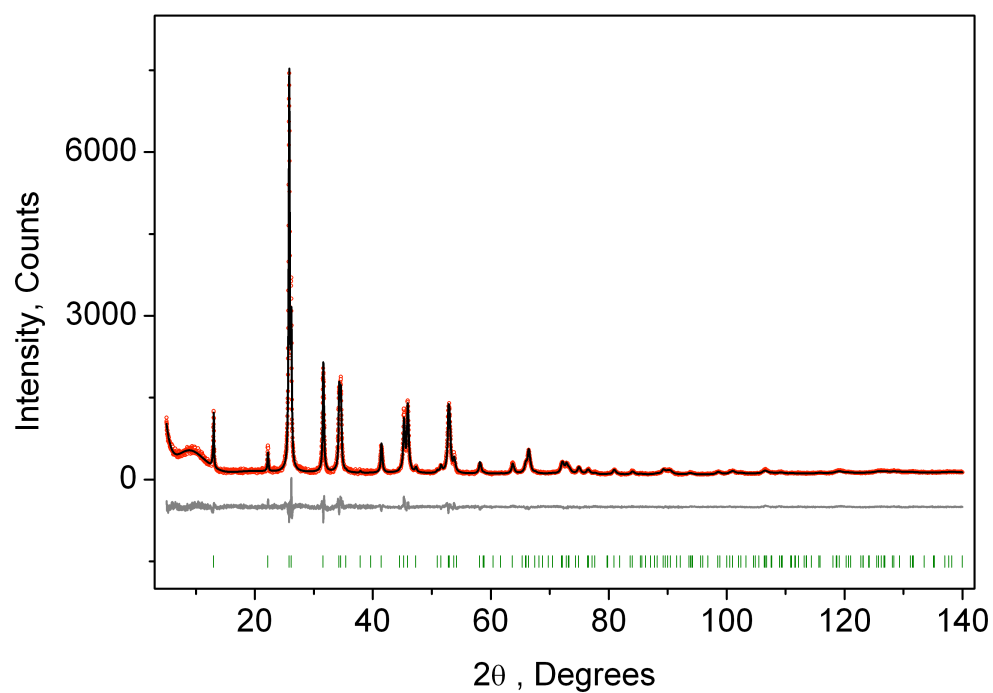
Supplementary Fig. 4. Rietveld difference plot of CsScF4 at 303 K (*Pmmn* phase).



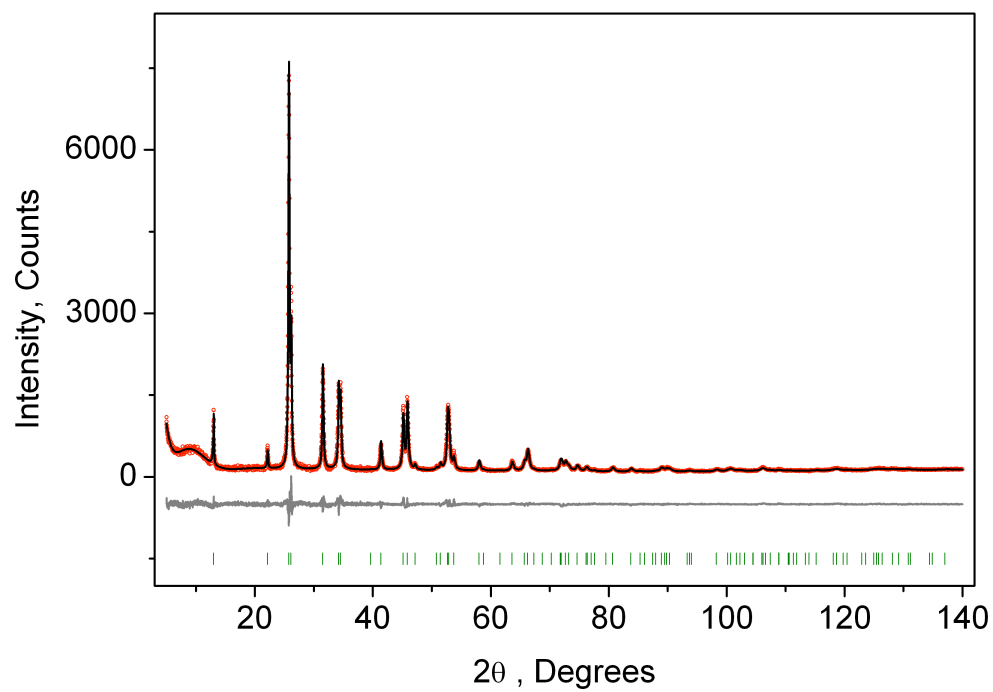
Supplementary Fig. 5. Rietveld difference plot of CsScF4 at 353 K ($P4/mbm$ phase).



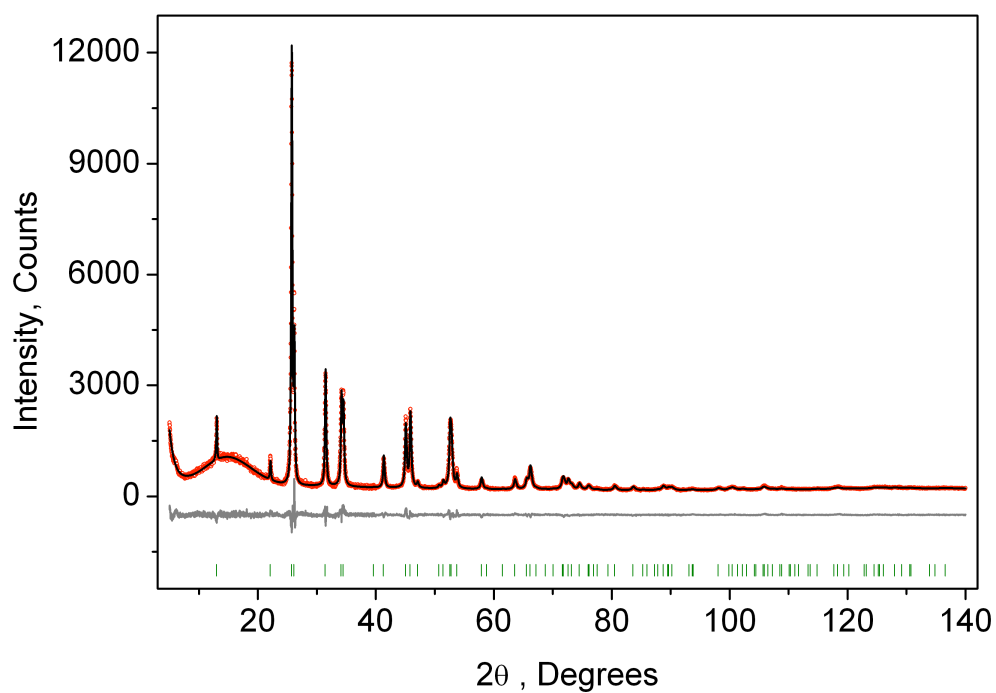
Supplementary Fig. 6. Rietveld difference plot of CsScF4 at 393 K ($P4/mbm$ phase).



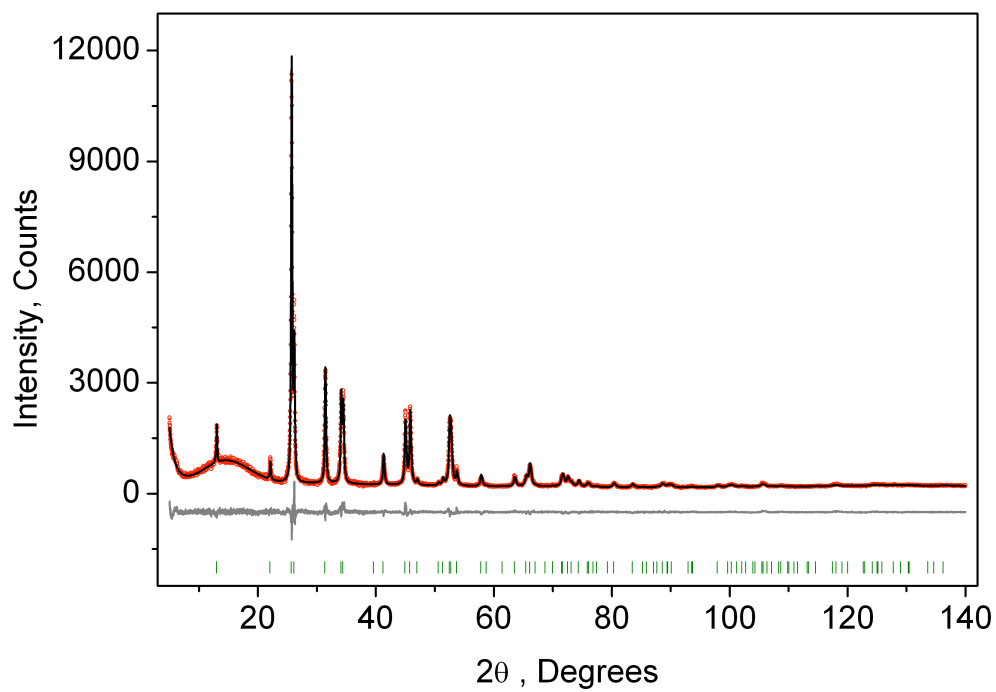
Supplementary Fig. 7. Rietveld difference plot of CsScF4 at 433 K ($P4/mbm$ phase).



Supplementary Fig. 8. Rietveld difference plot of CsScF4 at 503 K ($P4/mmm$ phase).



Supplementary Fig. 9. Rietveld difference plot of CsScF4 at 543 K ($P4/mmm$ phase).



Supplementary Fig. 10. Rietveld difference plot of CsScF4 at 583 K ($P4/mmm$ phase).