

Crystal structure and magnetic modulation in β -Ce₂O₂FeSe₂

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Table S1. Structure parameters of β -Ce₂O₂FeSe₂ from combined refinement using PXRD and PND data (Pna2₁ model) ^(a).

Space Group	Pna2 ₁ (33)					
<i>a</i> (Å)	17.18613(2)					
<i>b</i> (Å)	16.28510(2)					
<i>c</i> (Å)	3.962979(5)					
<i>V</i> (Å ³)	1109.150(3)					
<i>d</i> _{theory} (g/cm ³)	6.29987(2)					
<i>R</i> _{wp} (%)	2.02 (overall), 3.69 (lab X-ray), 3.06 (synchrotron X-ray), 3.68 (PND_bank1), 2.81 (PND_bank2), 1.82 (PND_bank3), 1.51 (PND_bank4), 1.41 (PND_bank5), 1.65 (PND_bank6).					
	Site	<i>x</i>	<i>y</i>	<i>z</i>	Occupancy	
Ce1	4 <i>a</i>	0.40755(9)	0.02273(10)	0.25	1	0.47(3)
Ce2	4 <i>a</i>	0.41325(8)	0.82595(12)	0.752(6)	1	0.47(3)
Ce3	4 <i>a</i>	0.08419(7)	0.82329(12)	0.752(6)	1	0.55(3)
Ce4	4 <i>a</i>	0.09070(8)	0.01866(10)	0.248(8)	1	0.39(3)
Se1	4 <i>a</i>	0.24988(10)	0.51258(3)	0.249(4)	1	0.749(16)
Se2	4 <i>a</i>	0.42625(6)	0.67052(10)	0.251(5)	1	0.77(2)
Se3	4 <i>a</i>	0.06484(6)	0.67184(9)	0.253(6)	1	0.72(2)
Se4	4 <i>a</i>	0.24917(9)	0.75113(3)	0.754(4)	1	0.813(16)
O1	4 <i>a</i>	0.13804(9)	0.87821(12)	0.245(8)	1	0.60(5)
O2	4 <i>a</i>	0.35996(10)	0.88037(11)	0.247(8)	1	0.31(4)
O3	4 <i>a</i>	0.45405(11)	0.96077(13)	0.750(10)	1	0.60(4)
O4	4 <i>a</i>	0.04539(11)	0.95885(13)	0.749(10)	1	0.67(4)
Fe1	4 <i>a</i>	0.24967(9)	0.88209(3)	0.262(4)	1	1.010(17)
Fe2	4 <i>a</i>	0.27581(10)	0.66217(10)	0.251(7)	0.797(3)	0.92(2)
Fe3	4 <i>a</i>	0.2352(3)	0.6605(3)	0.249(17)	0.203(3)	0.92(2)

^(a): The *z* coordinate of Ce1 was fixed to 0.25 to keep the center of mass near to that of the *Pnma* model.

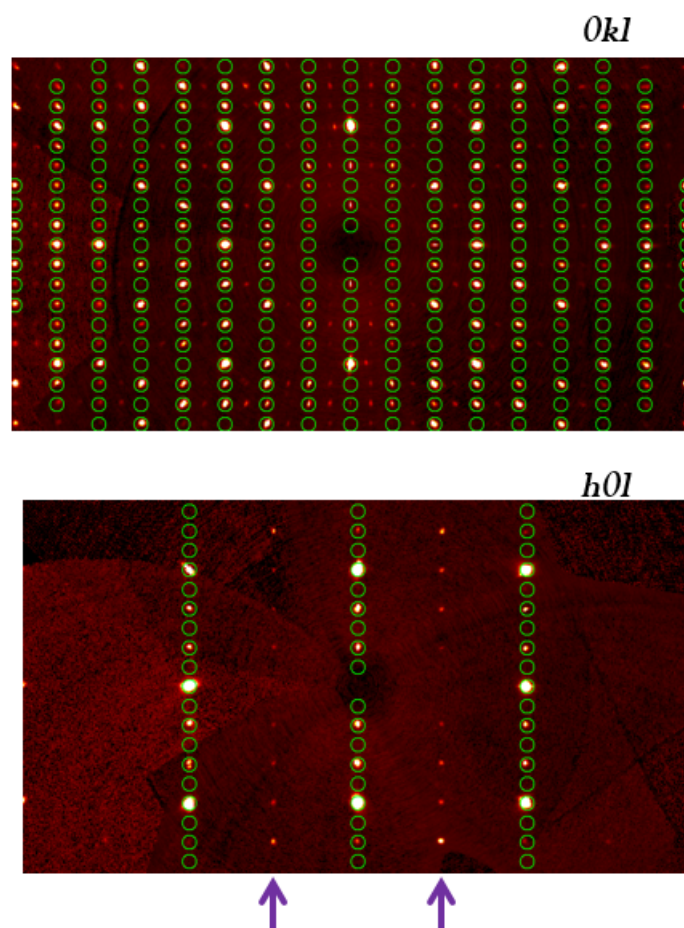


Fig. S1. Selected cross sections of single crystal XRD image of β - $\text{Ce}_2\text{O}_2\text{FeSe}_2$. Green circles are reflections predicted by $Amam$ space group. Extra reflections pointed by arrow were observed.

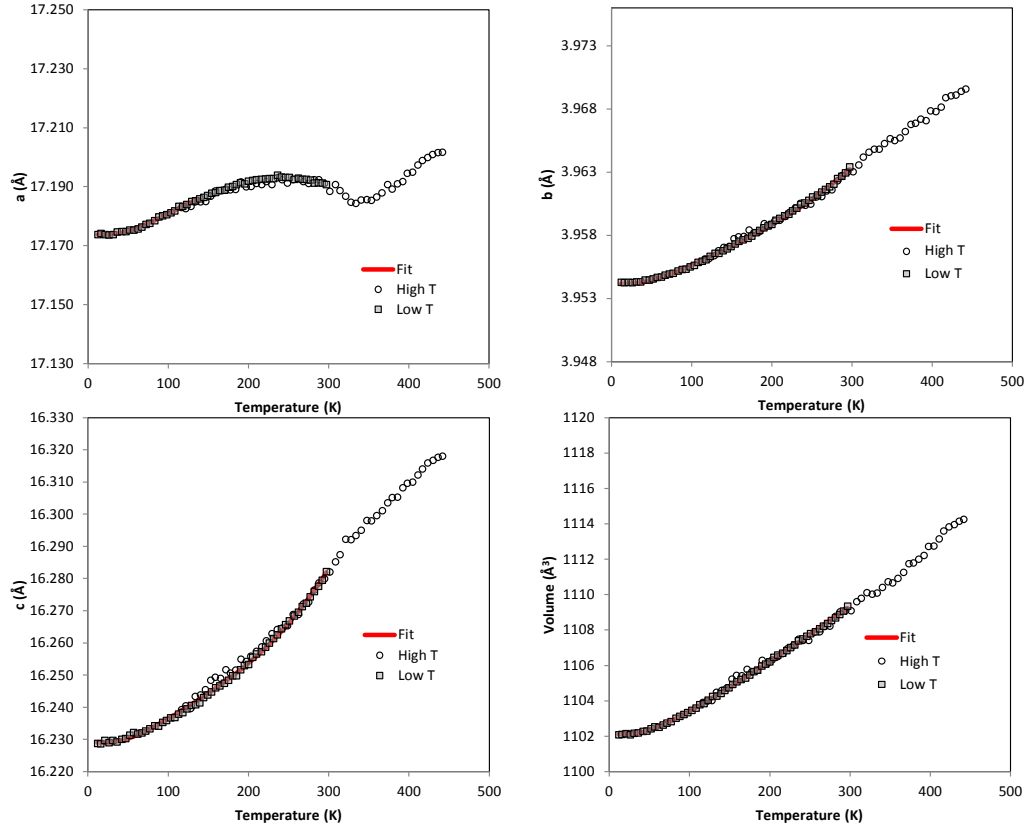
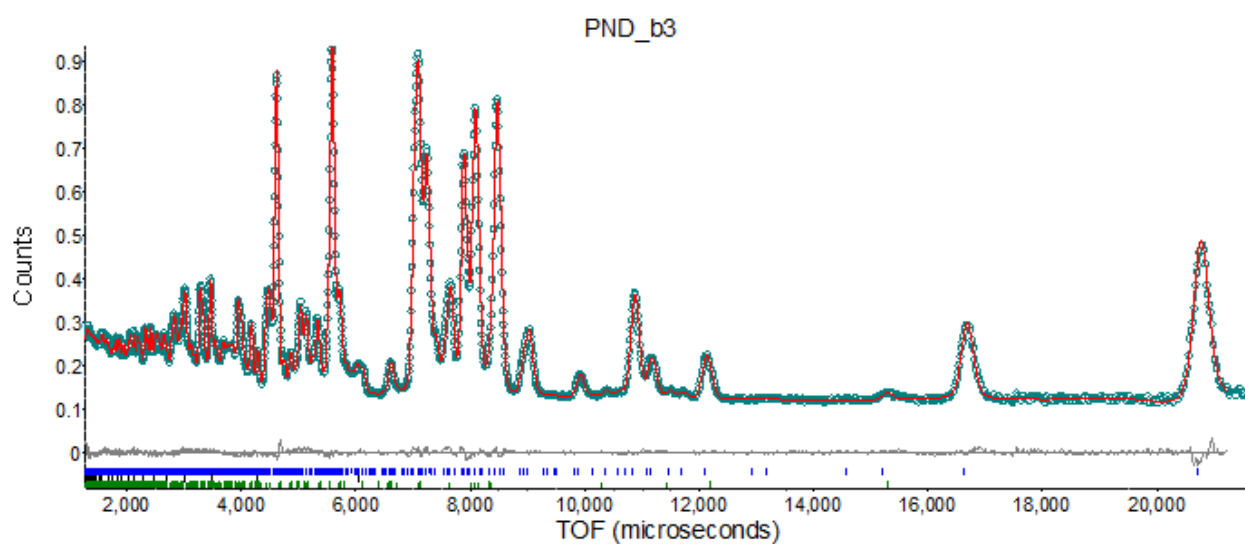
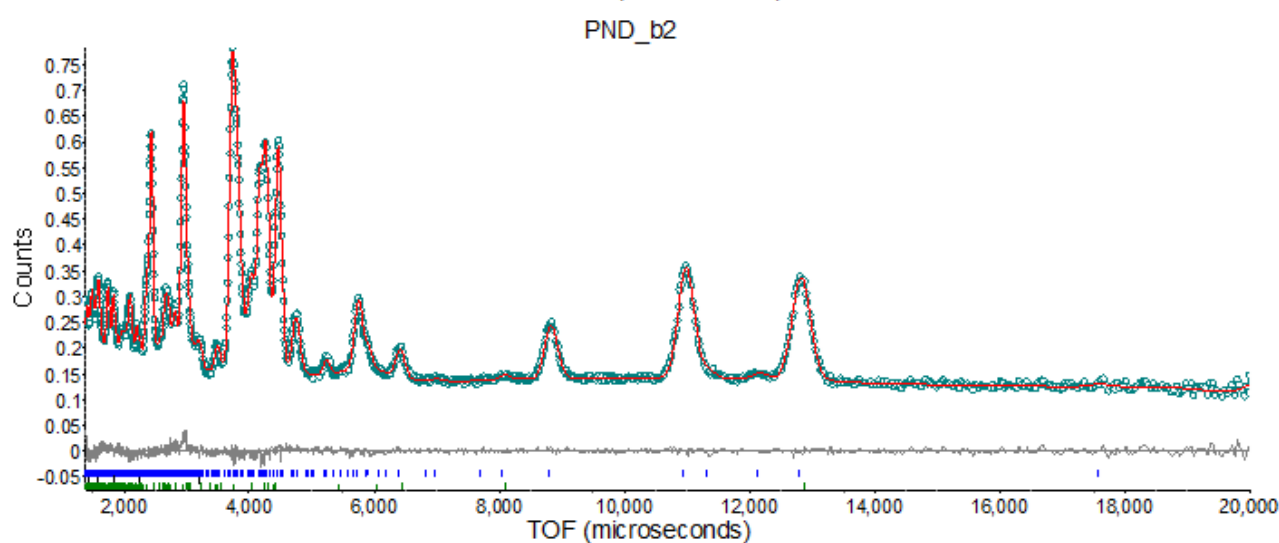
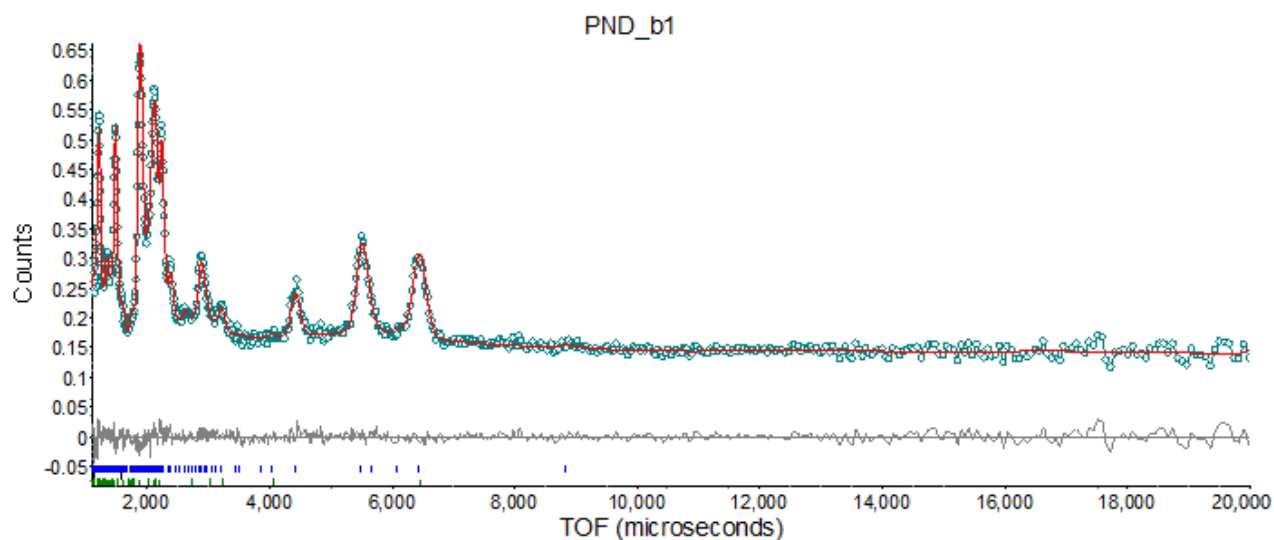
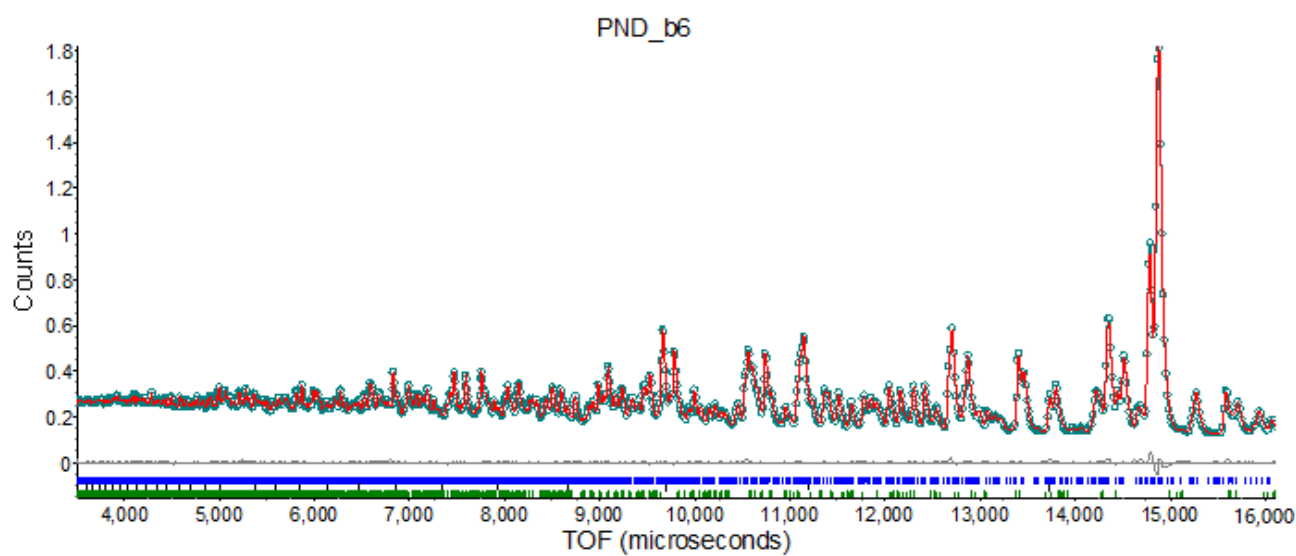
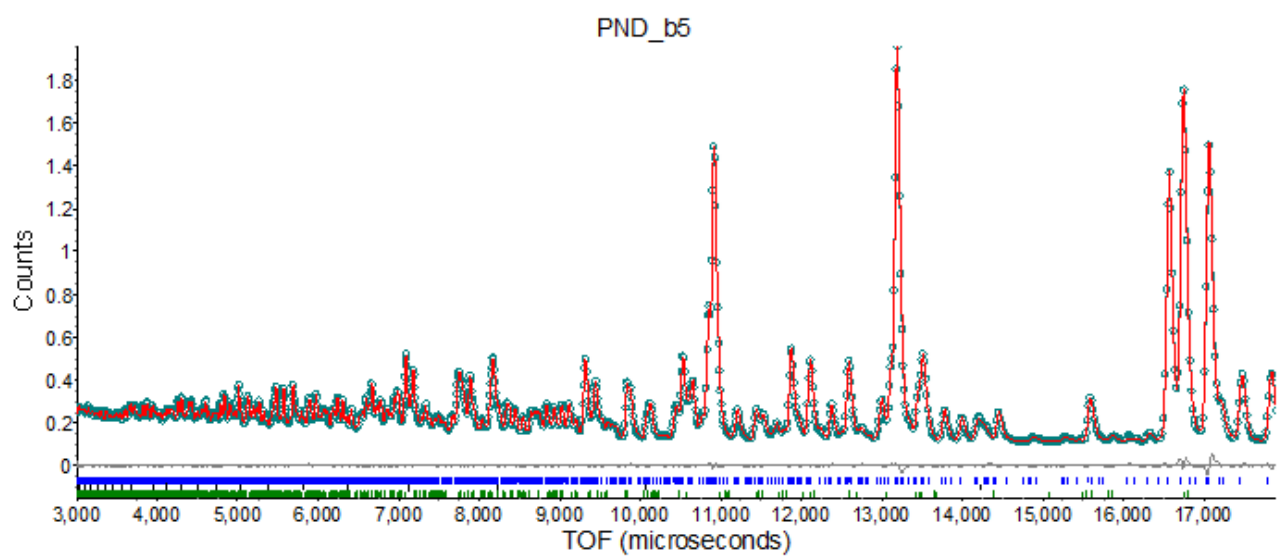
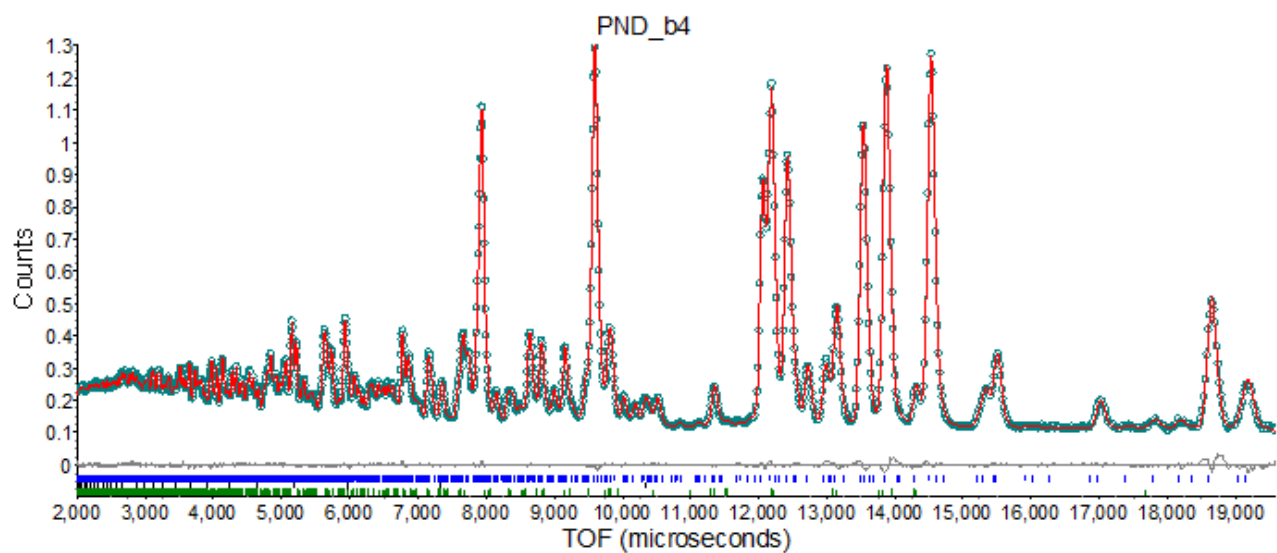


Figure S2. Temperature dependence of cell parameters of β - $\text{Ce}_2\text{O}_2\text{FeSe}_2$. The solid curves were fitted based on Eq. 2. Closed data points collected in Phenix cryostat in Bragg-Brentano mode; open data points using a capillary set up and Oxford cyrostream. Lower-quality capillary data have been offset by 0.009, 0.002 and 0.007 Å for a , b and c respectively.





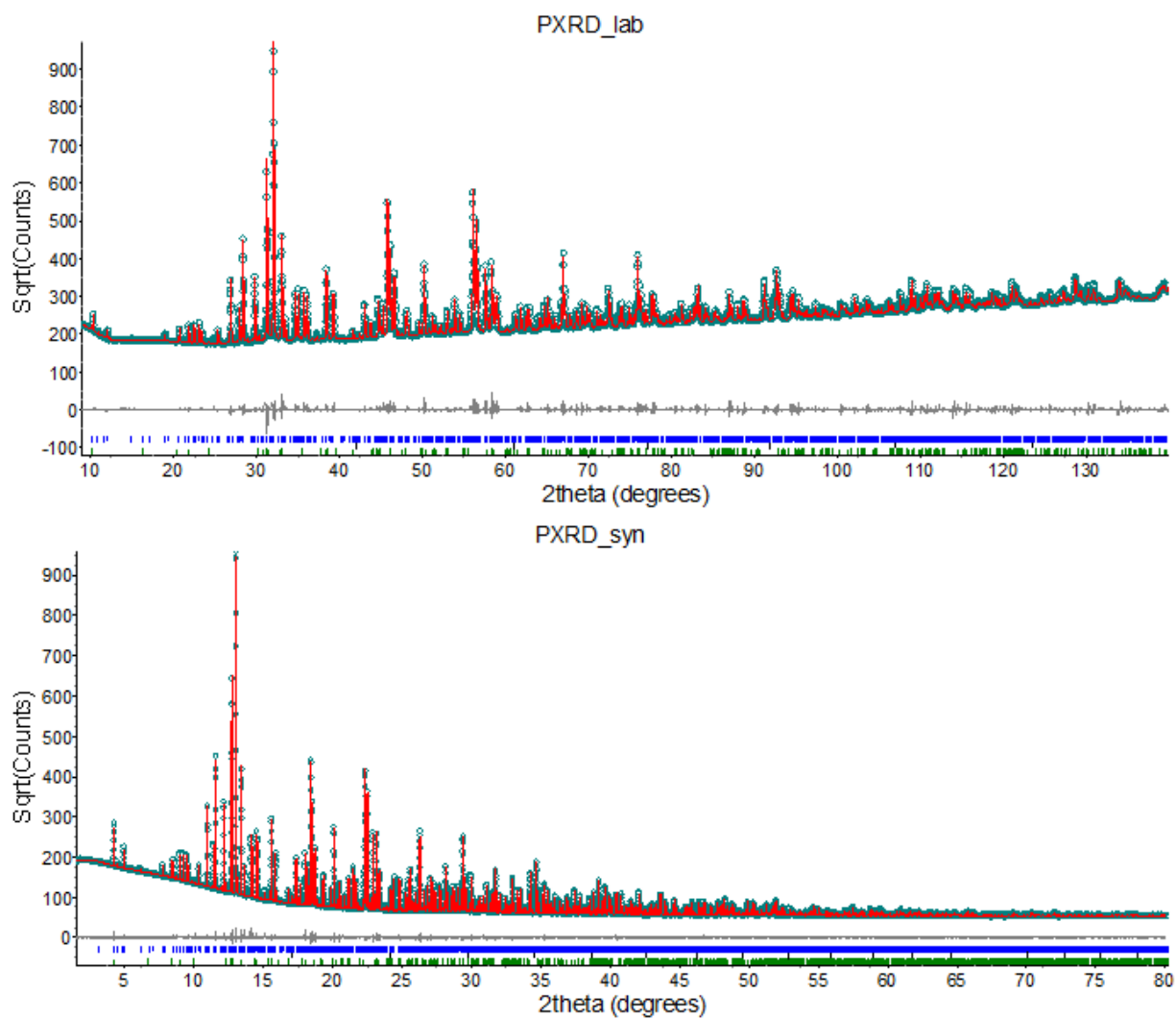
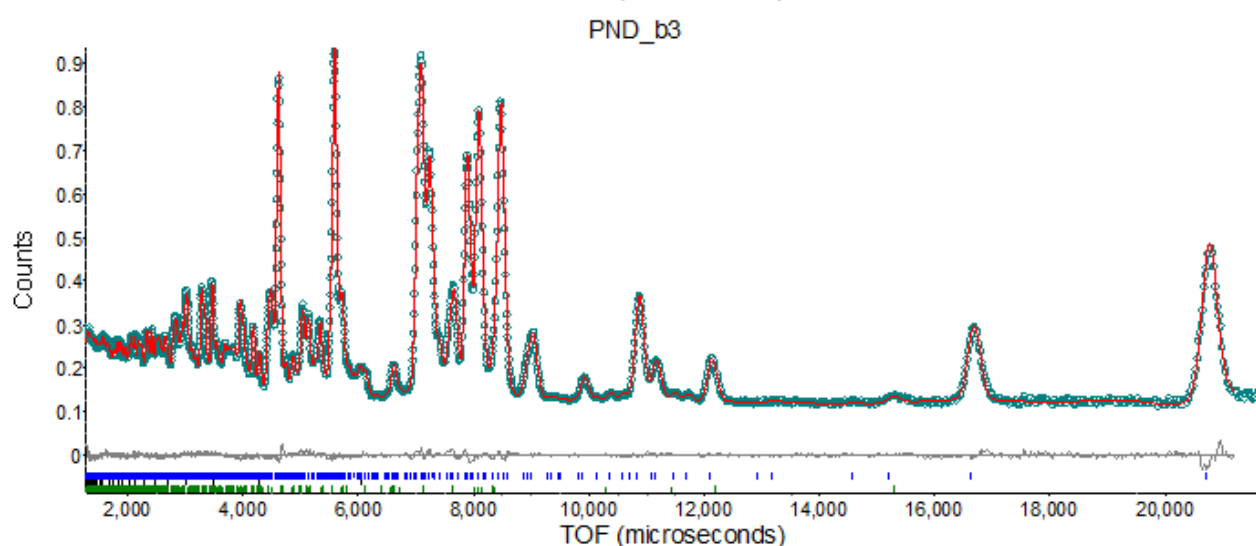
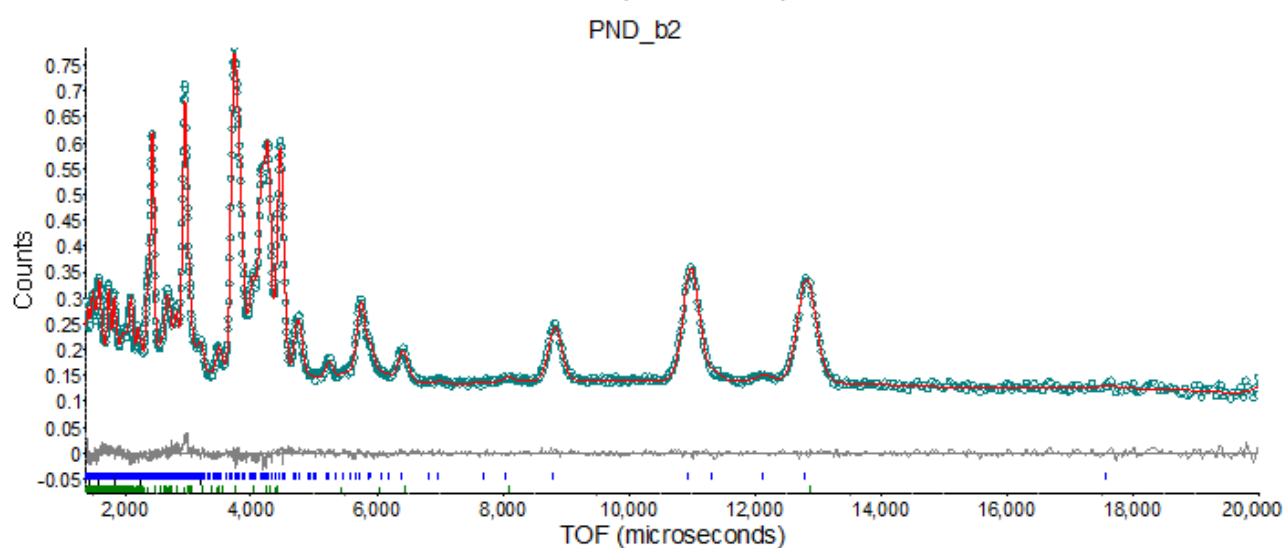
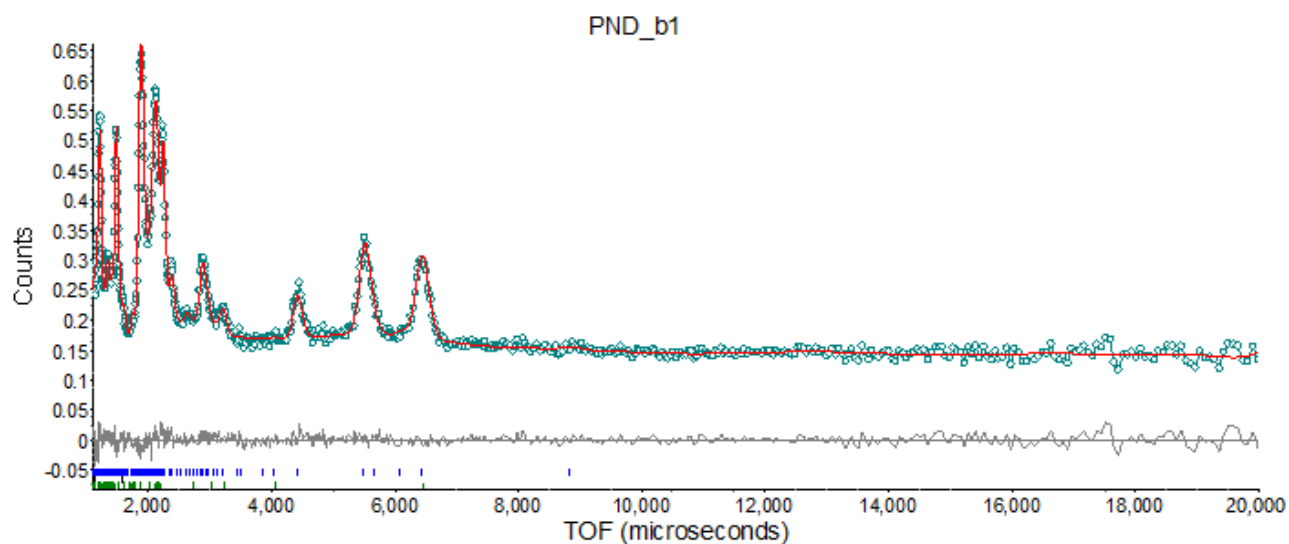
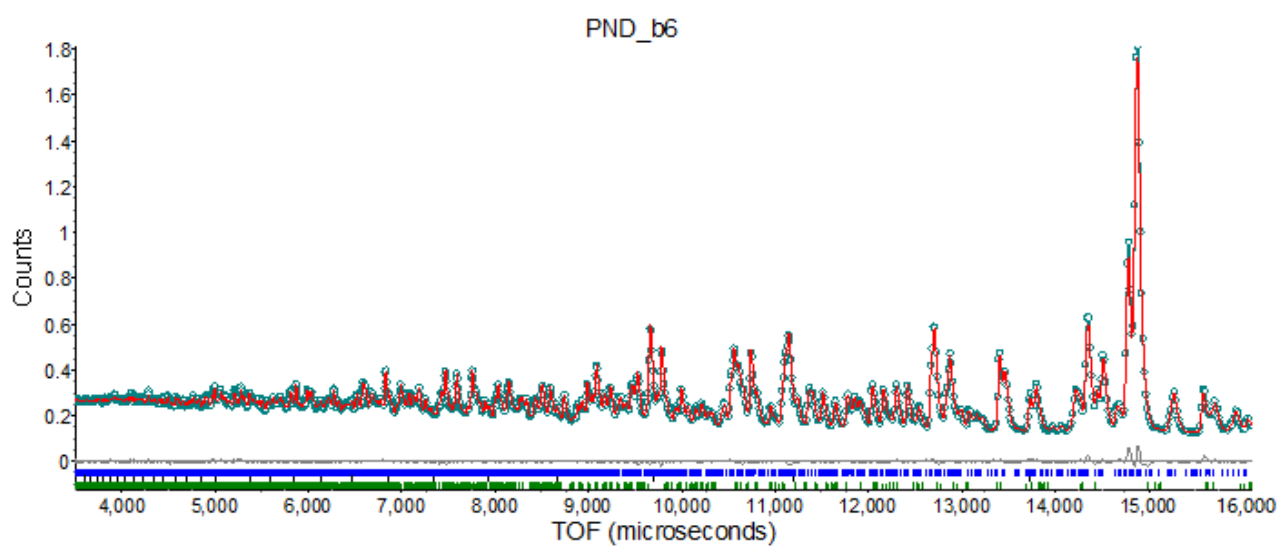
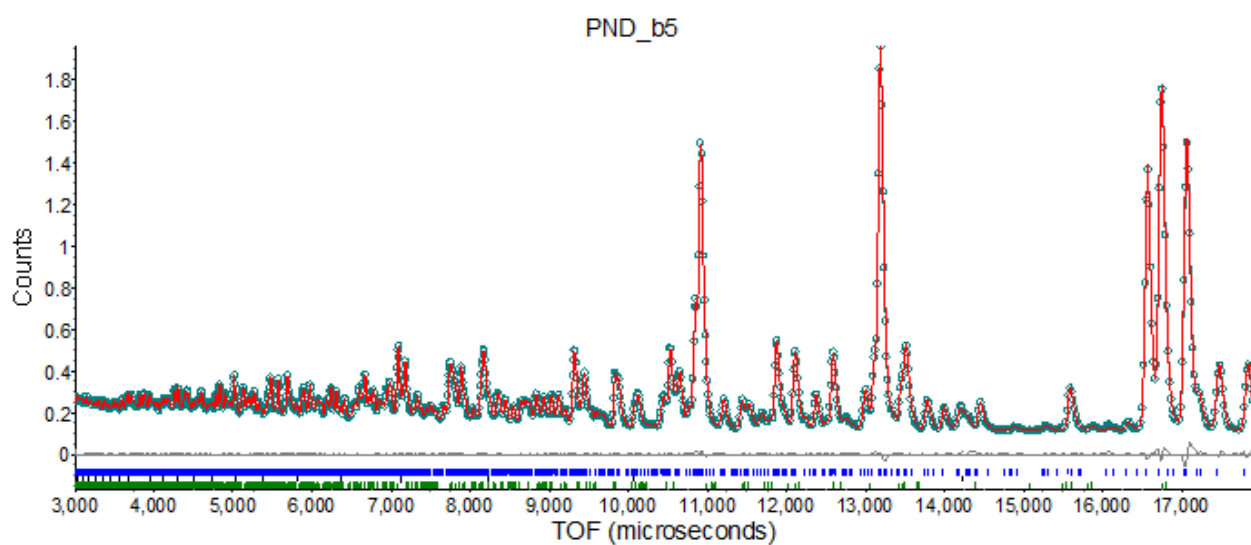
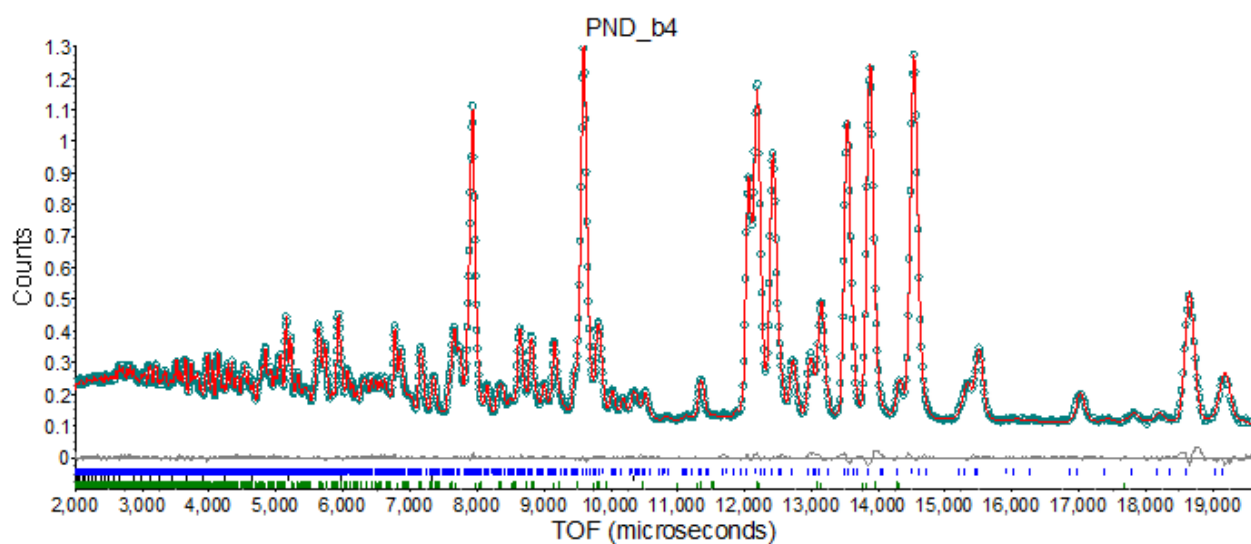


Fig. S3. Rietveld refinement profiles of $\text{Ce}_2\text{O}_2\text{FeSe}_2$ from combined refinement of room temperature data using $Pna2_1$ model. Dots: observed, solid line: calculated curve; grey line below: difference curve; vertical tick marks: peak positions.





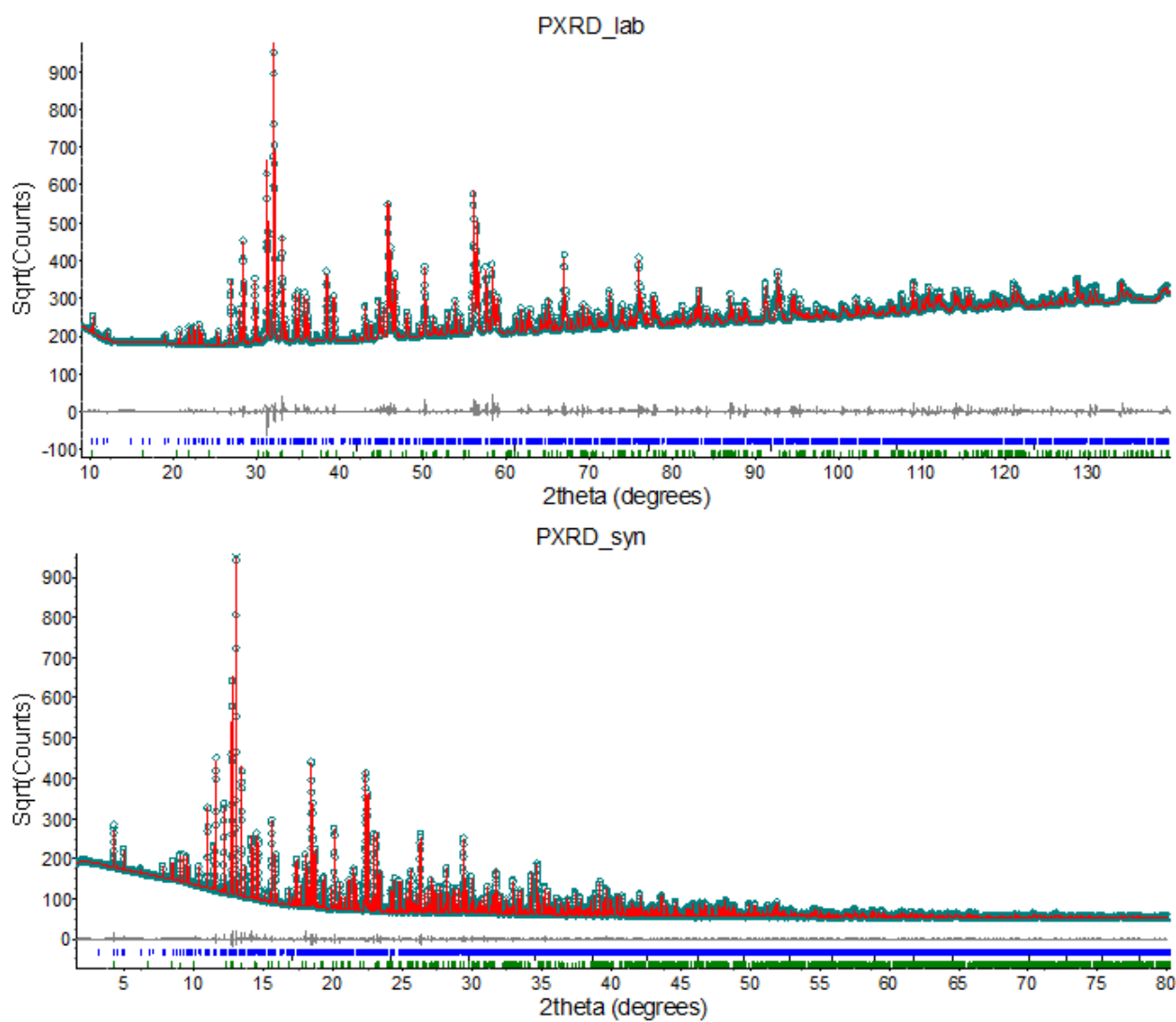


Fig. S4. Rietveld refinement profiles of $\text{Ce}_2\text{O}_2\text{FeSe}_2$ from combined refinement of room temperature data using *Pnma* model. Dots: observed, solid line: calculated curve; grey line below: difference curve; vertical tick marks: peak positions.

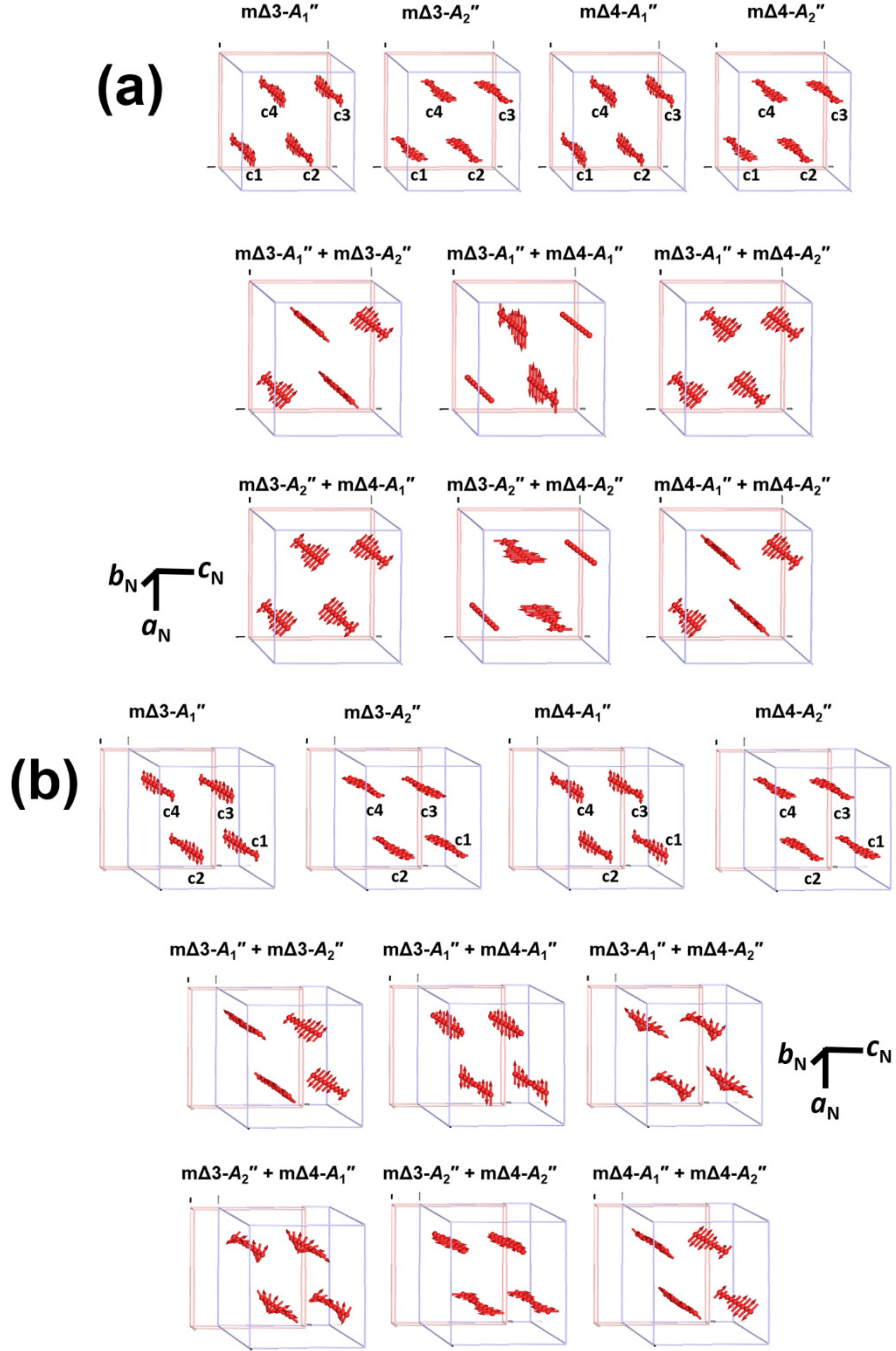


Fig. S5. The $m\Delta 3$ and $m\Delta 4$ magnetic moments modes in $a_N c_N$ plane of Fe1 (cf nuclear structure) and their combinations. (a) and (b) are two different phase choices between $m\Delta 3$ and $m\Delta 4$; c_1 to c_4 indicate the different chains along b_N axis and the amplitude of all modes are set to the same in the figure. The PND data was fitted best by $m\Delta 3-A_2'' + m\Delta 4-A_1''$ models (both choices).

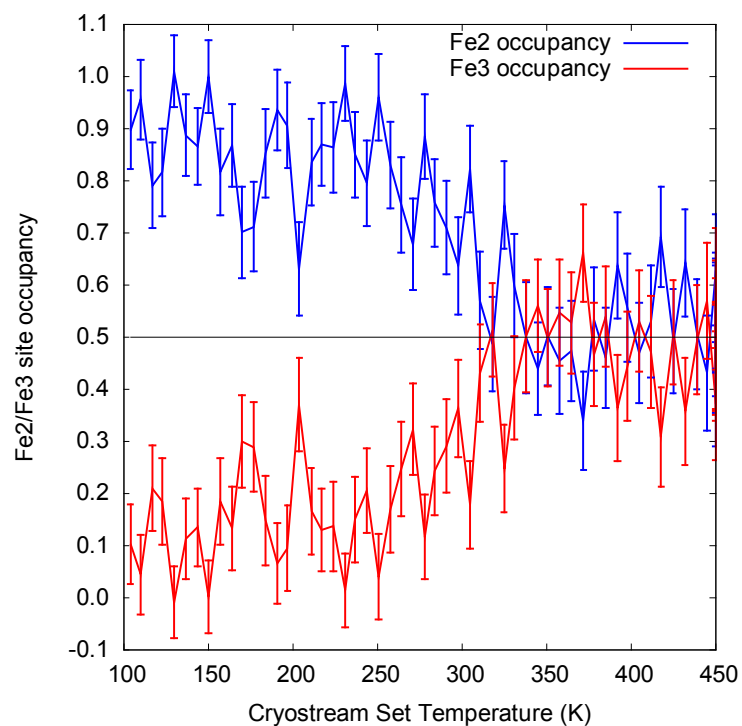


Fig. S6. Refined Fe site occupancies from “High T” variable temperature powder diffraction data discussed in the text. Data were collected relatively rapidly and the contribution of Fe2/Fe3 site ordering to diffraction data is relatively low. Despite this, the evolution of Fe site ordering with temperature can be observed.