Electronic Supplementary Information for "Crystal structure of the new $FeSe_{1-x}$ superconductor"

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Table 1S. Refined structural parameters and selected bond lengths (Å) and angles (°) for $FeSe_{1-x}$ obtained from combined Rietveld refinements of the synchrotron X-ray and neutron powder diffraction data at 5 and 295 K.

		5 K	295 K
Space group		*Cmma*	*P*4/*nmm*
a (Å)		5.30781(5)	3.77376(2)
b (Å)		5.33423(5)	
c (Å)		5.48600(5)	5.52482(5)
Volume (Å^3)		155.325(2)	78.680(1)
Fe	B_{iso} (Å^2)	0.60(2)	2.05(3)
	Occ.	1.00	1.00
Se	*z*	0.2653(1)	0.2652(1)
	B_{iso} (Å^2)	0.35(2)	1.50(2)
	Occ.	0.92(1)	0.91(1)
R_{wp} (%) (SXRPD)		8.34	7.87
R_{exp} (%) (SXRPD)		5.04	4.75
R_{wp} (%) (NPD)		3.77	5.80
R_{exp} (%) (NPD)		2.27	3.50
χ^2 (combined)		2.750	2.743
Fe-Fe (Å)		2.65391(3) (2x) 2.66713(3) (2x)	2.66845(1) (4x)
Fe-Se (Å)		2.3787(4) (4x)	2.3890(4) (4x)
Fe-Se-Fe (°)		104.54(2) (2x) 68.20(1) (2x) 67.82(2) (2x)	104.34(3) (2x) 67.90(1) (4x)

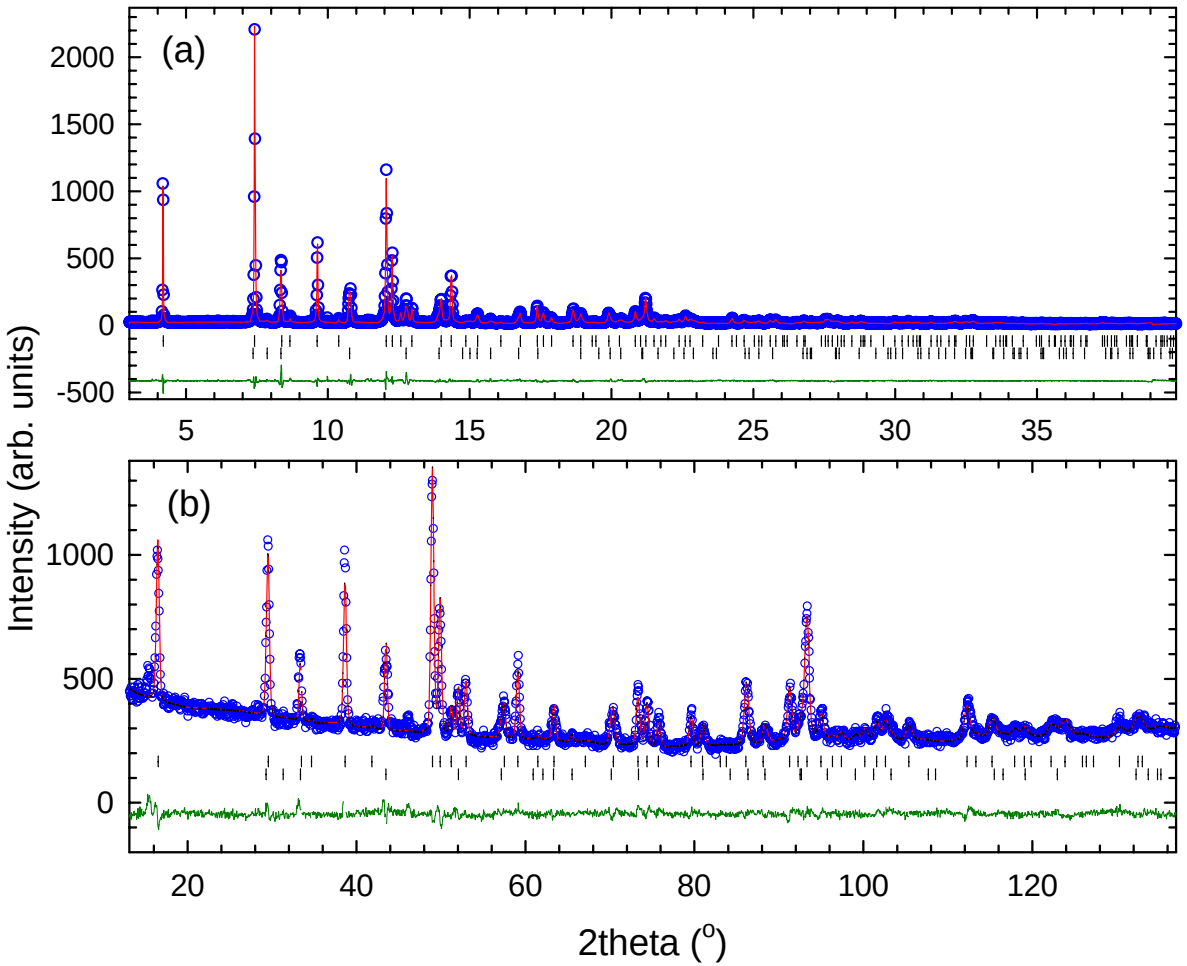

Figure 1S. Final observed (circles) and calculated (solid lines) **(a)** synchrotron X-ray (λ = 0.40301 Å) and **(b)** neutron (λ = 1.5944 Å) powder diffraction profiles for the α-$FeSe_{1-x}$ sample at 295 K. The lower solid lines show the difference profiles and the tick marks show the reflection positions of the α- (top) and β-$FeSe_{1-x}$ (bottom) phases.