Supplementary Information

Structural and magnetic characterization of the double perovskite Pb_2FeMoO_6.

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Table S1. Refined atomic parameters of Pb_2FeMoO_6 at room temperature.

Pb2FeMoO6 310 K

S.G. 225 (Fm-3m)
a=b=c=7.96477(7)Å
Vol.=505.265(14) Å³ (Z=1)
d=8.701 g/cm³

Atom (site)	x	y	z	occ.	U_{iso}(Å²)
PB1	0.2298(2)	0.2298(2)	0.2298(2)	0.25	0.0078(8)
FE1	0	0	0	0.825(12)	0.0072(3)
MO2	0	0	0	0.175(12)	0.0072 (3)
MO1	½	½	½	0.725(12)	0.0072 (3)
FE2	½	½	½	0.275(12)	0.0072 (3)
O1	0.7495(4)	0	0	1	0.0108(3)

Nobs = 11174
Number of parameters = 70
Rp = 0.0359
wRp = 0.0484

Table S2. Agreement factors of the refinement carried out on the individual histograms at RT.

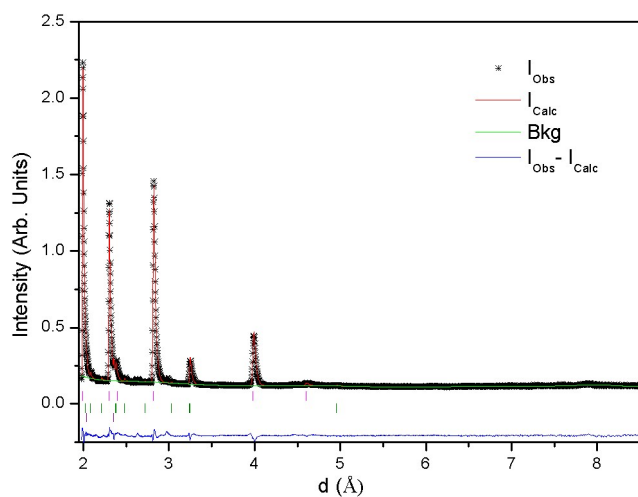| Histogram	wRp	Rp	Nobs	R(F²)
SPRD	0.0604	0.0359	1030	0.1509
TOF 2θ=58.3°	0.0373	0.0247	26	0.0458
TOF 2θ=90°	0.0505	0.0352	154	0.0890
TOF 2θ=121.6°	0.0370	0.0252	167	0.0891
TOF 2θ=152.8°	0.0527	0.0413	258	0.1021

Figure S1. Rietveld plot of the TOF data collected on bank 2 of WHISH (2θ=58.3°) at 310 K.

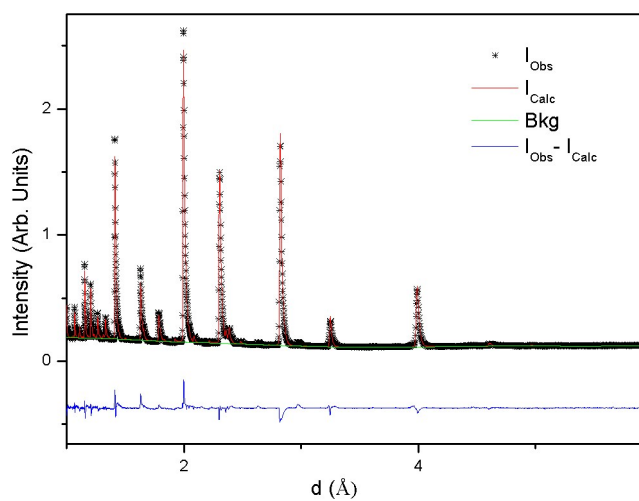**Figure S2.** Rietveld plot of the TOF data collected on bank 3 of WHISH (2θ=90°) at 310 K.

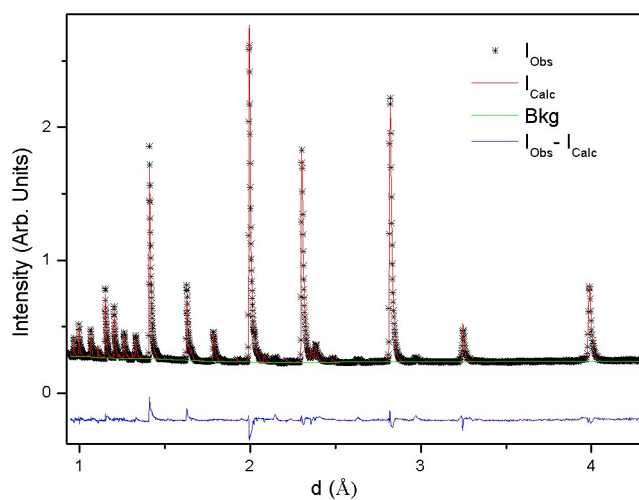**Figure S3.** Rietveld plot of the TOF data collected on bank 4 of WHISH (2θ=121.6°) at 310 K.

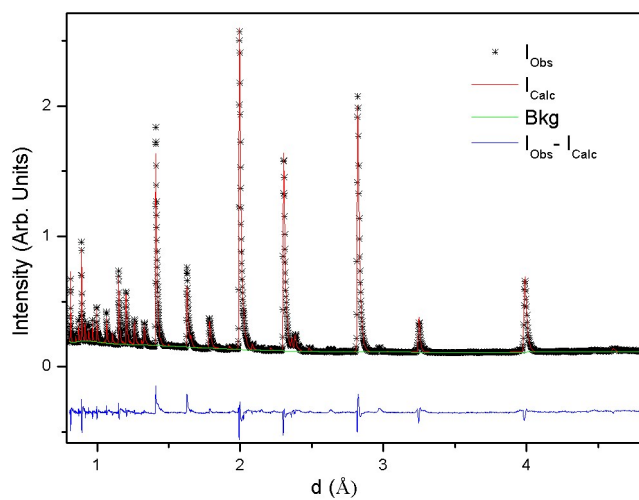**Figure S4.** Rietveld plot of the TOF data collected on bank 5 of WHISH (2θ=152.8°) at 310 K.

Figure S5. Comparison of the TOF diffraction data collected at 310 and 1.5 K.

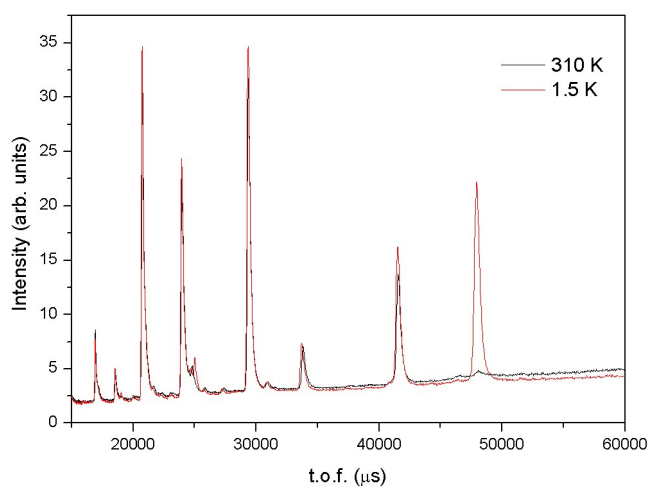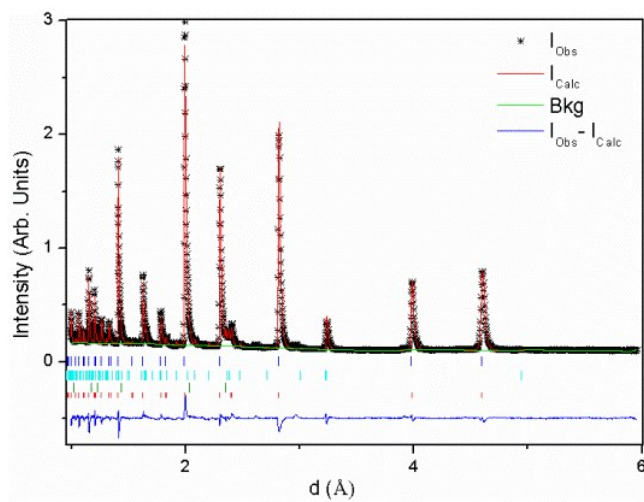**Figure S6.** Rietveld plot of the TOF data collected on bank 3 of WHISH (2θ=90°) at 1.5 K.

Table S3. Refined atomic parameters of Pb_2FeMoO_6 at 1.5 K.

		Pb2FeMoO6 1.5 K			
		S.G. 225 (Fm-3m) a=b=c=7.95579(3) Å Vol.= 503.559 (6) Å³ (Z=1)			
Atom (site)	x	y	z	occ.	$U_{iso}(Å^2)$
PB1	0.22981(15)	0.22981(15)	0.22981(15)	0.25	0.0027(3)
FE1	0	0	0	0.780	0.0021(2)
MO2	0	0	0	0.220	0.0021(2)
MO1	½	½	½	0.780	0.0021(2)
FE2	½	½	½	0.220	0.0021(2)
O1	0.7458(2)	0	0	1	0.0082(2)

Nobs = 9572
Number of parameters = 106
$R(F^2)$ = 0.052
Rp = 0.032
wRp = 0.043

Table S4. Agreement factors of the refinement carried out on the individual histograms at 1.5 K.

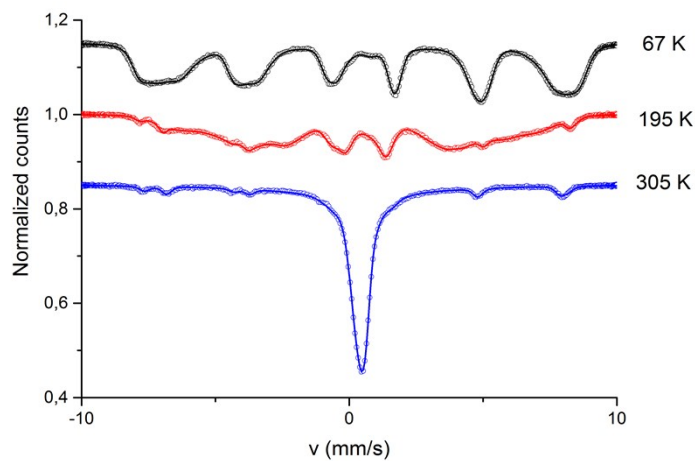| Histogram	wRp	Rp	Nobs	$R(F^2)$
TOF 2θ=58.3°	0.0359	0.0250	49	0.0582
TOF 2θ=90°	0.0337	0.0241	199	0.0582
TOF 2θ=121.6°	0.0498	0.0386	221	0.0898
TOF 2θ=152.8°	0.0496	0.0411	326	0.1078

Figure S7. Thermal evolution of Mössbauer spectra. Data fitting are reported as solid lines.

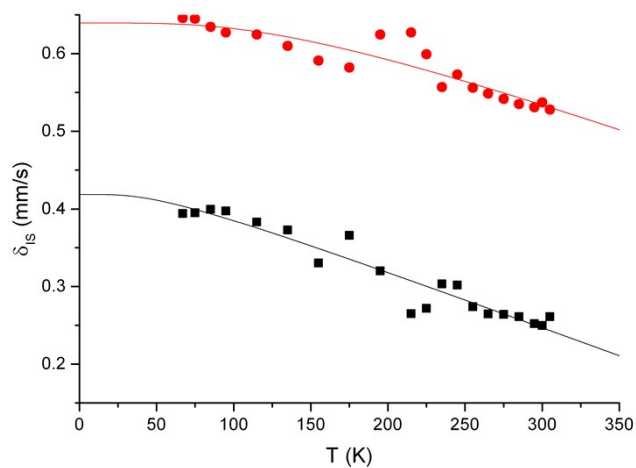**Figure S8.** Isomer shift vs T for both the subcomponents: the straight lines stand for the Debye model based fit.

Figure S9. Thermal trend of t_a with the related fit based on the Debye model.
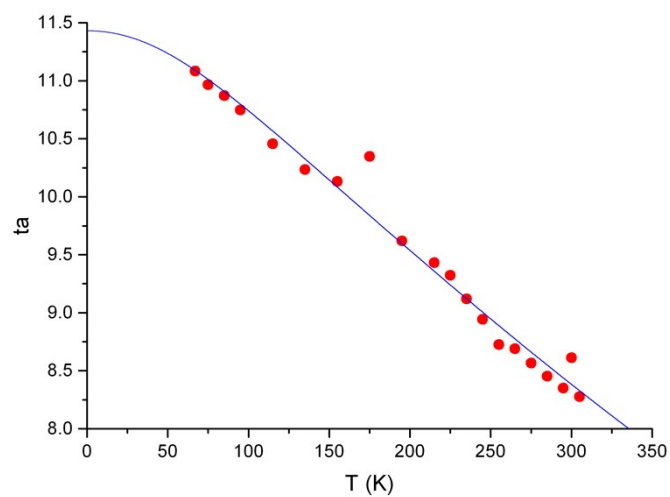
Figure S10. From top to bottom, hyperfine field density for the two contributions at 67, 195 and 305 K, respectively.