Indian Journal of Advanced Physics (IJAP)
ISSN: 2582-8983 (Online), Volume-2 Issue-2, October 2022

Synthesis, Structural and Optical Characterisation of Orthoferrites $Rfeo_3$ (R= Pr,Nd)

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Abstract: *Orthorhombic structure of rare earth perovskite type oxide ($RFeO_3$, R =Pr, Nd) nano particles prepared by metathesis method. Powders prepared were characterized by several measurements such as X-ray diffraction, scanning electron microscope, EDX, FTIR, and diffuse reflectance spectroscopy to understand their physio-chemical properties. $NdFeo_3$ and $PrFeo_3$, synthesized metathesis method crystallite size of 61nm and 60.5 nm respectively.*

Keywords: *Perovskite, Metathesis, $PrFeO_3$, $NdFeO_3$, Orthoferrite*

I. INTRODUCTION

Perovskite oxides of general formula ABO_3 (where A is rare earth and B is a transition metal ion). Have been the focus of intense research due to their fascinating properties since long [1][13]. These properties include metal insulator transition, colossal magnetoresistance, multiferroic behaviour etc. These systems are generally named on the basis of transition metal ion at B site e.g cobalites, Manganites, Orthoferrites, Ortho chromites etc. Among these materials rare earth orthoferrites ($RFeO_3$,R=Pr, Nd) found special status due to its multiferroic properties [2][9][10][11]. These materials have potential applications in spintronics and data storage, including high speed memory with magnetically and electrically addressable states magnetically tunable switches and sensors. $RFeO_3$ (R=Pr,Nd) powders are sysnthesised by metathesis method and structure and composition were analized byXRD and EDX [1]. The optical properties were analysed by UV-visible diffuse reflectance spectrometer. The vibration of specific set of chemical bonds are known by FTIR (Fourier-transforminfrared absorption spectra) which is recorded at room temperature within the wave number 4000-400 cm^{-1}.

Manuscript received on 20 September 2022 | Revised Manuscript received on 12 October 2022 | Manuscript Accepted on 15 October 2022 | Manuscript published on 30 January 2024.

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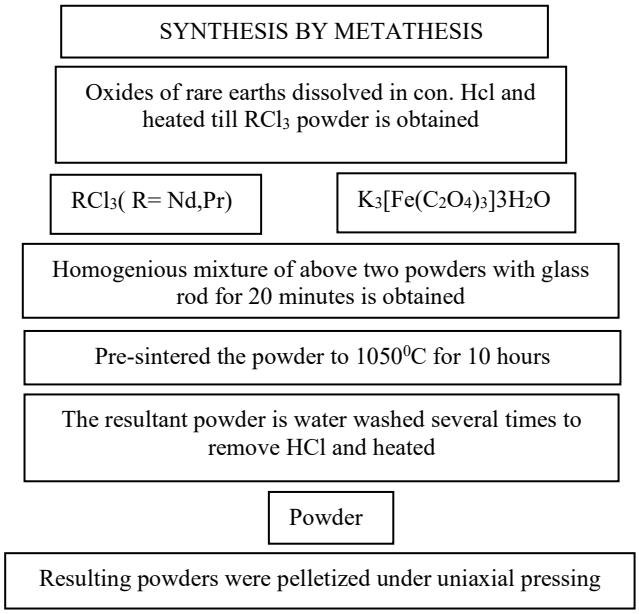
Experimental Details

K_3 $[Fe(c_2O_4)_3]$ $3H_2O$ and RCl_3 (R=Nd,Pr) were used as precursors. Nd_2O_3 and Pr_6O_{11} were converted into $NdCl_3$ and $PrCl_3$ using concentrated HCl. Then K_3 $[Fe(c_2O_4)_3]3$ H_2O and RCl_3 (R=Nd, Pr) were mixed well using glass rod. The resultant homogenized mixtures were calcinated to 1050 ^{0} C and 1050 ^{0} C for 10 hours Use the "Insert Citation" button to add citations to this document. to get $NdFeO_3$ and $PrFeO_3$ respectively. Collected powders were washed with distilled water several times to remove KCl and then heat treated. Resulting powders were pelletized under uniaxial pressing. The pellets were sintered at 1100 ^{0}C for 4 hours.These sintered pellets were used for various measurements.



II. RESULTS AND DISCUSSION

The XRD pattern of the powders shown in figure 1. It shows the products are pure perovskite oxides, $RFeO_3$ (R= Nd, Pr) with an orthorhombic structure of pbnm space group. The diffraction data are in good agreement with JCPD card of $NdFeO_3$ (JCPDS NO 74-1473) and $PrFeO_3$ (JCPDS NO 74-1472). The XRD pattern confirmed the single phase of $NdFeO_3$ and $PrFeO_3$.Lattice parameters were calculated using POWD software shown in the table 1. Which is in good agreement with the reported values.

a= 5.457Å b = 5.585 Å c= 7.780Å (NdFeO3-JCPDS No. 74-1473)

a= 5.48 Å b =5.578 Å c=7.786 Å (PrFeO3-JCPDS No. 74-1472)

The average size of particles were calculated by employing the Scherrer equation

$$D = K\lambda/\beta \cos\theta$$

Where D is the average crystallite size
K = 0.94
λ is the X- ray wavelength
B is the FWHM
θ is the Bragg angle

On the basis of this equation the mean particle size of $RFeO_3$(R= Nd, Pr). Orthoferrites were about 61nm and 60.5 nm respectively.

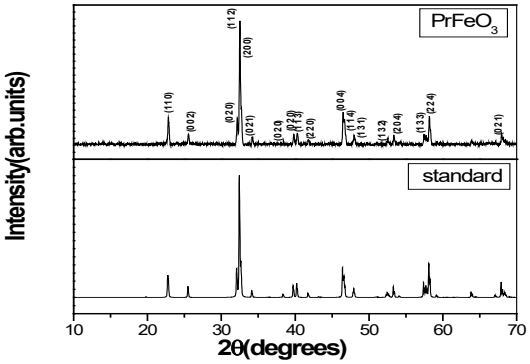


Fig. 1: XRD pattern of $PrFeO_3$

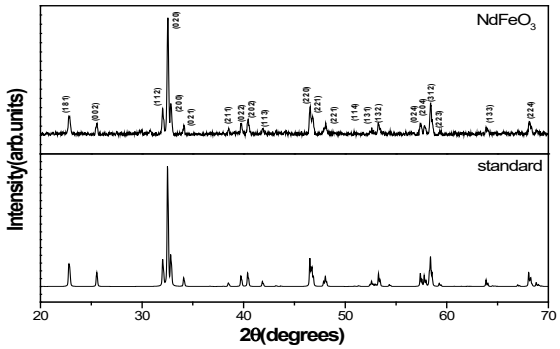


Fig. 2: XRD Pattern of NdFeO3

SEM:

The surface morphology was studied by using scanning electron microscopy (SEM). The SEM images are shown in fig. The SEM images reveal the nonuniformity in grain sizes and also existence of porosity.

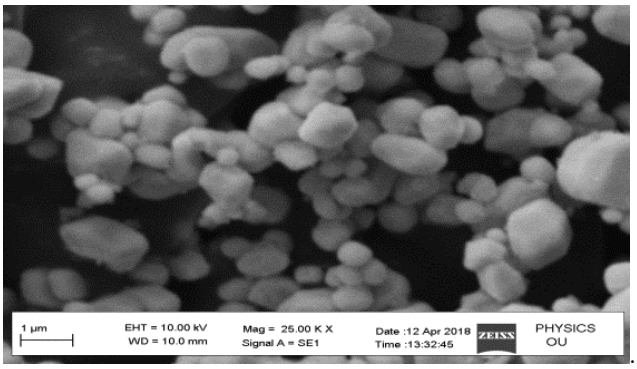


Fig. 3: Surface Morphology of PrFeO3

$PrFeO_3$

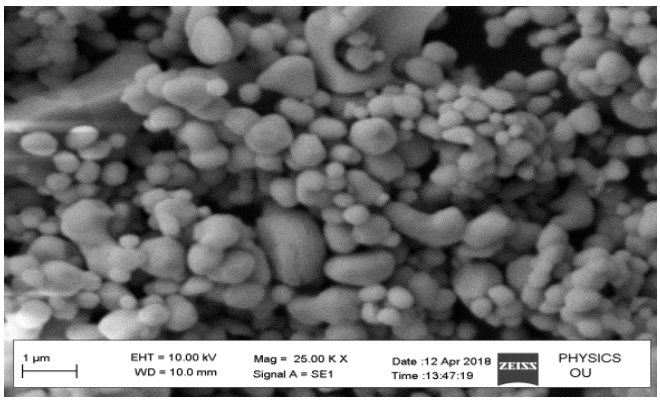


Fig. 4: Surface Morphology of NdFeO3

$NdFeO_3$

EDAX SPECTRA:

EDAX analysis was carried out for confirming the composition of synthesized powders. The data wascollected at different locations on the sample. The weight percentage and atomic percentage of the constituent elements are tabulated below.

Element	Weight%	Atomic%
O K	17.62	56.10
Fe L	26.49	24.16
Nd L	55.89	19.74
Totals	100.00	

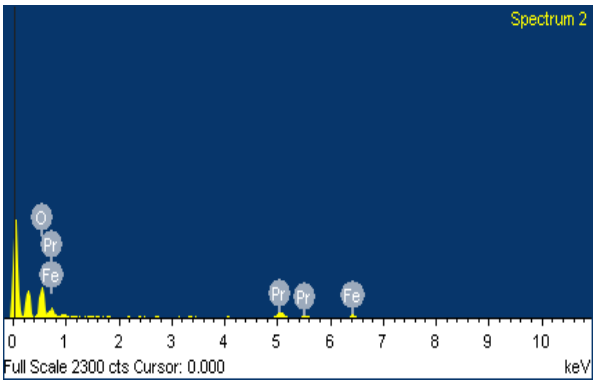


Fig. 5: Chemical Composition of PrFeO3 from EDAX

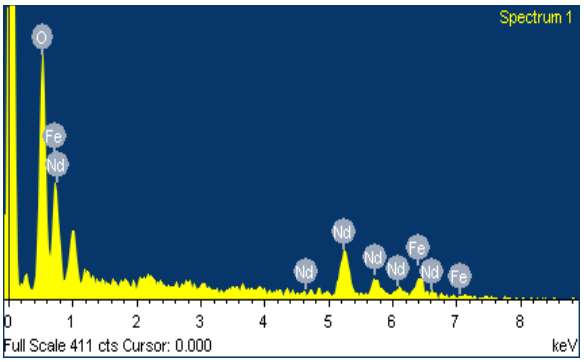


Fig. 6: Chemical Composition of NdFeO3 from EDAX

Element	Weight%	Atomic%
O K	22.36	65.08
Fe L	18.39	15.34
Pr L	59.25	19.58
Totals	100.00	100.00

DRS Spectroscopy:

The optical absorption spectrum of $PrFeO_3$ and $NdFeO_3$ powders were recorded. The direct band gap energy (E_g) was determined by fitting the absorption data to the direct transition using the following equation.

$Ah\nu = \sqrt{\alpha}(h\nu - E_g)$

Where A is the optical absorption coefficient, hν is the photon energy.E_g is the direct band gap and α is a constant. The band values are estimated as 1.975eV and 2.08 eV for $PrFeO_3$ and $NdFeO_3$ respectively which are lower than in the previous works. This shows that these orthoferrite samples are suitable for absorption of visible region of light spectrum to efficiently utilize the solar energy. So these materials can be used as photocatalysts.

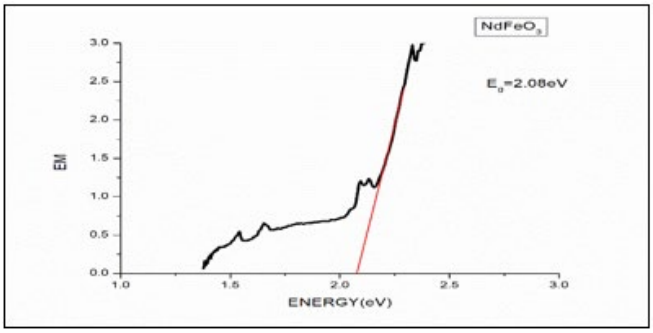


Fig. 7: UV-DRS Spectroscopy of NdFeO3

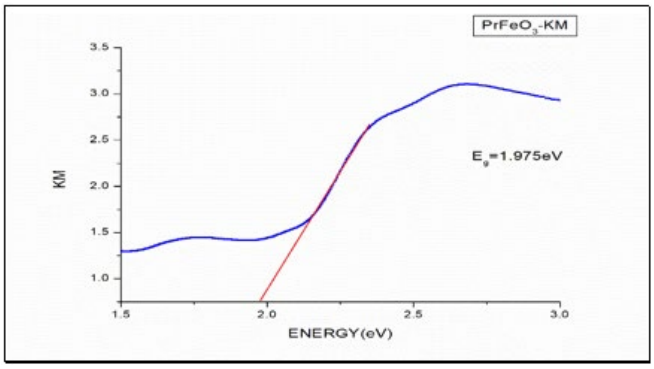


Fig. 8: UV-DRS Spectra of PrFeO3

FTIR:

The FTIR spectra of $PrFeO_3$ shows strong absorption bands at 432.07 cm^{-1} and 563.23 cm^{-1} and a few weak intensity bands in the range of 1300 -1500 cm^{-1} absorption at 432.07 corresponds to O-Fe-O bending vibrations, while that observed at 563.23 cm^{-1} corresponds to Fe-O stretching vibration as shown in the figure.

The FTIR spectrum of $NdFeO_3$ shows strong absorption bands at 437.07 cm^{-1} and 570.95 cm^{-1} absorption at 437.07 cm^{-1} corresponds to O-Fe-O bending vibrations, while that observed at 570.95 cm^{-1} to Fe-O stretching vibration as shown in the figure.

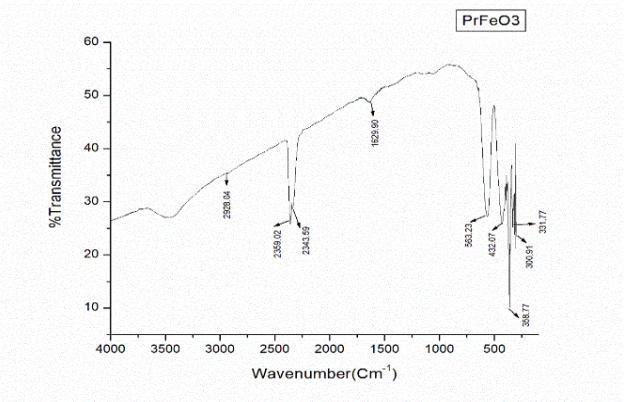


Fig. 9: FTIR Spectra of PrFeO3

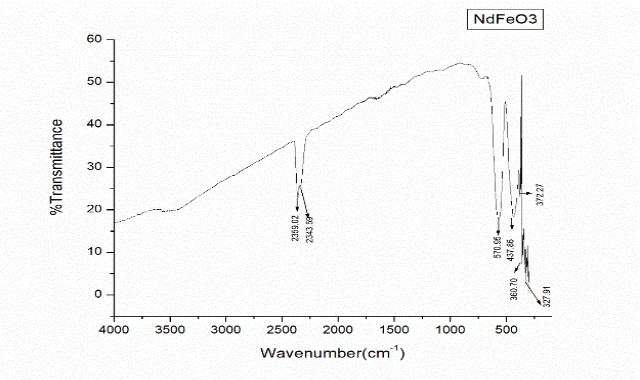


Fig. 10: FTIR Spectra of NdFeO3

III. CONCLUSION

$PrFeO_3$ and $NdFeO_3$ samples were synthesized by metathesis method. The crystalline nature was confirmed by powder XRD pattern. From XRD studies it is clear that the samples were formed of single-phase perovskite type crystalline compound with Orthorhombic structure. The chemical composition was confirmed through EDAX. These samples were characterized by SEM, UV-DRS and FTIR techniques. The UV-Visible diffuse reflectance spectroscopic analysis exhibited an optical band gap of approximately 1.975 eV and 2.08 eV of $PrFeO_3$ and $NdFeO_3$ respectively. These samples are capable of absorbing visible light hence these samples can utilize the solar energy. This is an interesting finding as such material could be potential source of visible light photocatalytic activity.

DECALARION STATEMENT

Funding	No, I did not receive.
Conflicts of Interest	No conflicts of interest to the best of our knowledge.
Ethical Approval and Consent to Participate	No, the article does not require ethical approval and consent to participate with evidence.
Availability of Data and Material/ Data Access Statement	Not relevant
Anthors Contributions	All authors have equal participation in this article.

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Prof. M. Vithal did his Ph.D. (1986) in Chemistry from University of Hyderabad and joined as faculty in Osmania University in 1986 and promoted as associate Professor in 1997 and as Professor in 2005. Superannuated in July 2017 and joined as UGC-BSR Faculty Fellow in November 2017. After completing the BSR term in November 2020, he has joined as CSIR- Emeritus Scientist in December 2020. Prof Vitthal has 160 publications in peer reviewed journals with an average impact factor of 1.8. His citations are 3084. The h- and i-10 indices are 25 and 69 respectively. He has 3 books and 2 book chapters to his credit. Prof Vitthal's research interests include preparation, characterization, magnetic, transport and catalytic properties of nanomaterials, oxide perovskites, borates, pyrochlores, delafossite, orthoferrites, fluorides, glasses and organic acid metal complexes. He has served as coordinator DST-FIST, deputy coordinator UGC-UPE, member DST PURSE- I and Director RDCC, OU. He is the coordinator Telangana Academy of Sciences for combined Karimanagar and Adilabad districts. He has successfully completed 14 major research projects from DST-SERB, CSIR, UGC, APCOST and one international project from TWAS (Third world Academy of Sciences). He is the recipient of Telangana state Best Teacher award in 2016. He is a Fellow of Andhra Pradesh Academy of Sciences (FAPAS) and Telangana Academy of Sciences (FTAS). He has supervised 18 students for PhD Programme and two students for M Tech project. He has mentored three UGC- DSKPDF fellows and three DST-Women Scientists (WOS- A). Presently, five PhD students and one CSIR-RA are working under his guidance..