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The structural and magnetic properties of $Cs_xFe_{2-y}Se_2$ as determined by x ray and neutron scattering of powder and single crystal samples KEITH TADDEI, Northern Illinois Univ, OMAR CHMAISSEM, Northern Illinois University and Argonne National Laboratory, MIHAI STURZA, Argonne National Laboratory, SEVDA AVCI, Bursa Technical University, HELMUT CLAUS, Argonne National Laboratory, MERCOURI KANATZIDIS, Northwestern University, STEPHAN ROSENKRANZ, RAY OSBORN, Argonne National Laboratory — The $A_xFe_{2-y}Se_2$ family of iron selenides (A = K, Rb and Cs) has proven an intricate system for the study of unconventional superconductivity, exhibiting high temperature superconductivity ($\sim$ 30 K) and a complex structural phase transition into a biphasic state coupled with a high temperature magnetic transition ($\sim$ 500 K). While isostructural to the 122 arsenides, significant structural differences are identified. In the selenides, iron vacancies in the tetrahedral FeSe layers become ordered below a high temperature structural transition defining a main phase $\sqrt{5} \times \sqrt{5}$ superstructure. Coexistent with the main phase, a secondary phase of a previously contested structure is observed and it is in this biphasic state that superconductivity arises at $\sim$ 30 K. Both powder and single crystal samples show similar phase separation and coexistence. In this talk, I will discuss structural results and lattice parameter evolution obtained from neutron powder diffraction as well as single crystal x-ray diffraction with an emphasis on a novel magnetic structural model, the identification of the secondary phase, and the nature of coincidence of the magnetic, structural and secondary phase transitions.

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