XRD characterization of orthoferrites $YFeO_3$ and $HoFeO_3$

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Outline

- Tasks
- Orthoferrites
- XRD measurements
- Crystallografic structure
- Results
- Conclusions

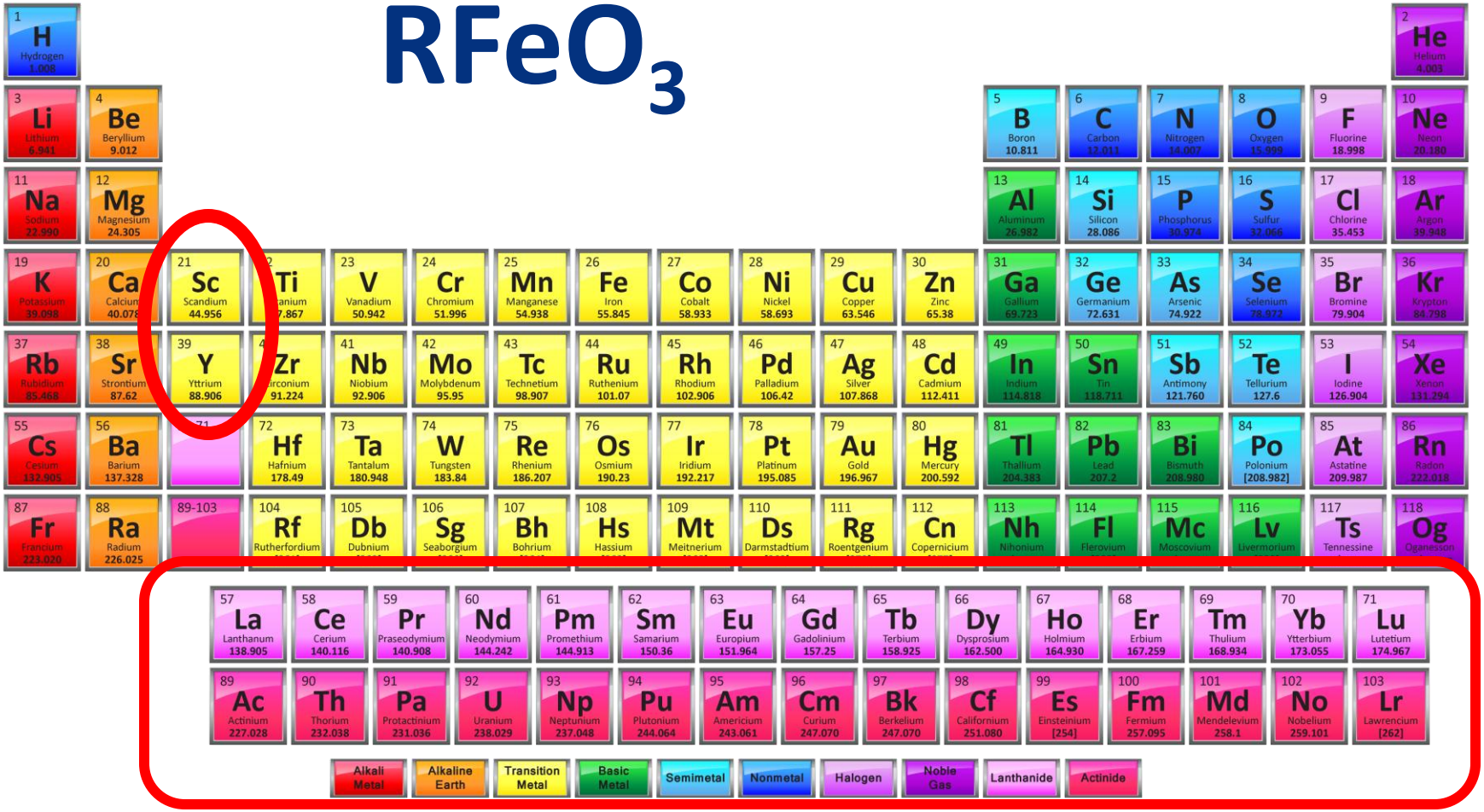
Tasks

1. Sample preparation for X-ray diffraction.
2. Realization of diffraction measurements.
3. Diffractograms analyzes – refinement of the structure by the Rietveld method.
4. Electron density distribution calculation.

Orthofferites

crystal structure: **orthorhombic**
space group: **Pbnm**

$RFeO_3$



STRUCTURE

ABX_3

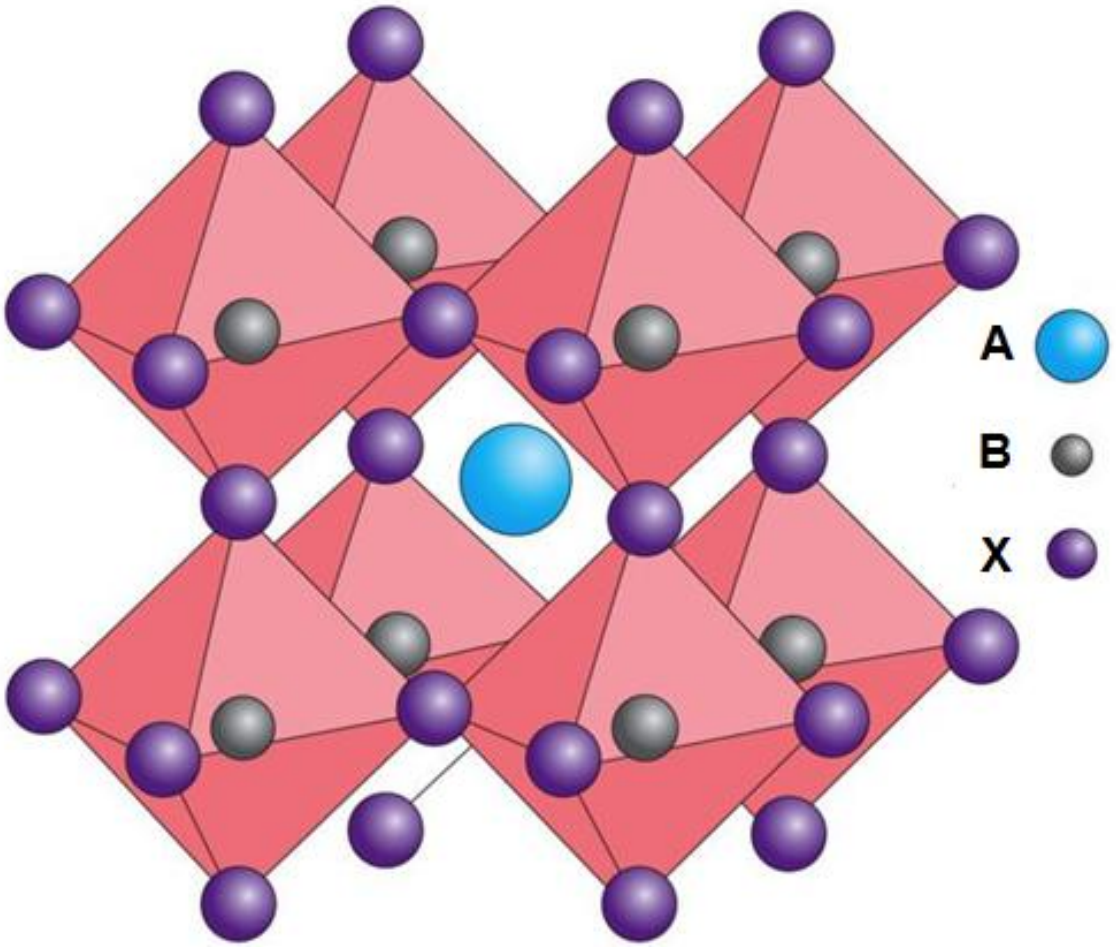


FIG.1. Crystallographic structure of perovskite ABX_3

Orthoferrites

- Mutiferroism (antiferromagnetism, ferromagnetism, ferroelectricity)
- small anisotropy of Fe spins in a – c plane, and large anisotropy towards b axis,
- spin reorientation.

The R ionic moments in orthoferrites $RFeO_3$ affect the crystal field of Fe ions. It can be expected that R may affect the magnetic properties of orthoferrites $RFeO_3$ in aspects.

APPLICATION:

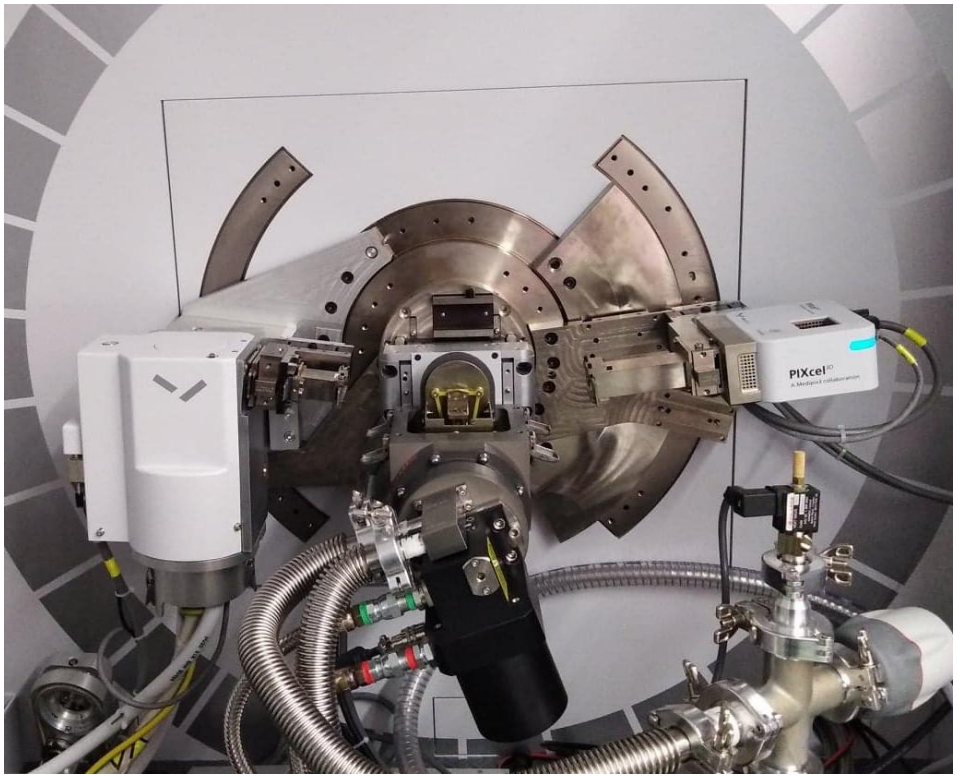
- Catalysis,
- gas separating,
- fuel cells,
- Sensing,
- magnetooptic device,
- environmental monitoring,
- spin valves,
- advanced information storage
- etc.

XRD measurements

15° - 118°
step 0.001°

Co $K_{\alpha 1}$ (λ = 1.7890 A) $K_{\alpha 2}$ (λ = 1.7929 A)

T = 20, 90, 160, 230, 295 K



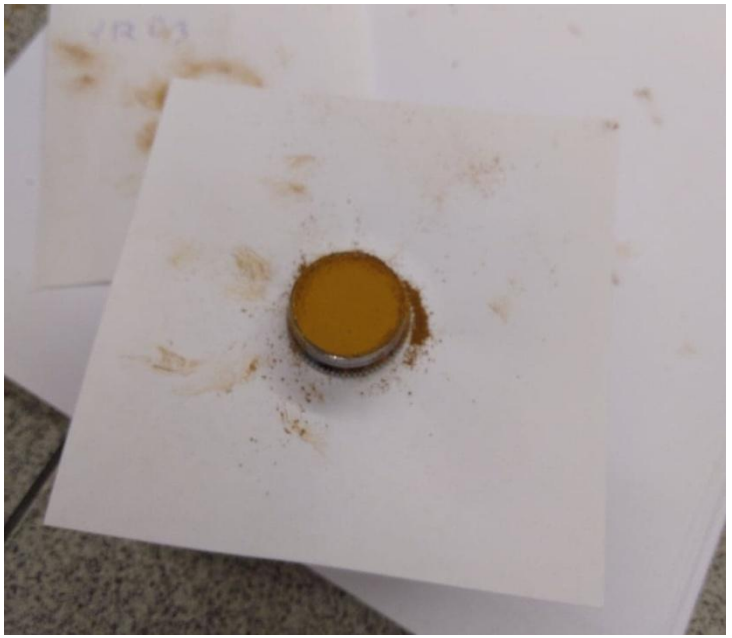


FIG.2. X-ray diffractometer Empyrean PANalytical (left) and sample holder (left)

XRD

Malvern Panalytical
a spectris company

HighScore

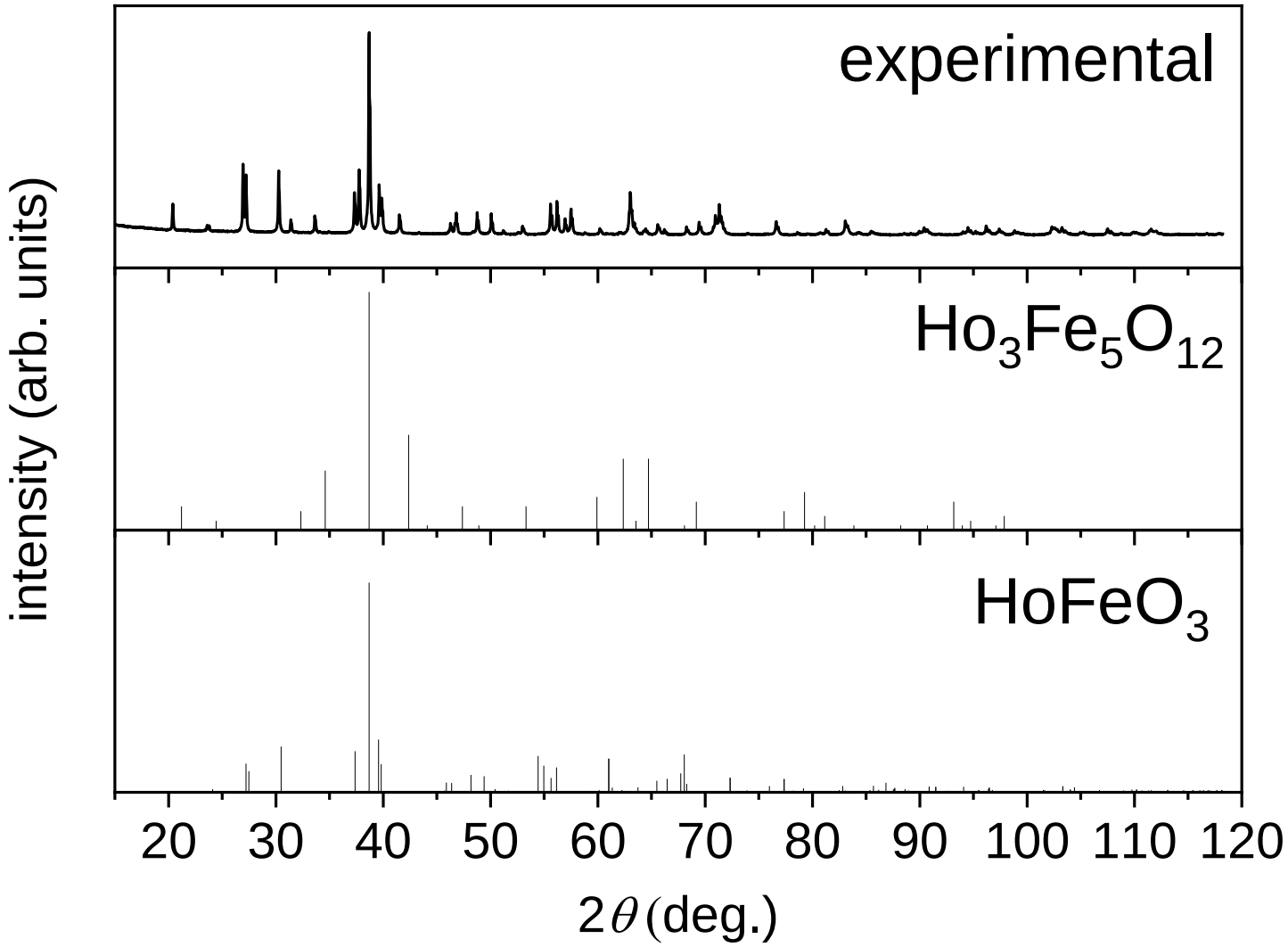


FIG.3. X-ray diffraction pattern of orthoferrite $HoFeO_3$. Sample revealed additional phase $Ho_3Fe_5O_{12}$

XRD

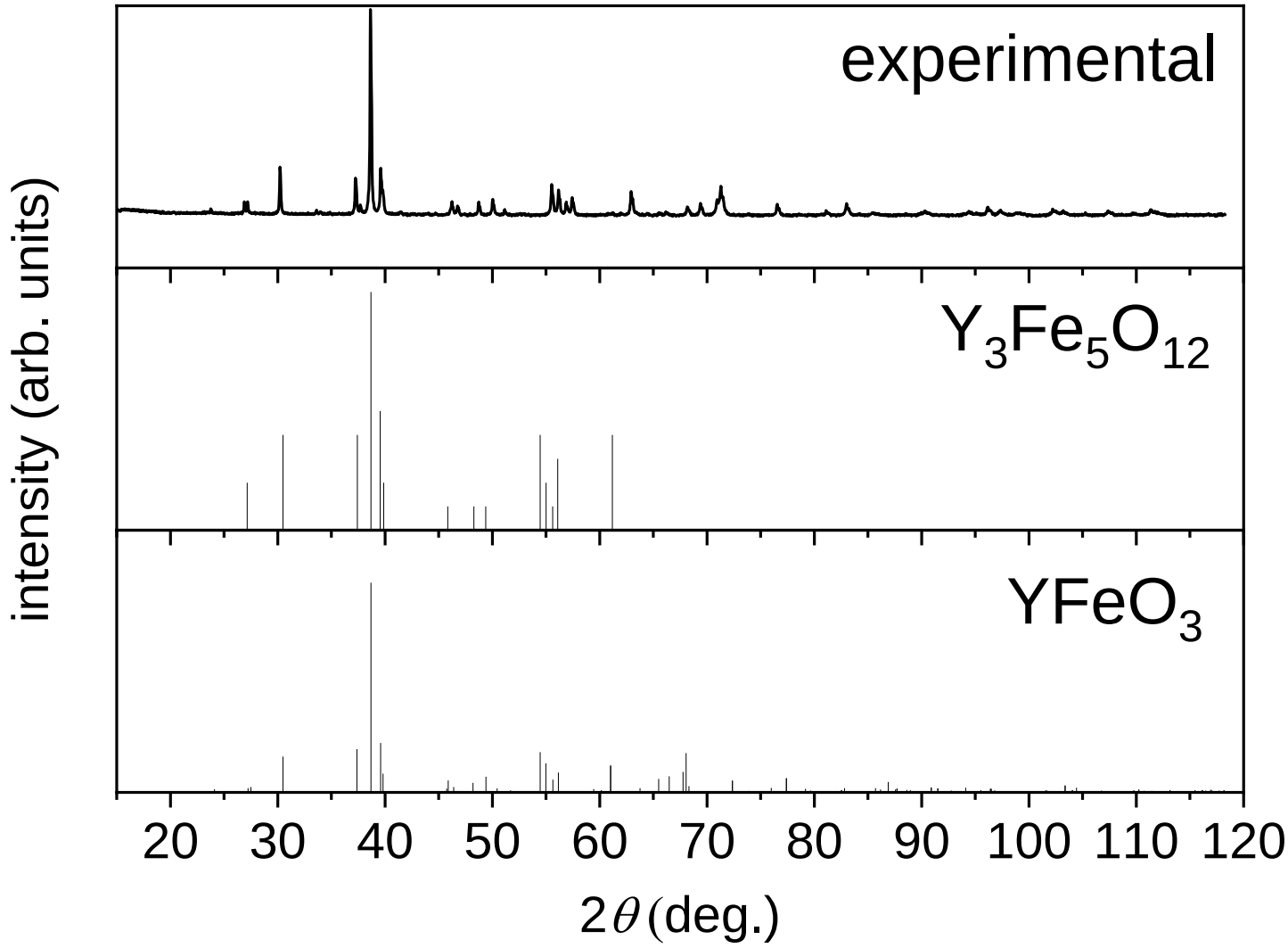
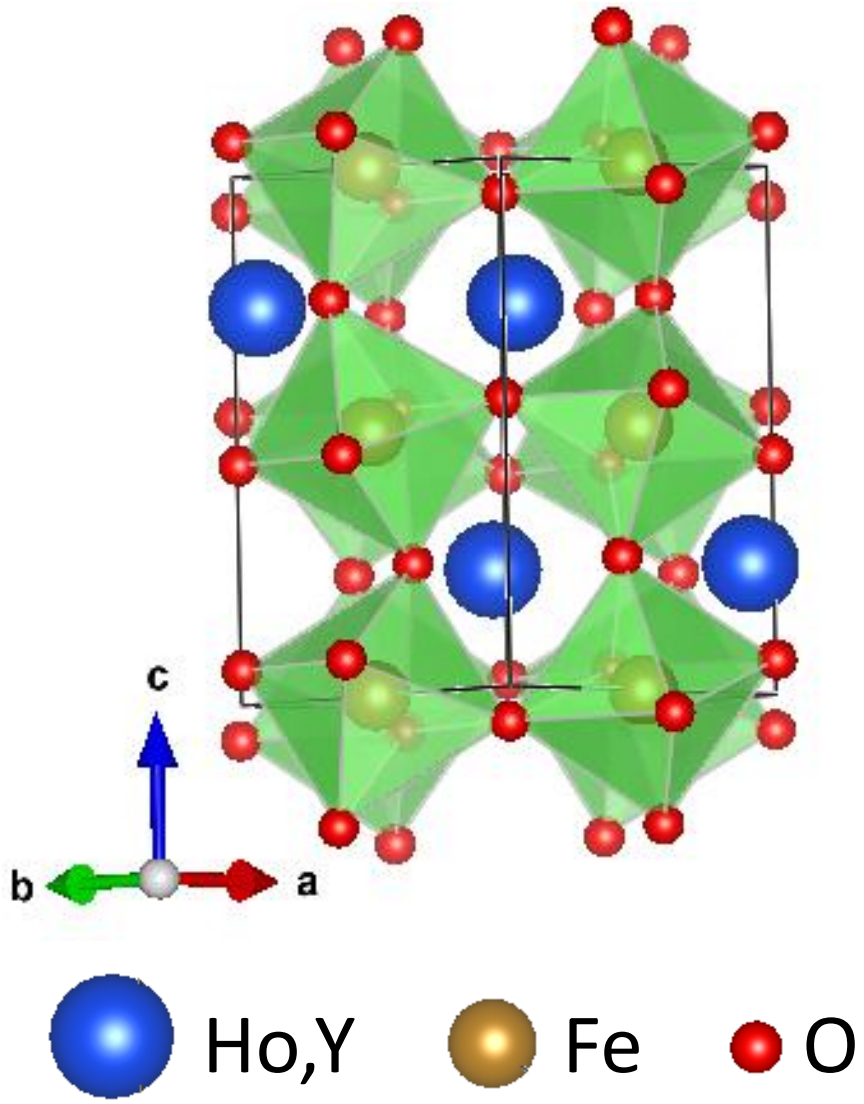


FIG.4. X-ray diffraction pattern of orthoferrite $YFeO_3$. Sample revealed additional phase $Y_3Fe_5O_{12}$

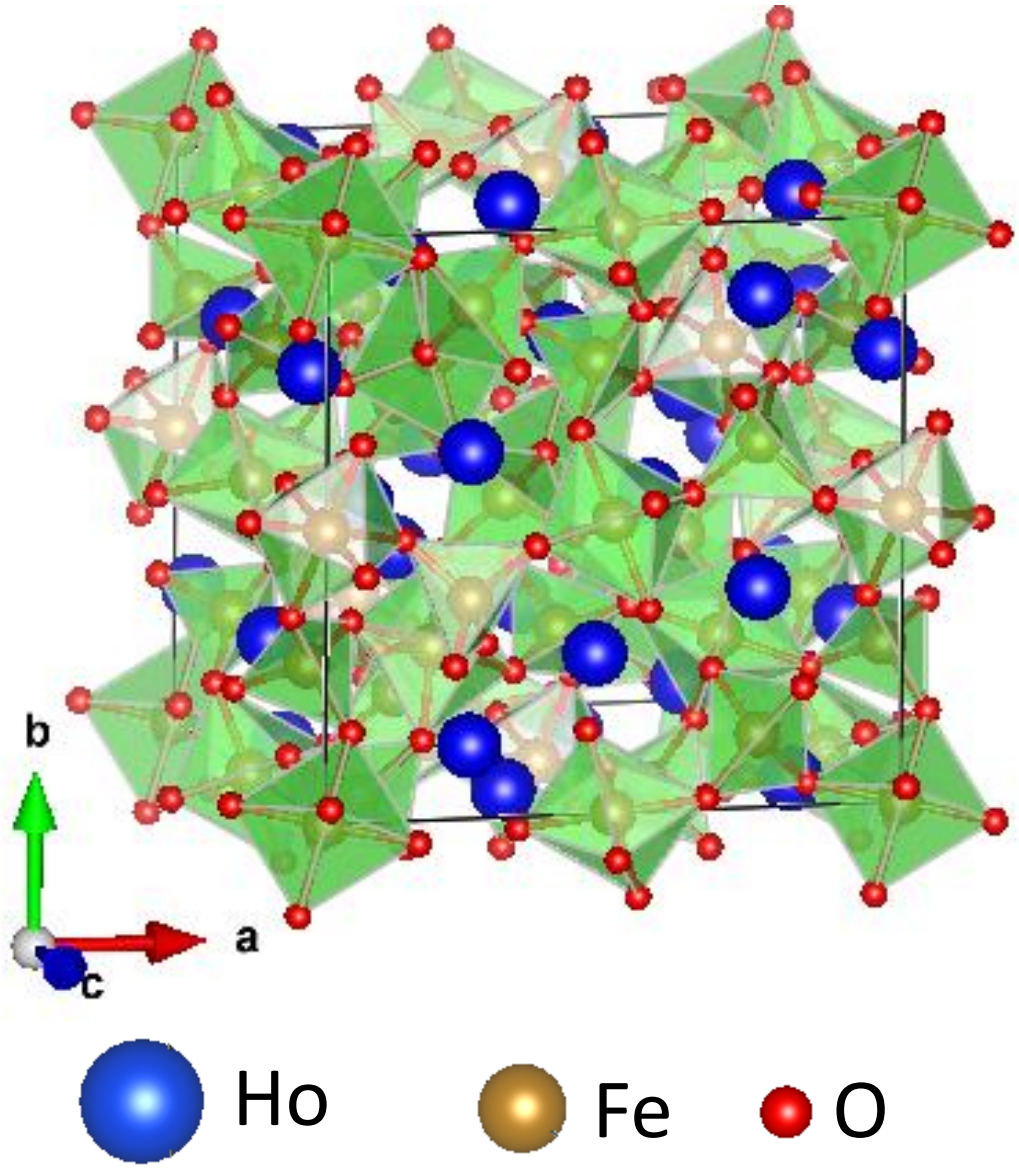
Crystallographic structure



$HoFeO_3$	
Unit cell	a = 5.278 Å b = 5.591 Å c = 7.602 Å
Space group	Pbnm (n° 62) Ohrthorombic

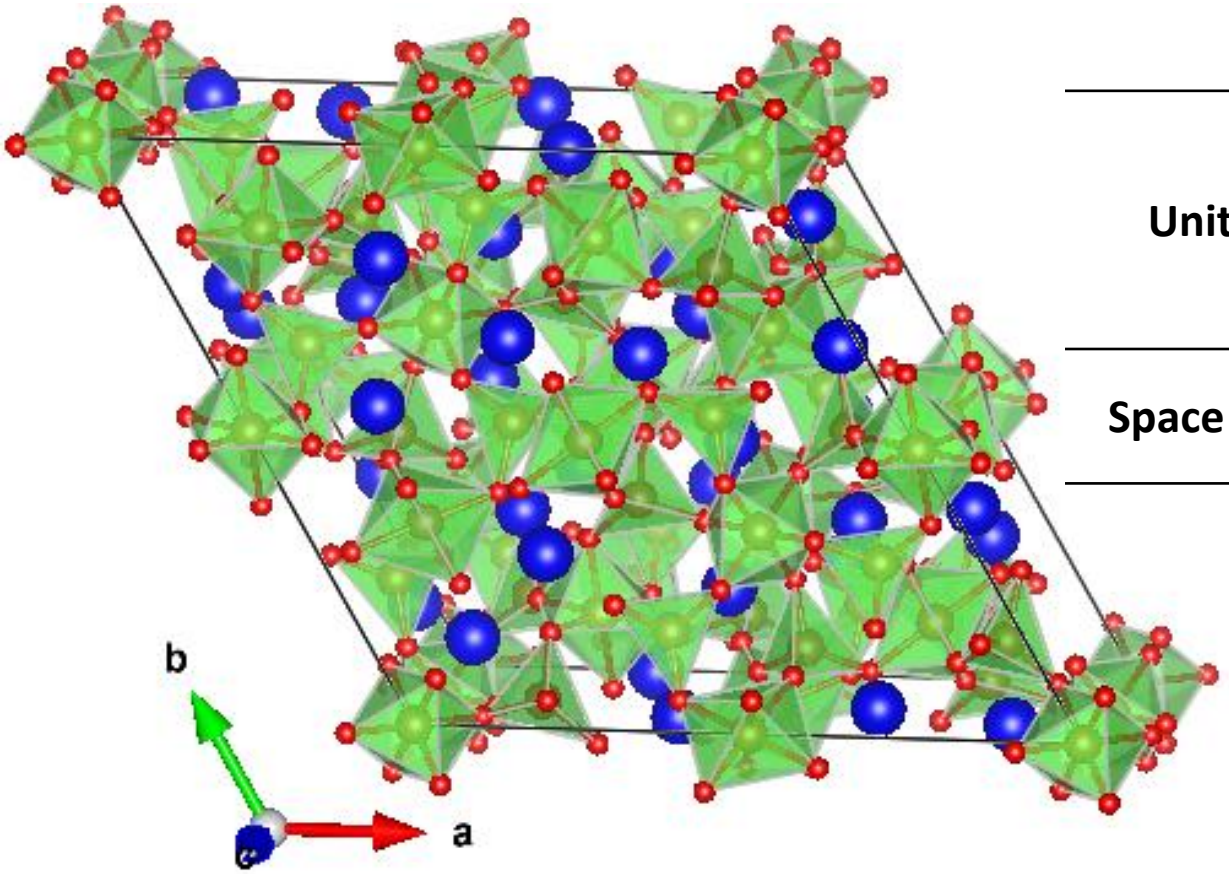
$YFeO_3$	
Unit cell	a = 5.2819 Å b = 5.5957 Å c = 7.6046 Å
Space group	Pbn21 (n° 33) Ohrthorombic

Crystallographic structure



$Ho_3Fe_5O_{12}$	
Unit cell	a = b =c = 12.376 Å
Space group	Ia-3d (n° 230) Cubic

Crystallographic structure



$Y_3Fe_5O_{12}$	
Unit cell	a = b = 17.484 Å c = 10.69 Å
Space group	R-3 (n° 148) hexagonal

Y Fe O

Rietveld method $HoFeO_3$

77.73% - $HoFeO_3$

22.27% - $Ho_3Fe_5O_{12}$

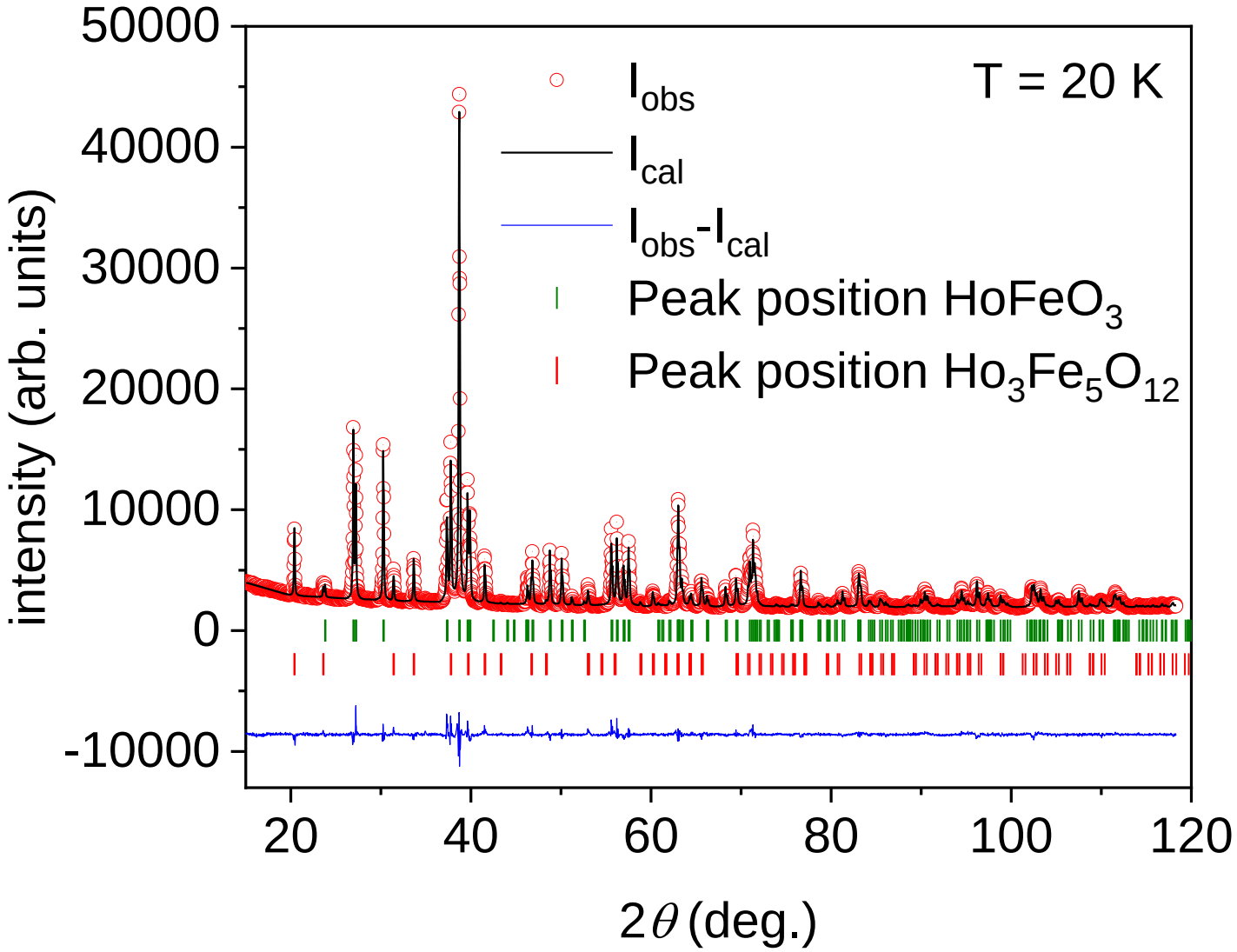
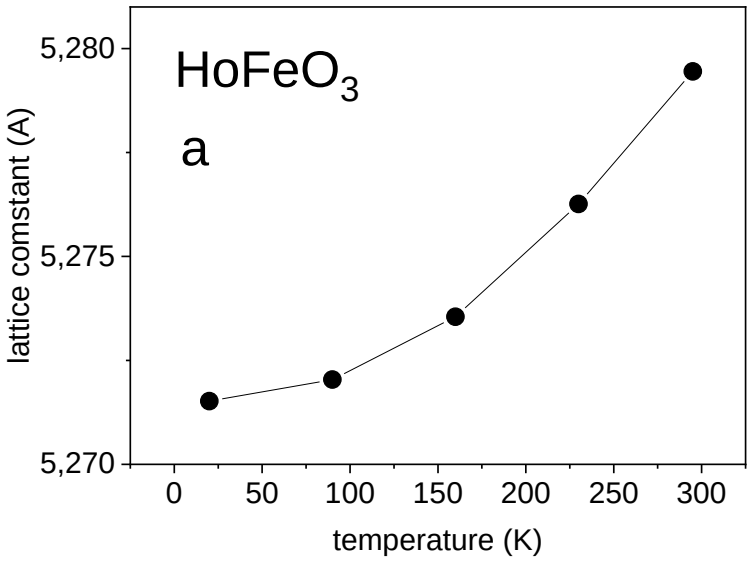
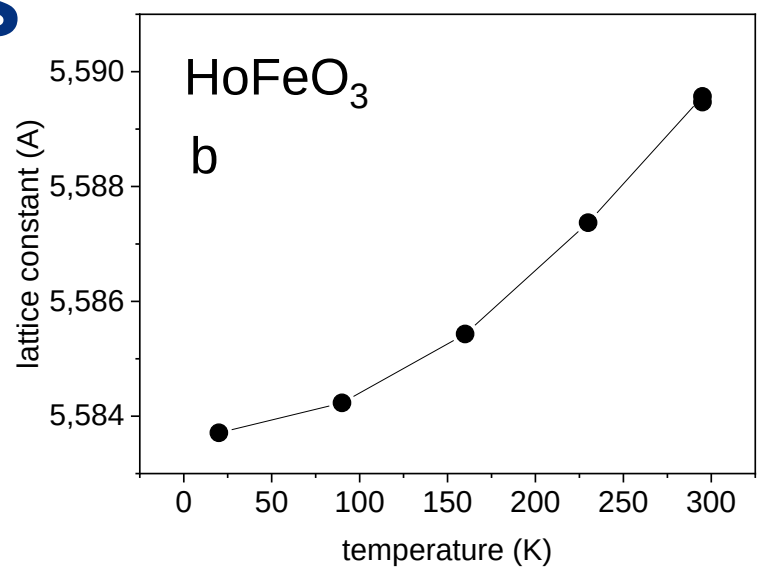


FIG.5. X-ray diffraction pattern of orthoferrite $HoFeO_3$. Sample revealed additional phase $Ho_3Fe_5O_{12}$

Temperature dependence of lattice constants





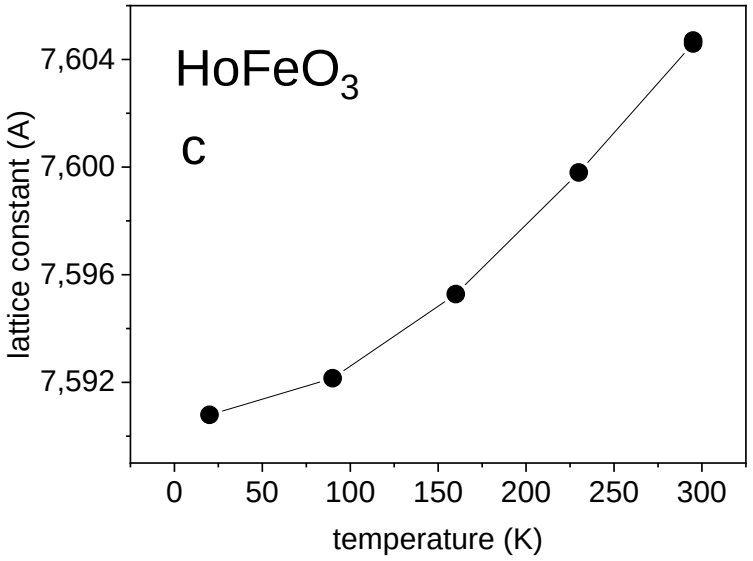


FIG.6. Temperature dependences of lattice constants a,b,c of $HoFeO_3$ compound

Rietveld method $YFeO_3$

95.8% - $YFeO_3$

4.2% - $Y_3Fe_5O_{12}$

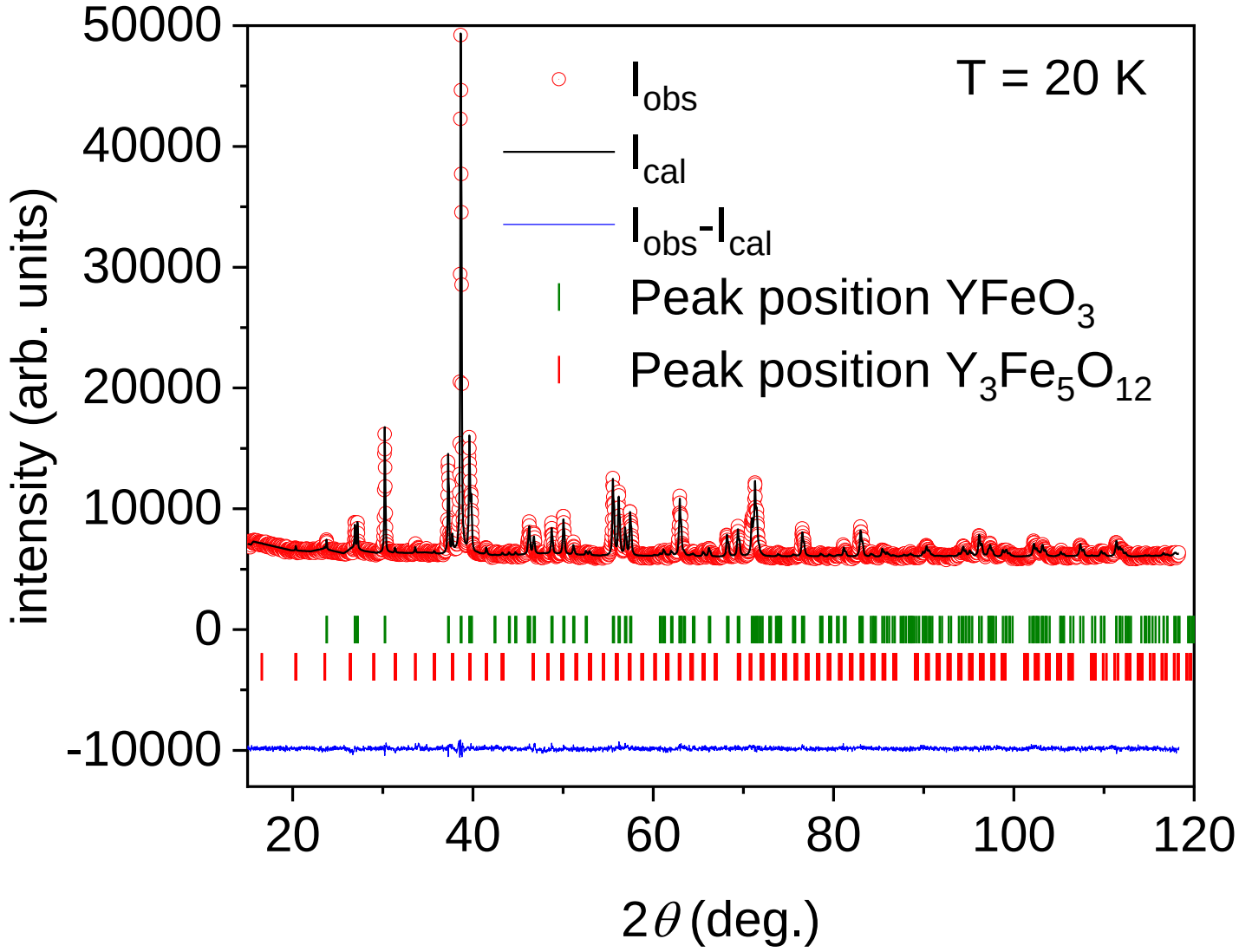
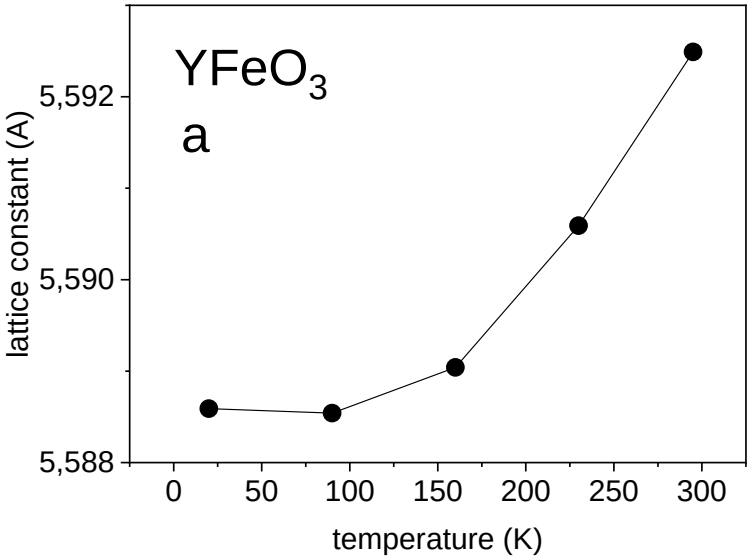
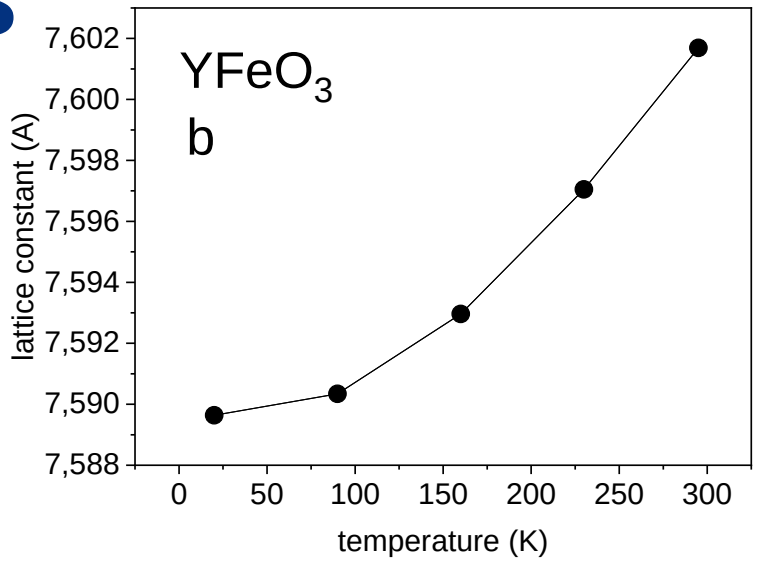


FIG.7. X-ray diffraction pattern of orthoferrite $YFeO_3$. Sample revealed additional phase $Y_3Fe_5O_{12}$

Temperature dependence of lattice constants





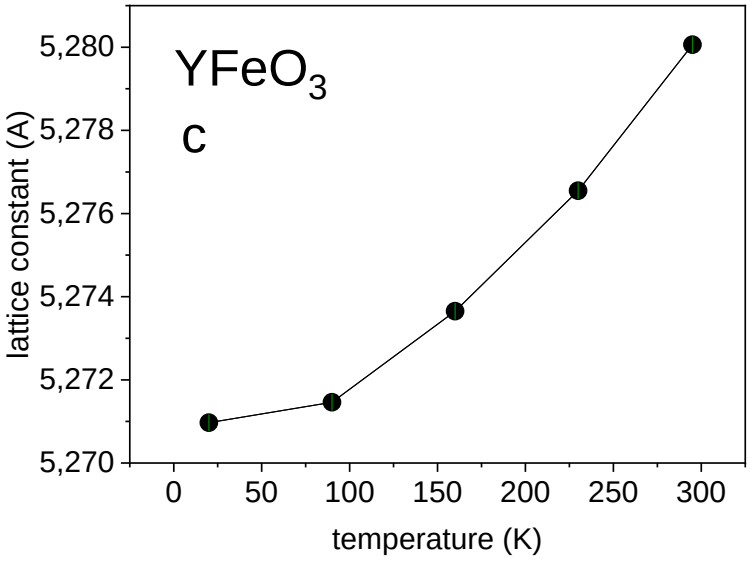


FIG.8. Temperature dependences of lattice constants a,b,c of $YFeO_3$ compound

Conclusions

1. Crystal structure of the compounds $HoFeO_3$ and $YFeO_3$, was studied by powder X-ray diffraction (XRD).
2. In both material two phases were noticed: $(Ho,Y)FeO_3$ (orthoferrite) and $(Ho,Y)_3Fe_5O_{12}$.
3. Rietveld refinement was applied for this samples.
4. The precentage contents of both phases were determinated:

- 77.73% - $HoFeO_3$, 22.27% - $Ho_3Fe_5O_{12}$
- 95.8% - $YFeO_3$, 4.2% - $Y_3Fe_5O_{12}$

5. Temperature dependences of lattice constatnts a,b,c were determinated.

Thank you for your attention!