

# INVESTIGATION OF CRYSTAL AND MAGNETIC STRUCTURES OF MULTIFERROIC MATERIAL UNDER HIGH PRESSURE



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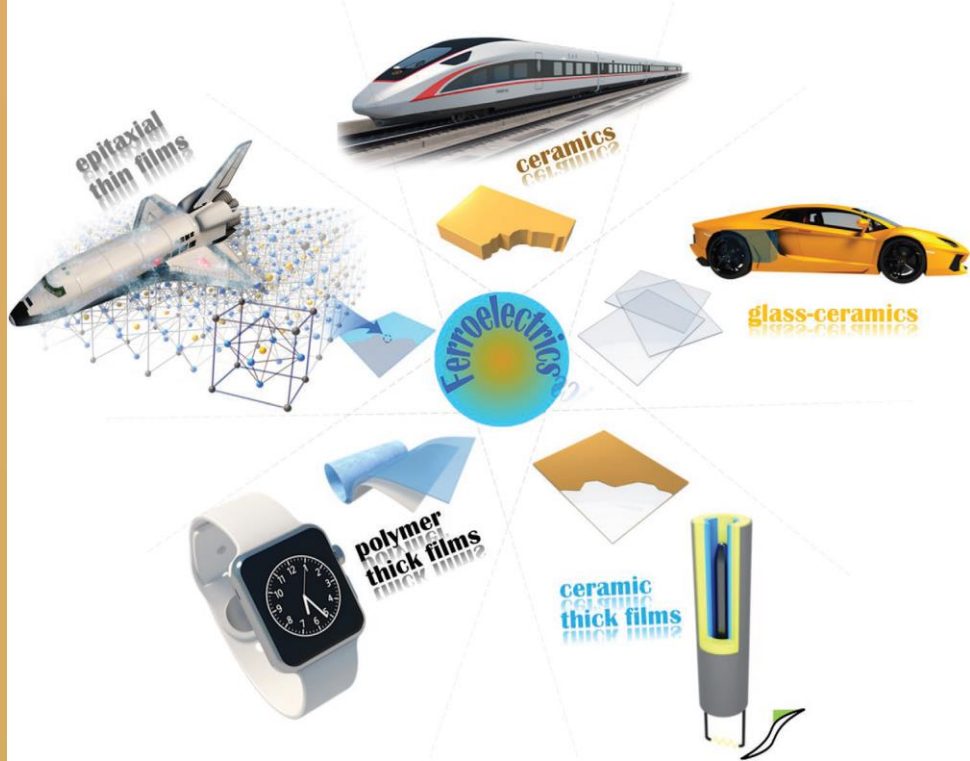
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## Relevance

Multiferroic materials, showing ordering of both electrical and magnetic degrees of freedom, are promising candidates enabling the design of novel electronic devices. Various mechanisms ranging from geometrically or spin-driven improper ferroelectricity via lone-pairs, charge-order or -transfer support multiferroicity in single-phase or composite compounds. The search for materials showing these effects constitutes one of the most important research fields in solid-state physics during the last years, but scientific interest even traces back to the middle of the past century. Especially, a potentially strong coupling between spin and electric dipoles captured the interest to control via an electric field the magnetization or via a magnetic field the electric polarization. This would imply a promising route for novel electronics.



But apart from potential application, the multiferroic compounds are attractive for great number of scientific research

## High Pressure

The knowledge of relationship between magnetic and crystal structure of such compounds, which can be obtained from high-pressure investigations, is very essential for understanding the nature and mechanism of physical phenomena observed in it.

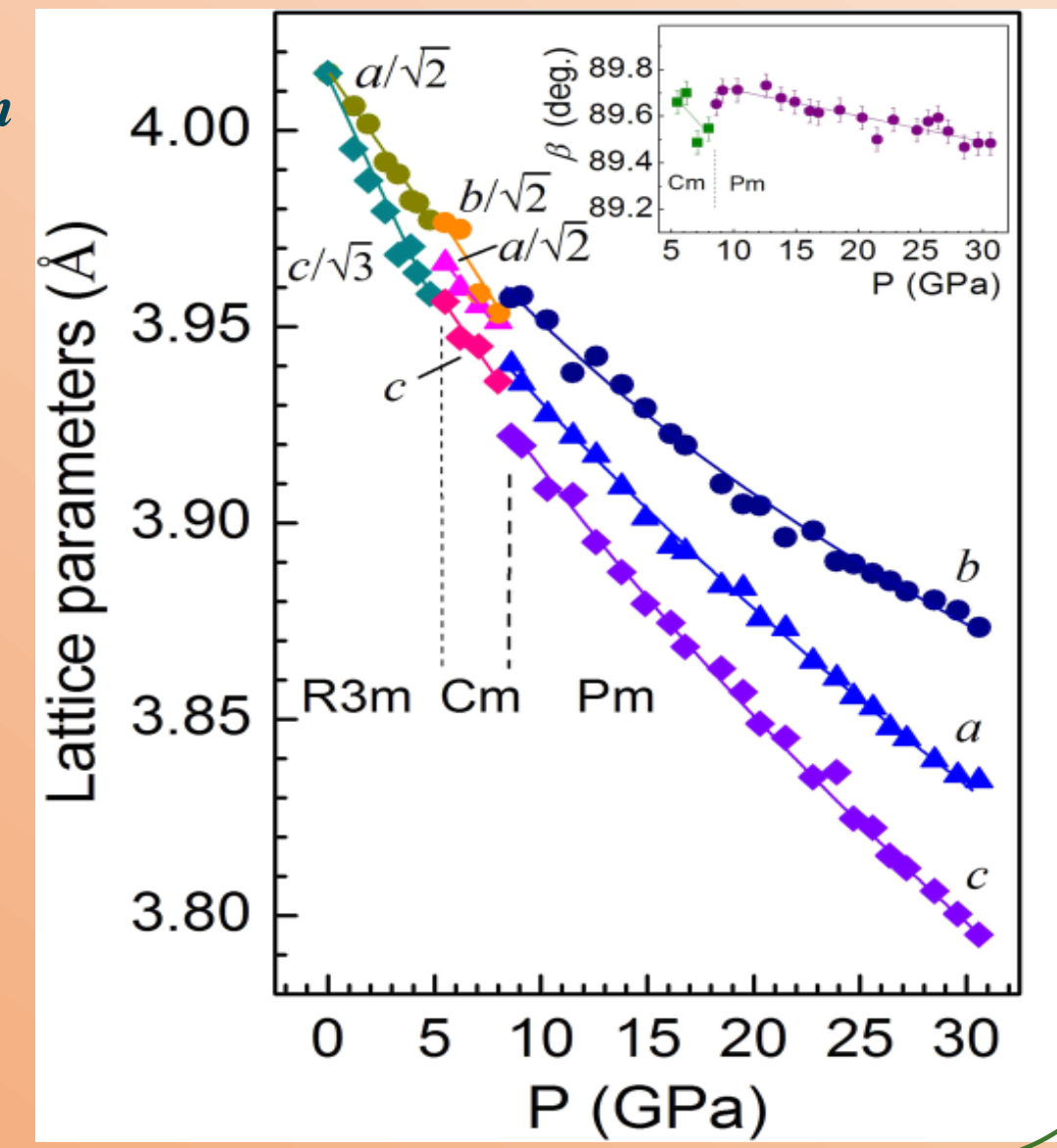
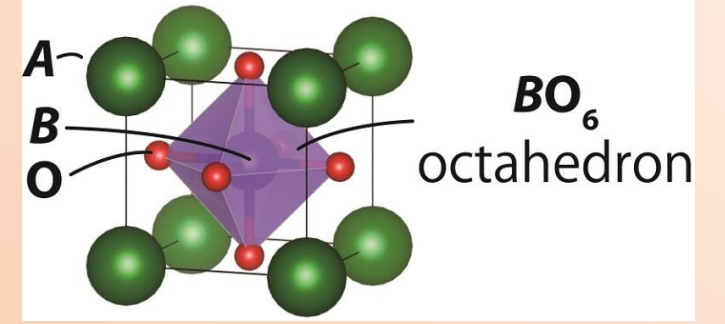
For example, in similar  $\text{PbFe}_{1/2}\text{Nb}_{1/2}\text{O}_3$  are observed: in paramagnetic phase with sp.g.  $\text{Pm-3m}$

Below  $T_C = 376\text{K}$  – tetragonally distorted structure  $\text{P4mm}$

Below  $T_I = 355$  – another polar phase  $\text{R3m/Cm}$

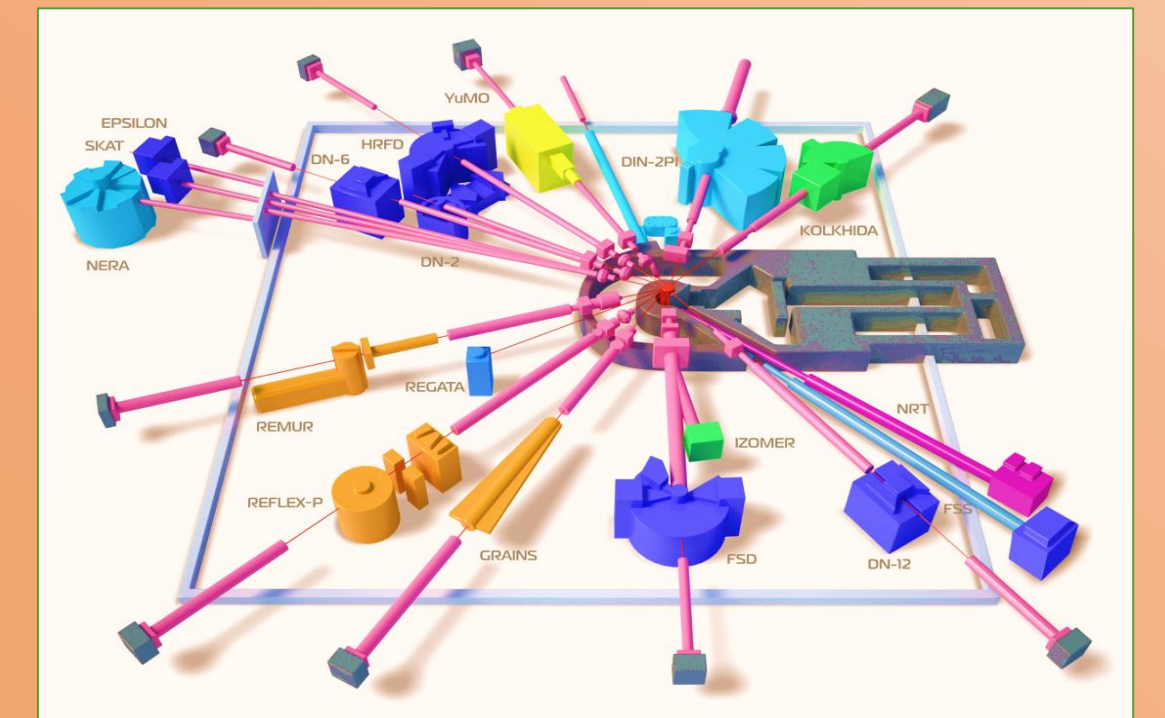
$T_N = 155\text{K}$  – AFM G-type

Under high pressure:  $\text{R3m} \rightarrow \text{Cm} \rightarrow \text{Pm}$



## Experimental methods

In present work was performed neutron diffraction studies of PFWO at high pressures and low temperature. Neutron powder diffraction measurements at high pressures up to 7 GPa were performed with the DN-12 diffractometer at the IBR-2 high-flux pulsed reactor [FLNP, JINR, Dubna, Russia] using the sapphire anvil high-pressure cell. In order to improve the understanding of the lattice instabilities the Raman spectroscopy studies of the vibration spectra of the compound under pressure up to 30 GPa were performed.

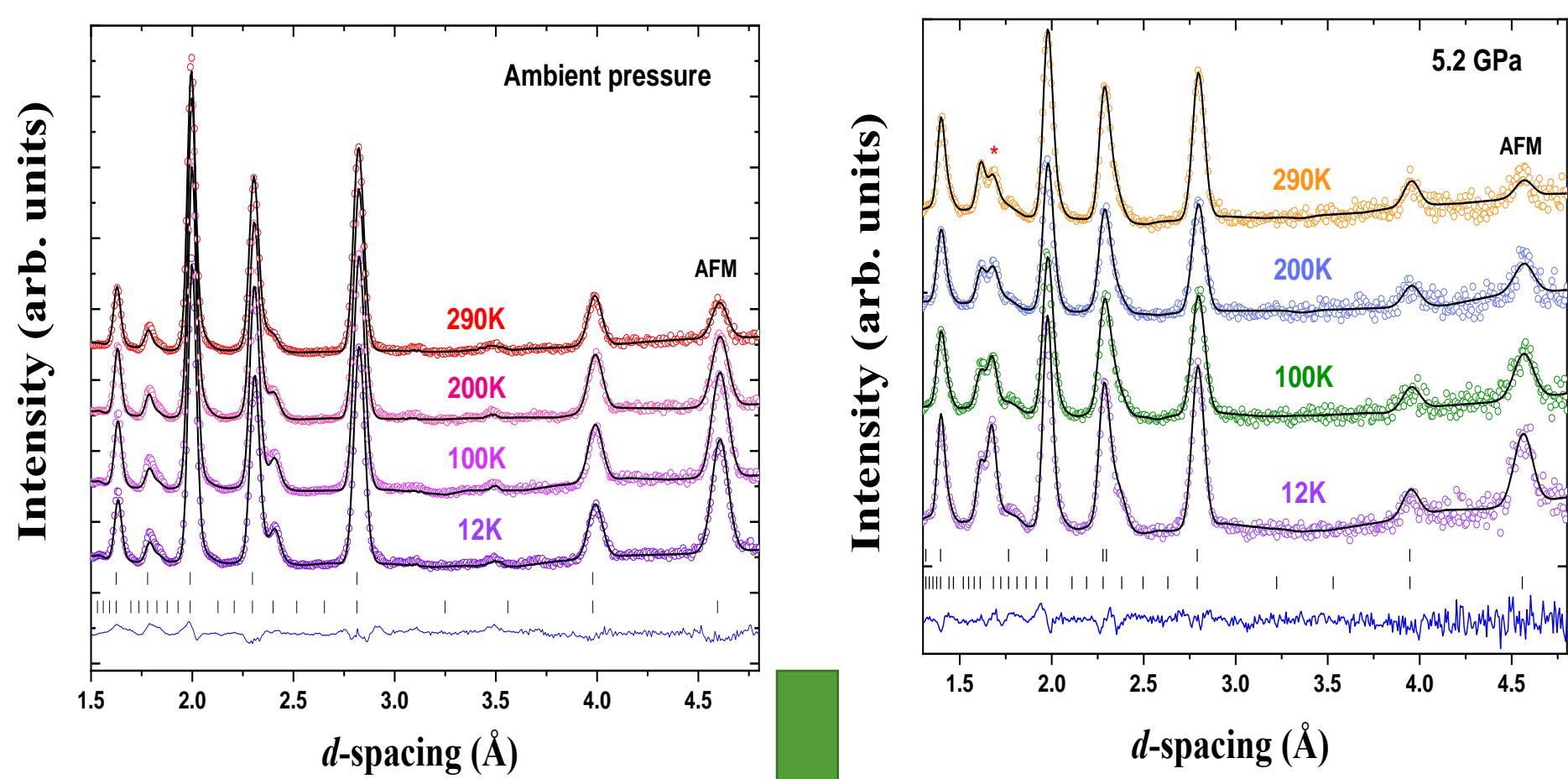


## Results

$\text{PbFe}_{2/3}\text{W}_{1/3}\text{O}_3$  - With cubic perovskite structure (space group  $\text{Pm-3m}$ )

PFW is ferroelectric and antiferromagnetic showing a perovskite-type structure, in which the two kinds of cations ( $\text{Fe}^{3+}$  and  $\text{W}^{6+}$ ) are randomly distribute at the octahedral B-site positions.

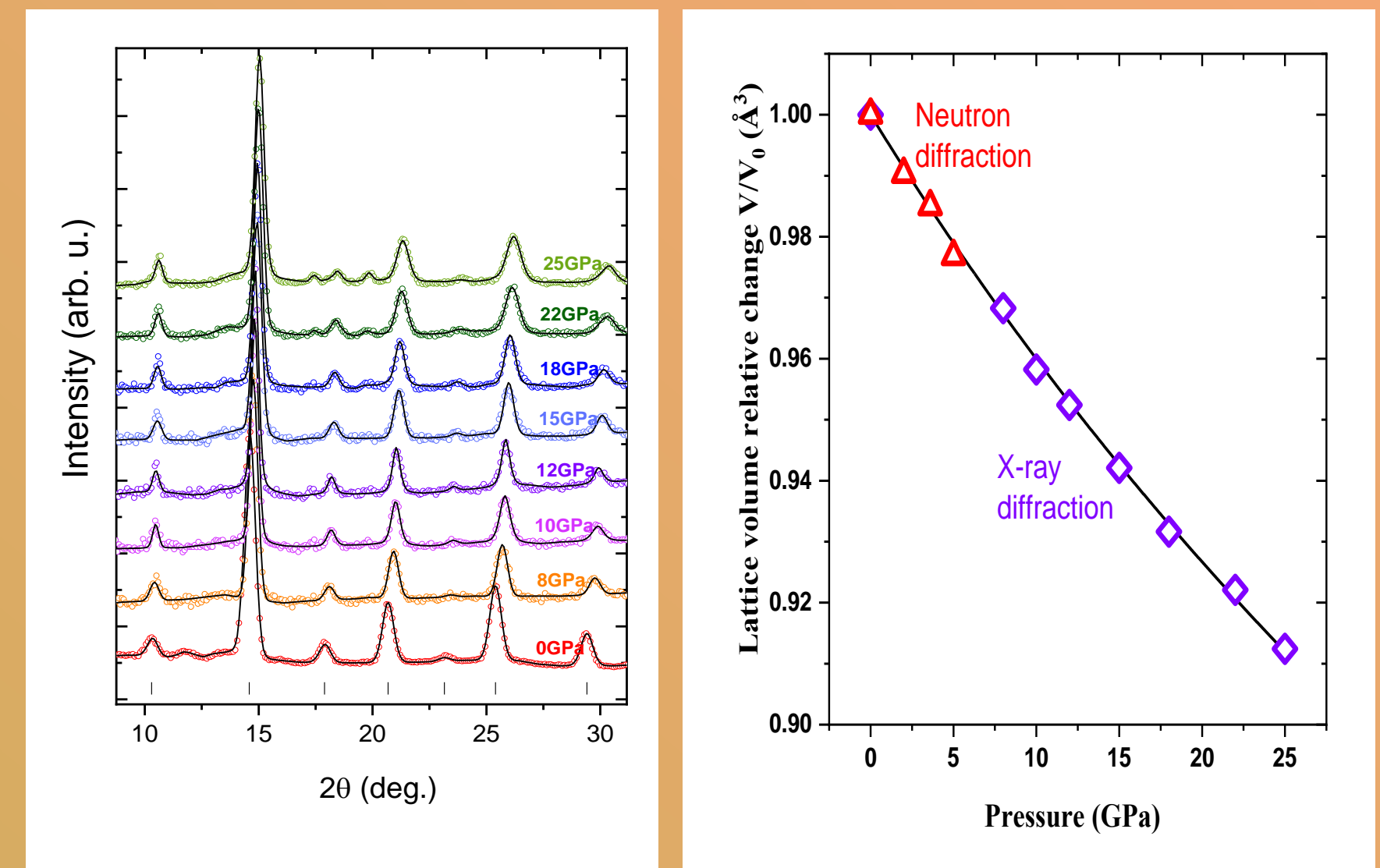
### Neutron diffraction



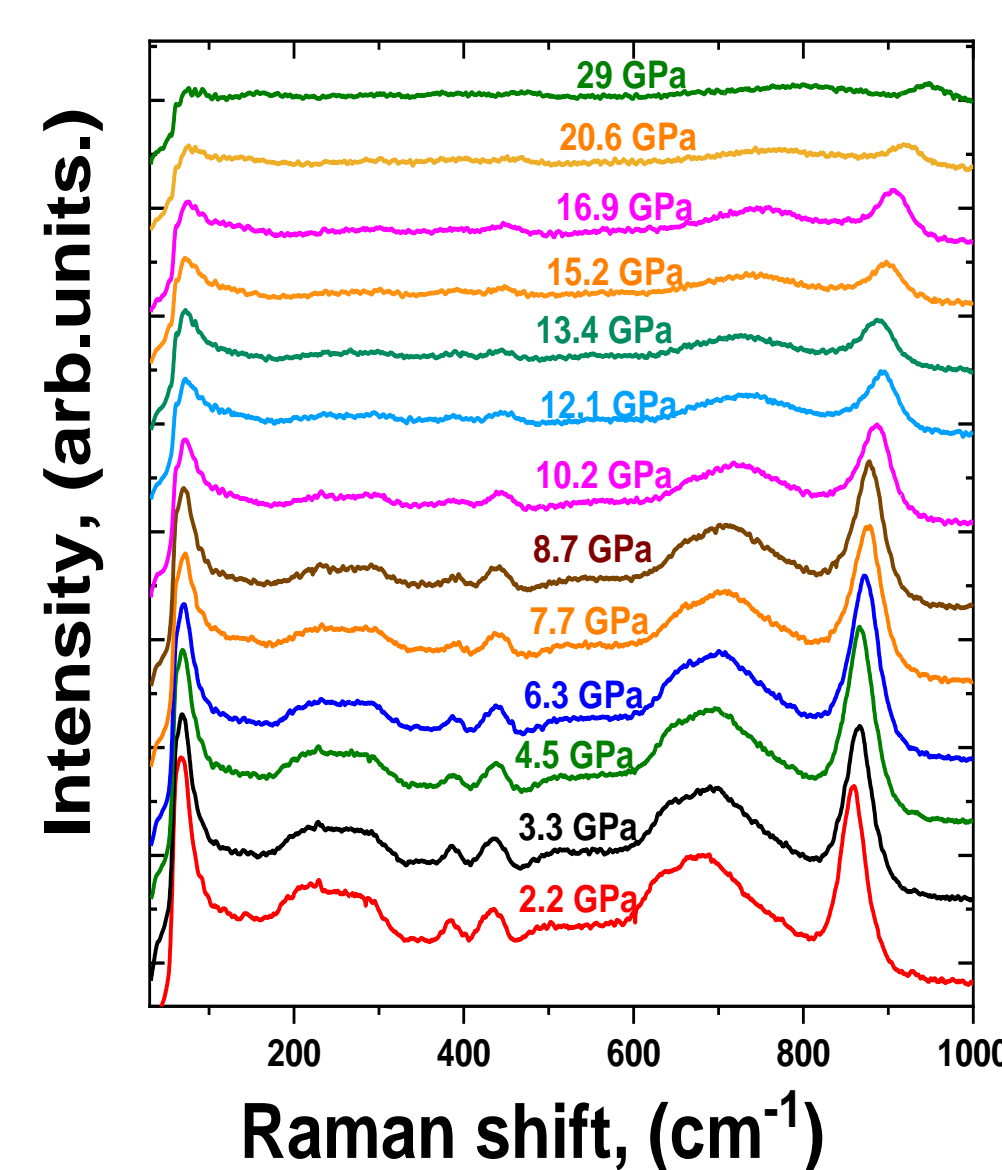
Space group:  $\text{Pm-3m}$   
 $a = b = c = 3.984(1) \text{ \AA}$  at 300K  
 $\alpha = \beta = \gamma = 90^\circ$   
 Magnetic moment:  $\mu_{\text{Fe}} = 3, 22 \mu_B$  at 12 K

Atom	x	y	z
Pb	0.0000	0.0000	0.0000
Fe/W	0.5000	0.5000	0.5000
O	0.5000	0.5000	0.00000

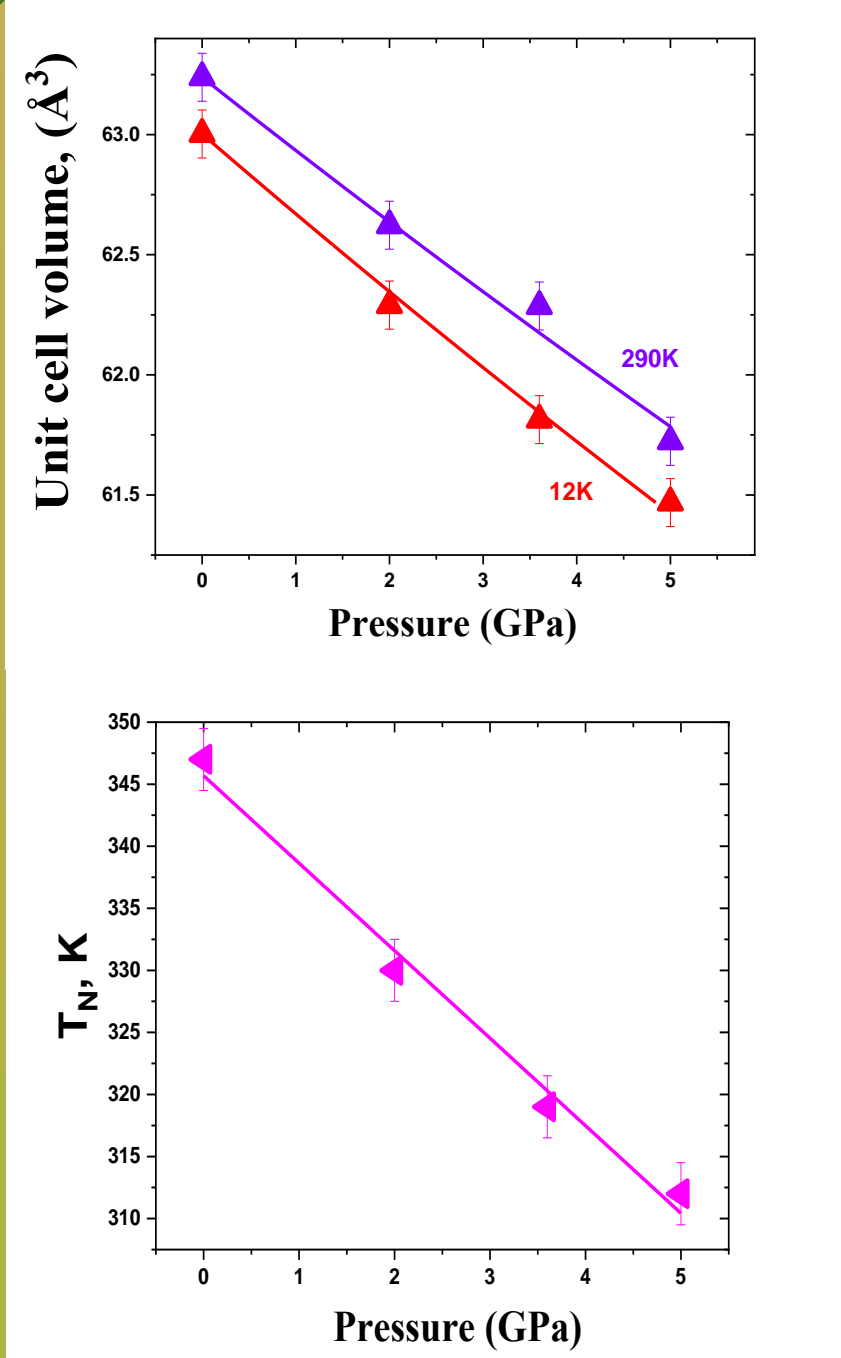
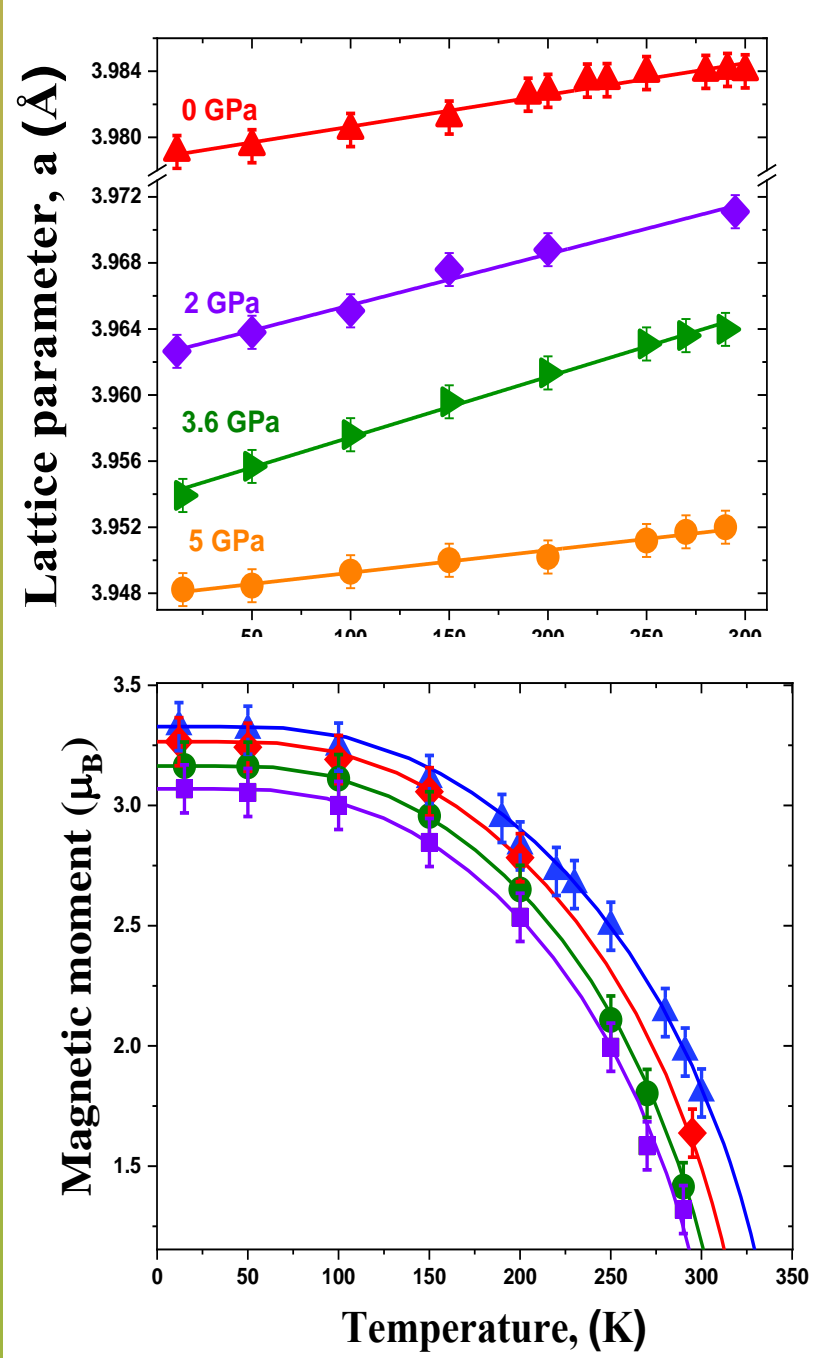
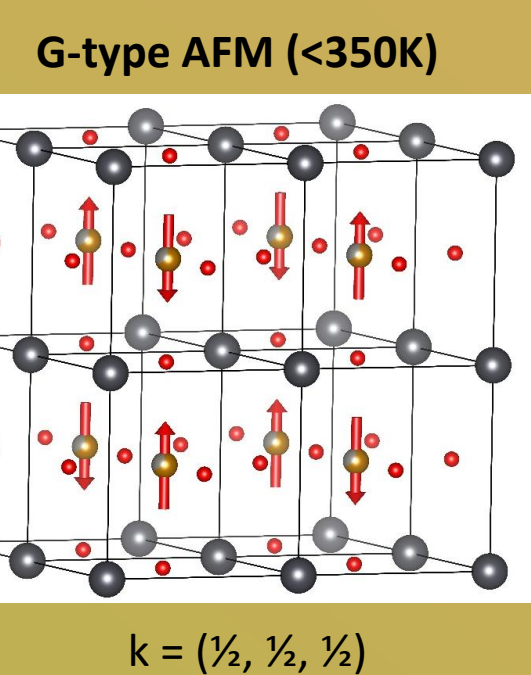
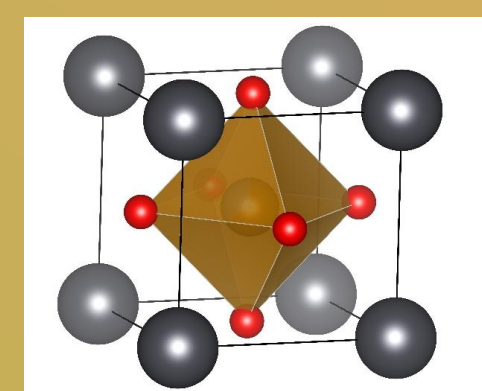
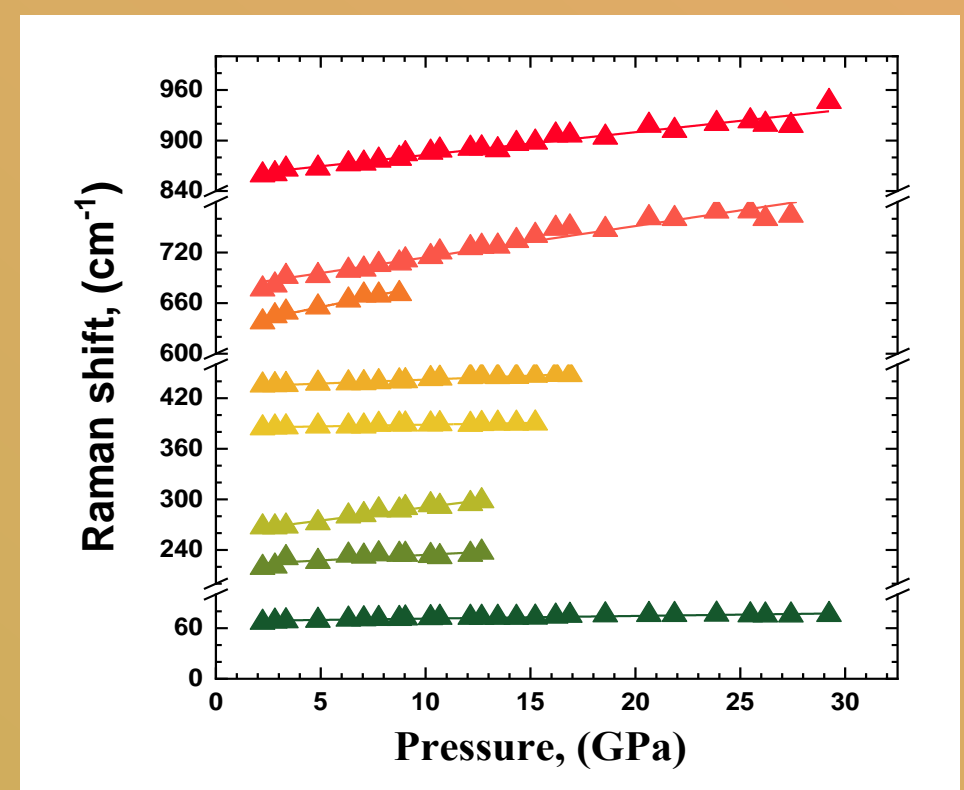
### X-ray diffraction



### Raman spectroscopy



Raman shift (cm <sup>-1</sup> )	Assignment
200-300	Localized asymmetric Pb-O modes
300-500	bending modes W-O-W and Fe-O-Fe
630 - 750	stretching mode W-O
860	stretching mode of Fe-O-W bonds



The obtained baric and temperature dependences of the lattice parameter, unit cell volume, magnetic moment and Neel temperature

## Summary

The crystal and magnetic structure of  $\text{PbFe}_{2/3}\text{W}_{1/3}\text{O}_3$  were investigated by means of neutron and x-ray diffraction, Raman spectroscopy. Pressure dependences of the volume, unit cell parameters and magnetic moments of antiferromagnetic (AFM) phase, Neel temperature were also calculated. With increasing temperature and pressure, slight decreasing of the magnetic moments of iron ions in PFWO were observed, however, although the crystal structure remains stable up to high pressures with a space group  $\text{Pm-3m}$ . Some Raman modes have been found on the Raman spectra, which in such compounds are correlated with the existence of nanoregions, however, with increasing pressure, these modes noticeably widen and vanish.