

XRD characterization of orthoferrites

YFeO_3 and HoFeO_3



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Outline

- Tasks
- Orthoferrites
- XRD measurements
- Crystallographic 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.



Orthoferites

crystal structure: orthorhombic
space group: Pbnm



The periodic table is color-coded by groups. A red circle highlights Scandium (Sc) in the transition metal block. A red box highlights the lanthanide and actinide series at the bottom of the table.

1 H Hydrogen 1.008																	2 He Helium 4.003																																																																																																																																																																																																																																																												
3 Li Lithium 6.941	4 Be Beryllium 9.012																	5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180																																																																																																																																																																																																																																																						
11 Na Sodium 22.990	12 Mg Magnesium 24.305																	13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948																																																																																																																																																																																																																																																						
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.631	33 As Arsenic 74.922	34 Se Selenium 78.972	35 Br Bromine 79.904	36 Kr Krypton 84.798																																																																																																																																																																																																																																																												
37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.95	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.711	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.294																																																																																																																																																																																																																																																												
55 Cs Cesium 132.905	56 Ba Barium 137.328	57 La Lanthanum 138.905	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.085	79 Au Gold 196.967	80 Hg Mercury 200.592	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987	86 Rn Radon 222.018																																																																																																																																																																																																																																																												
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103 Lanthanide series	104 Rf Rutherfordium	105 Db Dubnium	106 Sg Seaborgium	107 Bh Bohrium	108 Hs Hassium	109 Mt Meitnerium	110 Ds Darmstadtium	111 Rg Roentgenium	112 Cn Copernicium	113 Nh Nihonium	114 Fl Flerovium	115 Mc Moscovium	116 Lv Livermorium	117 Ts Tennessine	118 Og Oganesson																																																																																																																																																																																																																																																												
57 La Lanthanum 138.905																		58 Ce Cerium 140.116																		59 Pr Praseodymium 140.908																		60 Nd Neodymium 144.242																		61 Pm Promethium 144.913																		62 Sm Samarium 150.36																		63 Eu Europium 151.964																		64 Gd Gadolinium 157.25																		65 Tb Terbium 158.925																		66 Dy Dysprosium 162.500																		67 Ho Holmium 164.930																		68 Er Erbium 167.259																		69 Tm Thulium 168.934																		70 Yb Ytterbium 173.055																		71 Lu Lutetium 174.967																	
89 Ac Actinium 227.028																		90 Th Thorium 232.038																		91 Pa Protactinium 231.036																		92 U Uranium 238.029																		93 Np Neptunium 237.048																		94 Pu Plutonium 244.064																		95 Am Americium 243.061																		96 Cm Curium 247.070																		97 Bk Berkelium 247.070																		98 Cf Californium 251.080																		99 Es Einsteinium [254]																		100 Fm Fermium 257.095																		101 Md Mendelevium 258.1																		102 No Nobelium 259.101																		103 Lr Lawrencium [262]																	
Alkali Metal			Alkaline Earth			Transition Metal			Basic Metal			Semimetal			Nonmetal			Halogen			Noble Gas			Lanthanide			Actinide																																																																																																																																																																																																																																																		



STRUCTURE

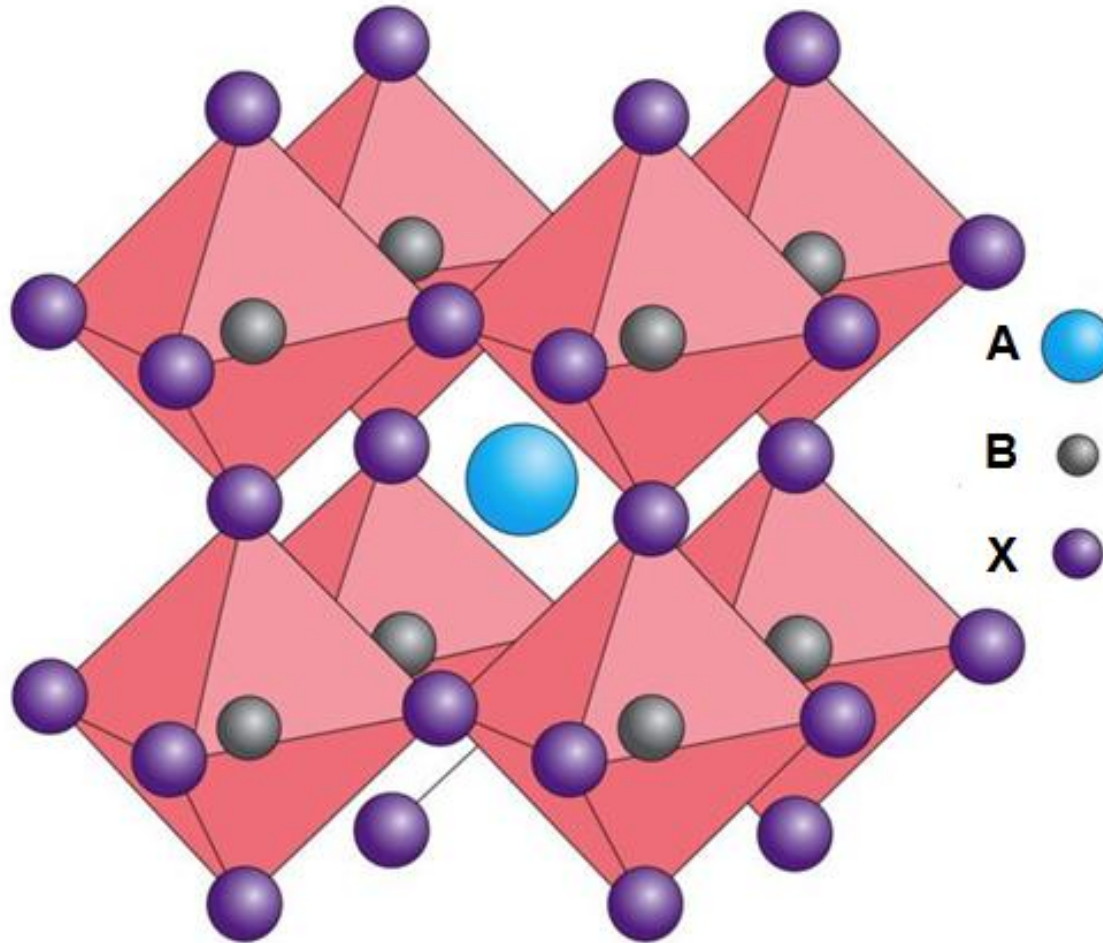


FIG.1. Crystallographic structure of perovskite ABX_3



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 $R\text{FeO}_3$ affect the crystal field of Fe ions. It can be expected that R may affect the magnetic properties of orthoferrites $R\text{FeO}_3$ in aspects.

APPLICATION:

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



XRD measurements

Co $K_{\alpha 1}$ ($\lambda = 1.7890 \text{ \AA}$) $K_{\alpha 2}$ ($\lambda = 1.7929 \text{ \AA}$)

$15^\circ - 118^\circ$
step 0.001°

$T = 20, 90, 160, 230, 295 \text{ K}$

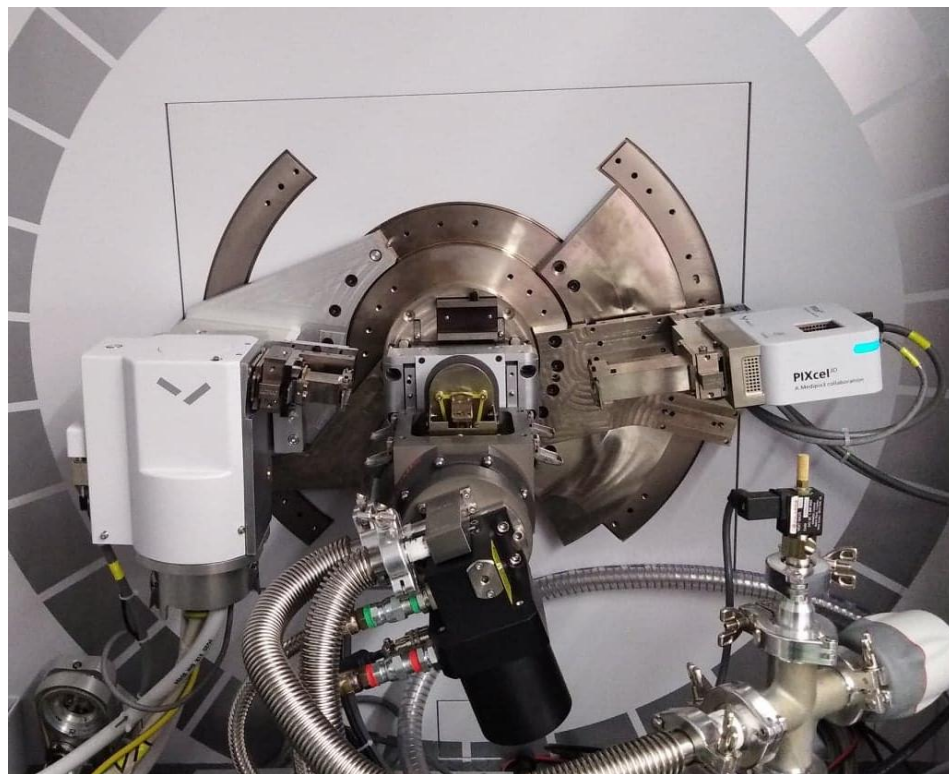


FIG.2. X-ray diffractometer Empyrean PANalytical (left) and sample holder (left)



XRD

Malvern
Panalytical
a spectris company

HighScore

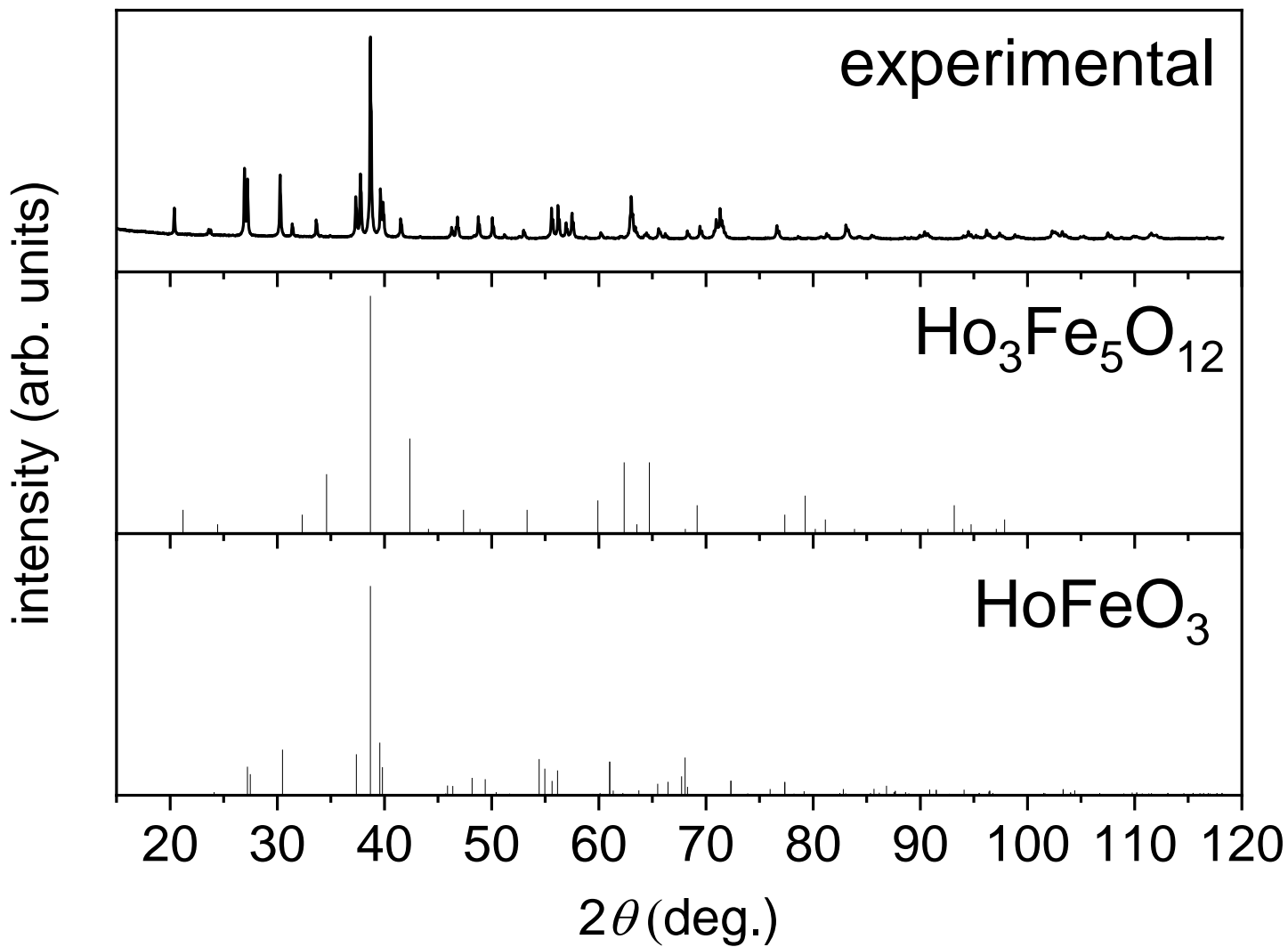


FIG.3. X-ray diffraction pattern of orthoferrite HoFeO_3 . Sample revealed additional phase $\text{Ho}_3\text{Fe}_5\text{O}_{12}$



XRD

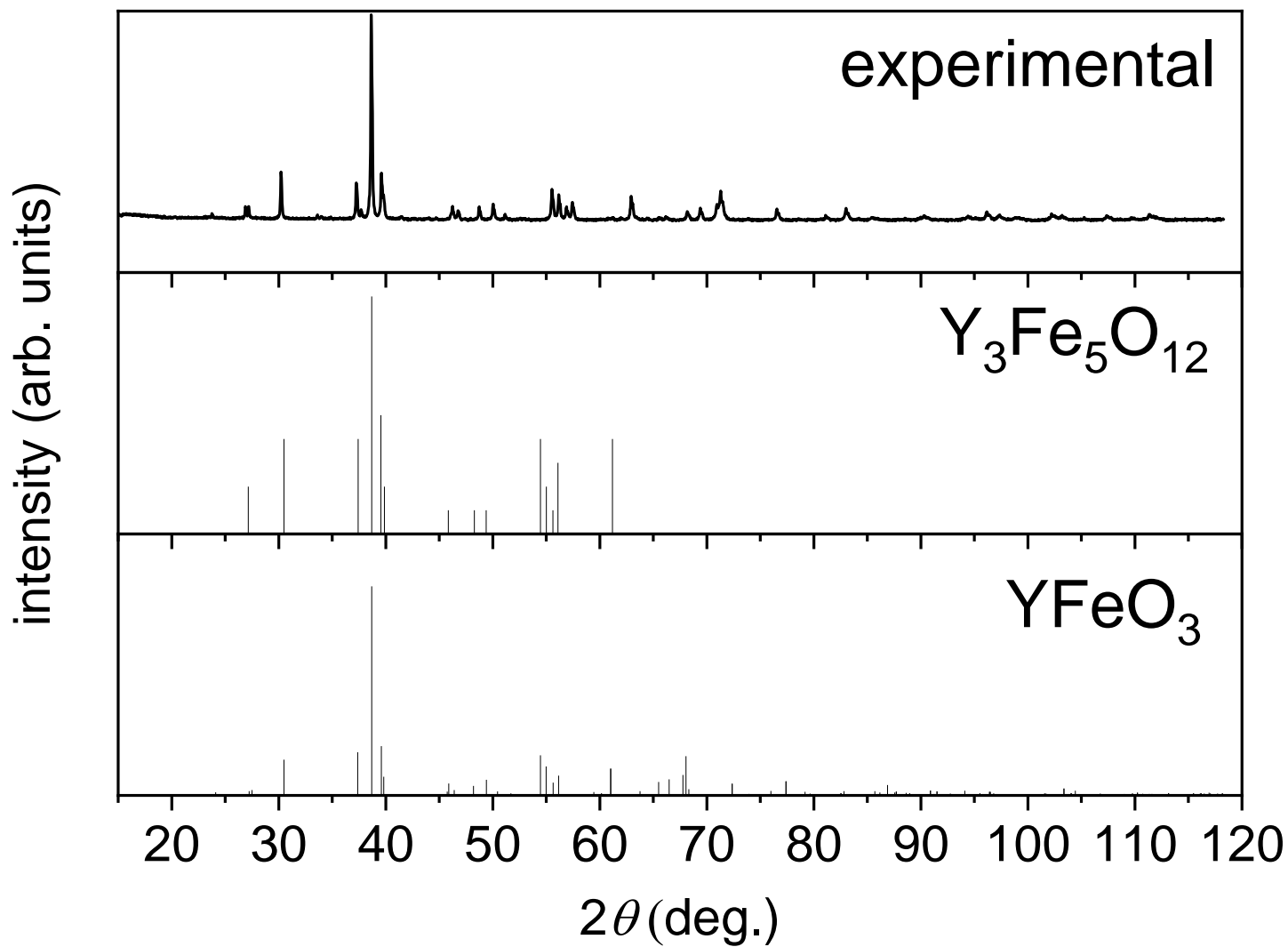
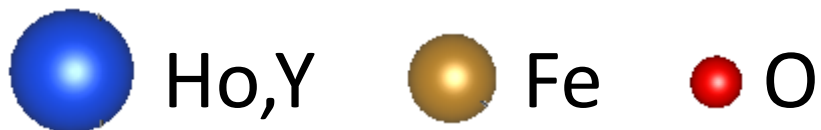
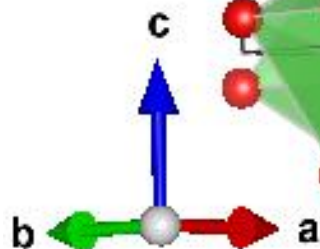
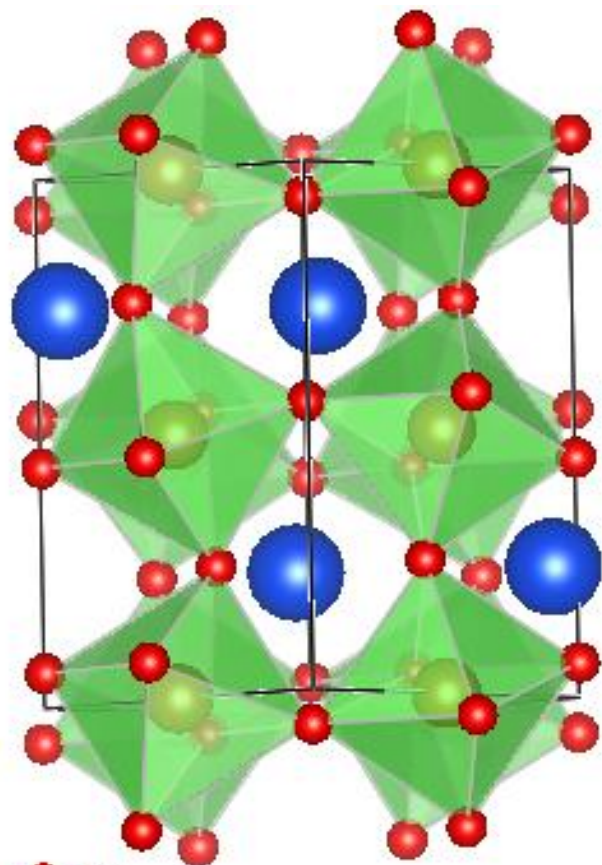


FIG.4. X-ray diffraction pattern of orthoferrite YFeO₃. Sample revealed additional phase Y₃Fe₅O₁₂



Crystallographic structure



HoFeO₃

Unit cell	$a = 5.278 \text{ \AA}$ $b = 5.591 \text{ \AA}$ $c = 7.602 \text{ \AA}$
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Space group	Pbnm (n° 62) Orthorhombic
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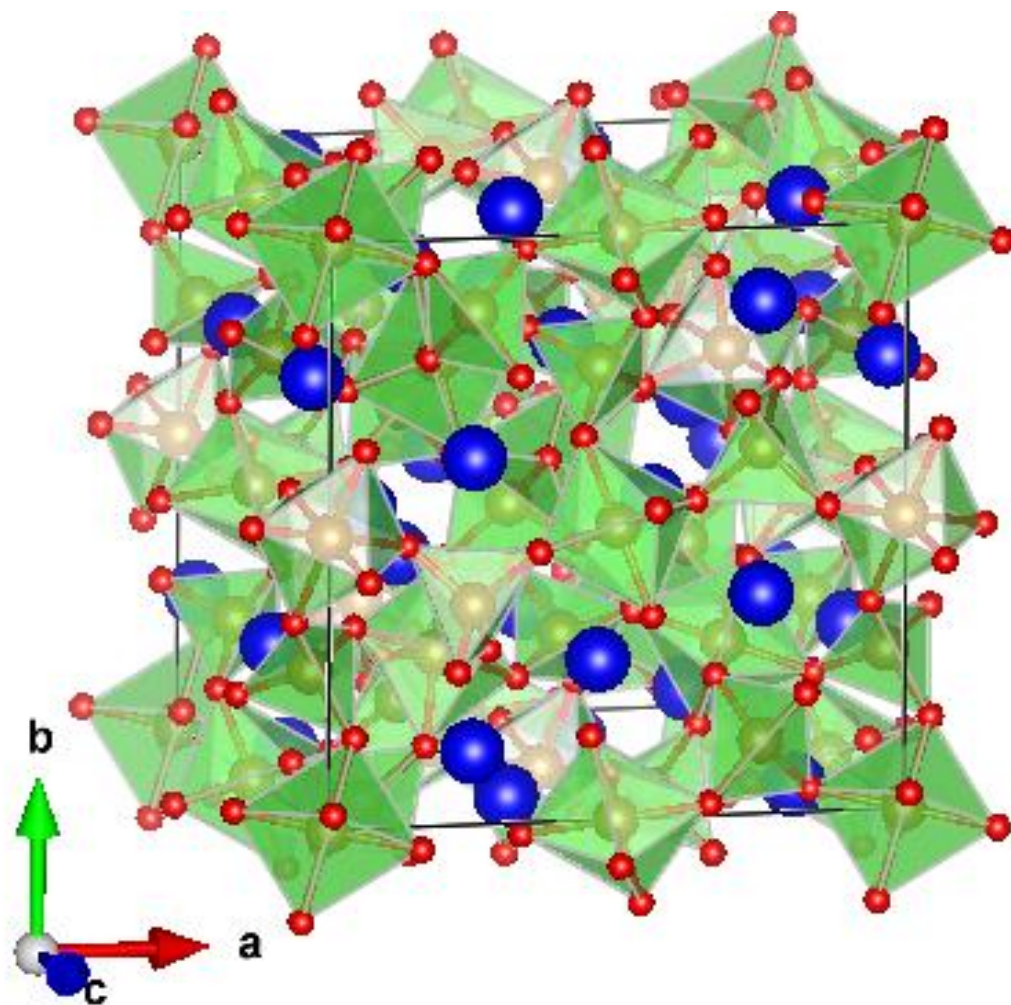
YFeO₃

Unit cell	$a = 5.2819 \text{ \AA}$ $b = 5.5957 \text{ \AA}$ $c = 7.6046 \text{ \AA}$
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Space group	Pbn21 (n° 33) Orthorhombic
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Crystallographic structure

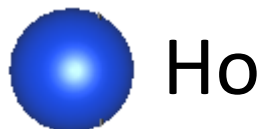


Unit cell

$$a = b = c = 12.376 \text{ \AA}$$

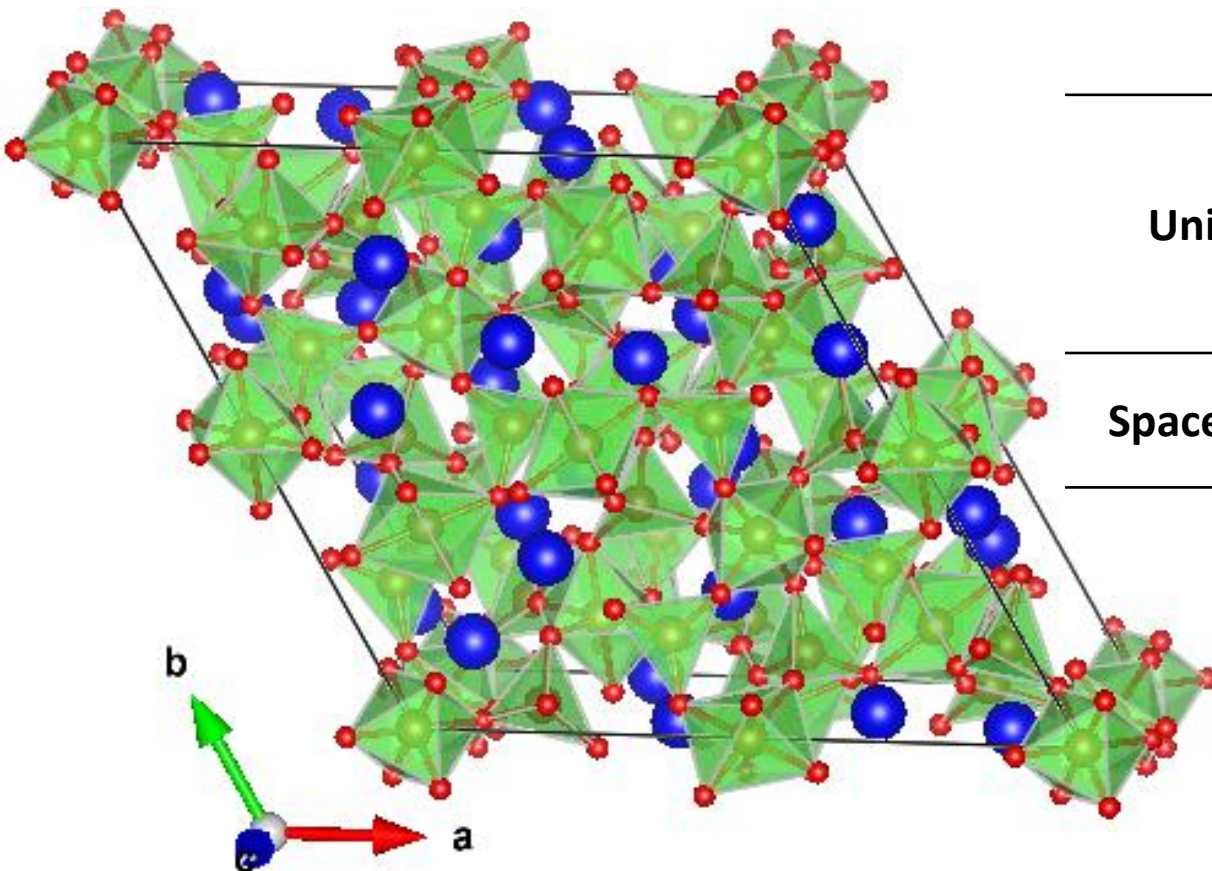
Space group

$Ia\text{-}3d$ (n° 230)
Cubic





Crystallographic structure

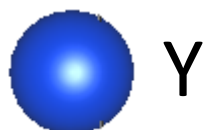


Unit cell

$$a = b = 17.484 \text{ \AA}$$
$$c = 10.69 \text{ \AA}$$

Space group

R-3 (n° 148)
hexagonal





Rietveld method HoFeO_3

77.73% - HoFeO_3

22.27% - $\text{Ho}_3\text{Fe}_5\text{O}_{12}$

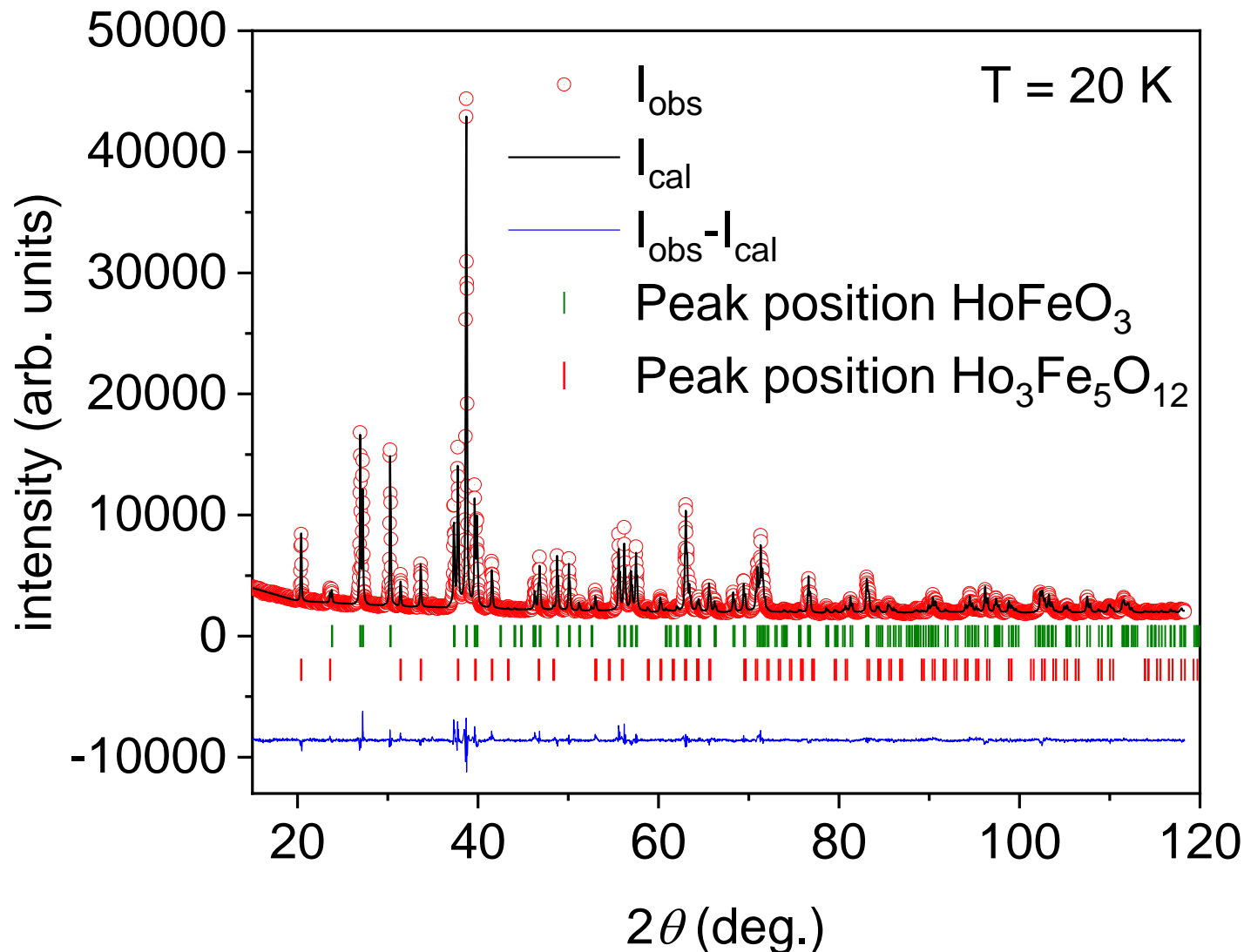


FIG.5. X-ray diffraction pattern of orthoferrite HoFeO_3 . Sample revealed additional phase $\text{Ho}_3\text{Fe}_5\text{O}_{12}$



Temperature dependence of lattice constants

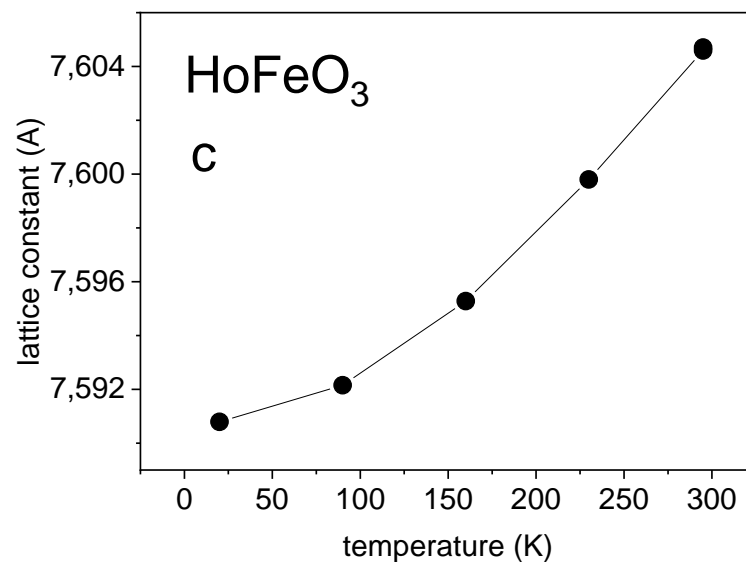
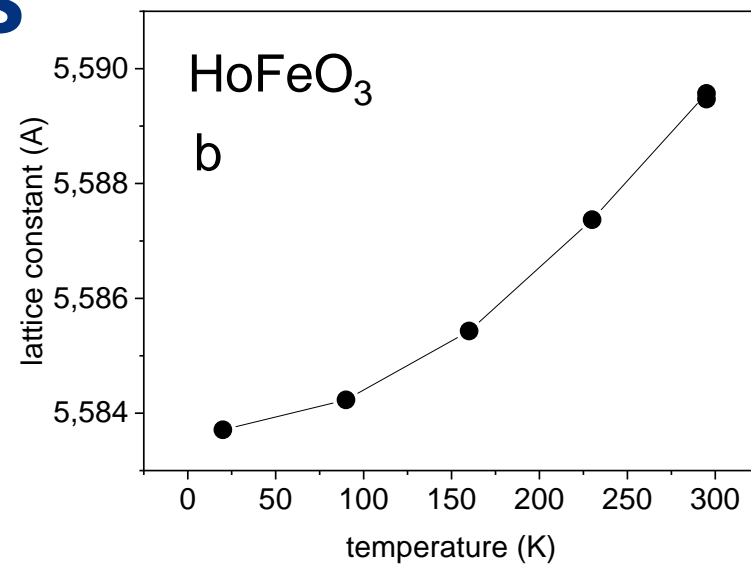
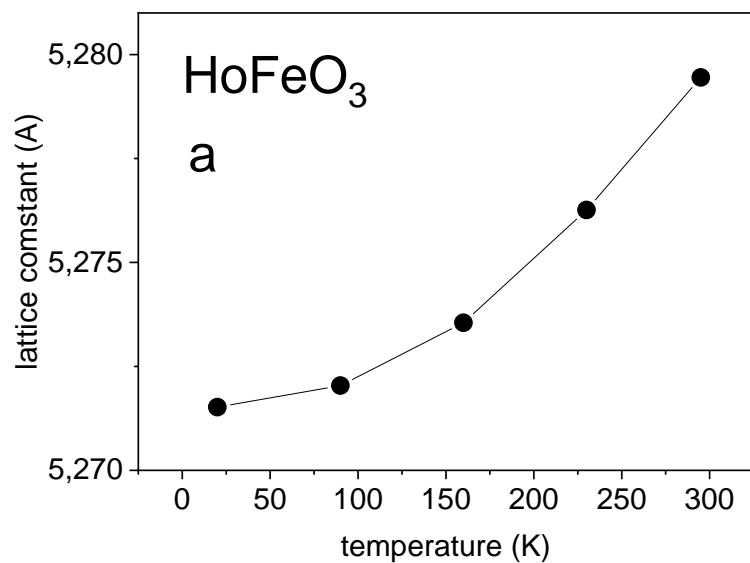


FIG.6. Temperature dependences of lattice constants a, b, c of HoFeO_3 compound



Rietveld method YFeO_3

95.8% - YFeO_3

4.2% - $\text{Y}_3\text{Fe}_5\text{O}_{12}$

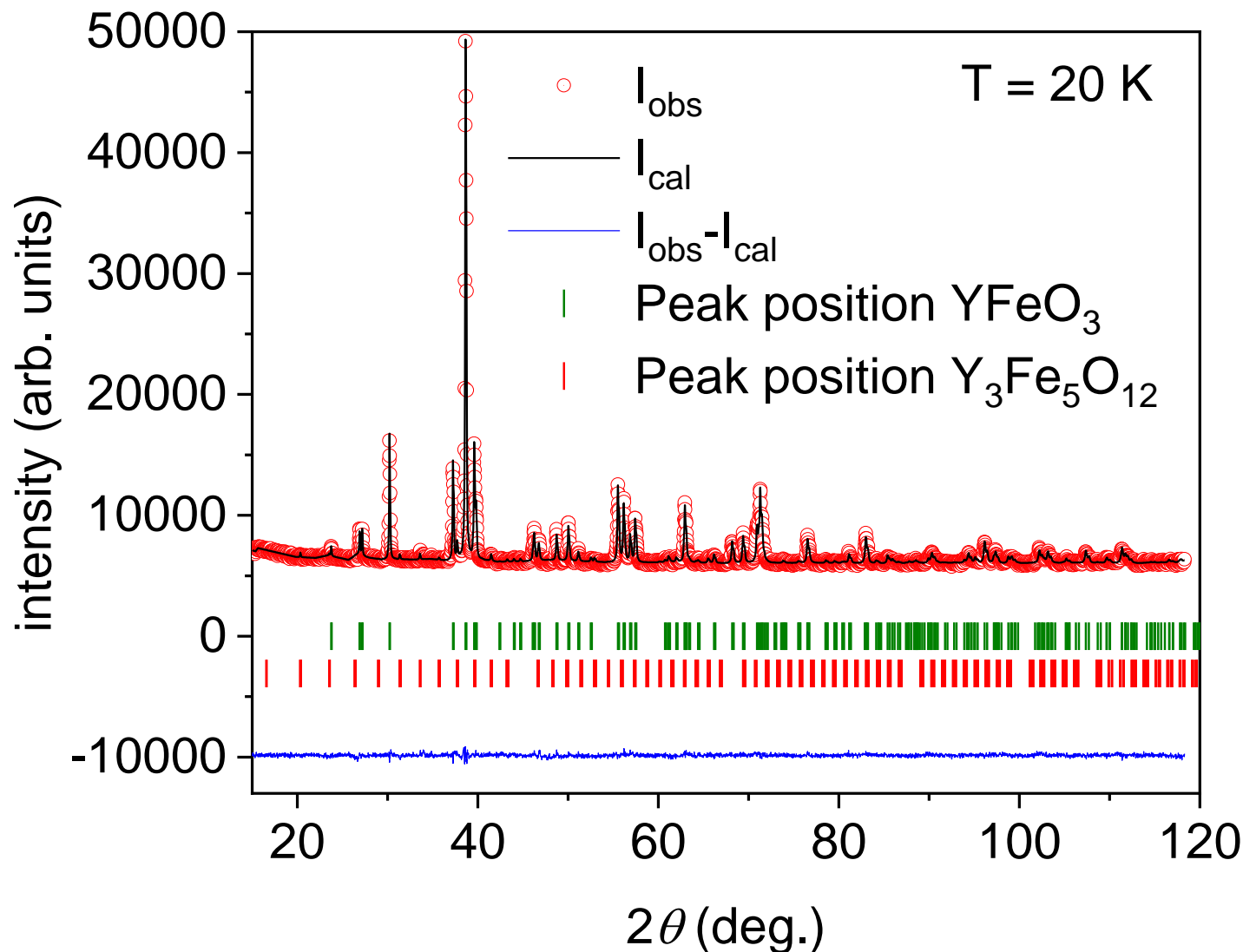


FIG.7. X-ray diffraction pattern of orthoferrite YFeO_3 . Sample revealed additional phase $\text{Y}_3\text{Fe}_5\text{O}_{12}$



Temperature dependence of lattice constants

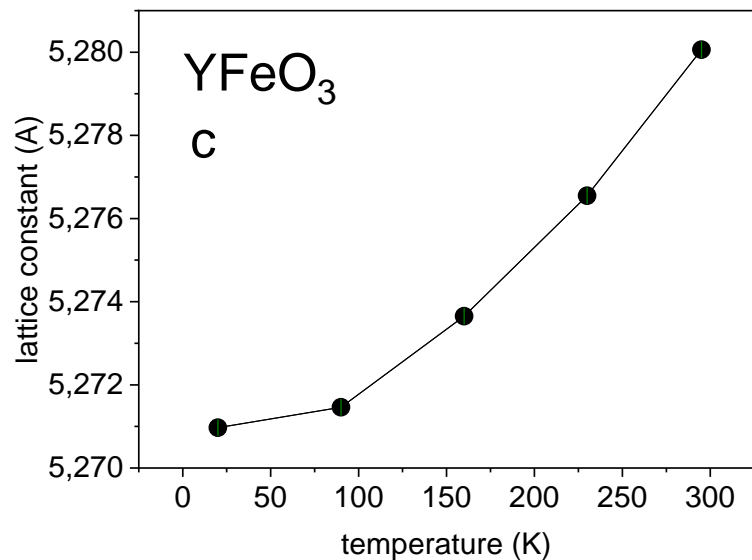
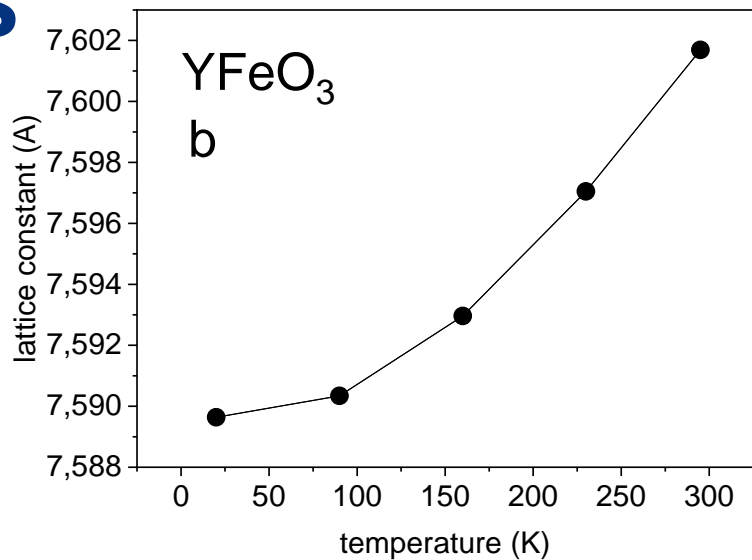
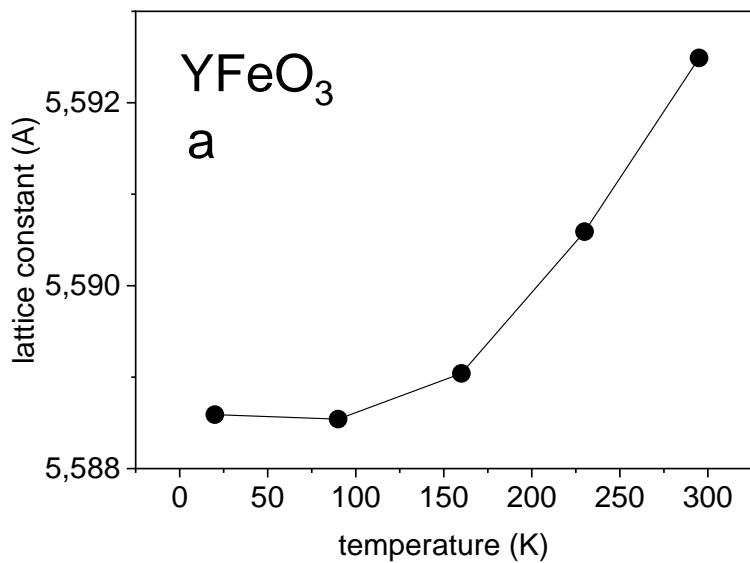


FIG.8. Temperature dependences of lattice constants a,b,c of YFeO₃ compound



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: $(\text{Ho},\text{Y})\text{FeO}_3$ (orthoferrite) and $(\text{Ho},\text{Y})_3\text{Fe}_5\text{O}_{12}$.
3. Rietveld refinement was applied for this samples.
4. The precentage contents of both phases were determinated:
 - 77.73% - HoFeO_3 , 22.27% - $\text{Ho}_3\text{Fe}_5\text{O}_{12}$
 - 95.8% - YFeO_3 , 4.2% - $\text{Y}_3\text{Fe}_5\text{O}_{12}$
5. Temperature dependences of lattice constatnts a,b,c were determinated.



Thank you for your attention!

