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Research department of
Physics & Chemistry


INTERNATIONAL CONFERENCE ON
ADVANCES & APPLICATION OF NANOMATERIALS IN MULTIDISCIPLINARY RESEARCH
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17th February, 2024.


Dr. M. Latha Beatrice

HOD Dept of Physics


Dr. S. Mary Helen

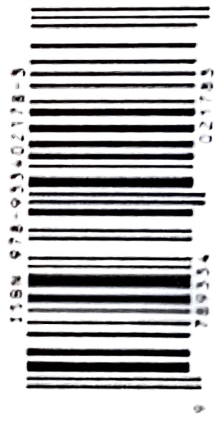
HOD Dept of Chemistry


Dr. J. Johnson

Principal

ADVANCES AND APPLICATIONS OF NANOMATERIALS IN MULTIDISCIPLINARY RESEARCH

Edited by
ANNAI VELANKANNI COLLEGE
PG & RESEARCH DEPARTMENT OF PHYSICS & CHEMISTRY
Thalayavattam, Kanyakumari District,
Tamil Nadu, India-629157



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PG & RESEARCH DEPARTMENT OF PHYSICS & CHEMISTRY
Thalayavattam, Kanyakumari District,
Tamil Nadu, India-629157

INVESTIGATIONS OF PHYSICAL AND STRUCTURAL PROPERTIES OF ALUMINO SILICATE GLASSES DOPED WITH V_2O_5

V. Geetha^a, R.P.Jebin^b

^aReg. No: 22213092132008, Department of Physics and Research centre, Muslim Arts College, Thiruvithancode, Tamil Nadu, India.

^bAssistant Professor, Department of Physics and Research centre, Muslim Arts College, Thiruvithancode, Tamil Nadu, India.

ABSTRACT

Pr_2O_3 and V_2O_5 doped with Calcium aluminosilicate glasses were prepared by conventional melt-quenching technique. The structure of the glasses was characterized using the Fourier transform infrared spectrometer. The FTIR analysis indicated the presence of various bonds comprising Ca-O, Si-O-Si, Al-O, V-O which were attributed to different vibrations. Density was measured using Archimedes principle, and the physical properties such as the ion concentrations, interatomic distance, polaron radius, and field strength were calculated.

Keywords: Oxide glasses and FTIR.

Introduction

Oxide glasses are well known as excellent hosts for co-doped of rare earth and transition metal ions. Borosilicate glasses have the properties of being extremely transparent, physically durable, low thermal expansion, thermally stable by nature and diverse applications. Adding B_2O_3 to SiO_2 glasses increases their chemical inert, thermal stability and corrosion resistance [1]. Micro-hardness and thermal stability are both improved by adding B_2O_3 to SiO_2 glass host. Transition metal ions are used in glass science due to their presence in one or more valence states that alters the structural and optical characters.

Experimental Method

The present glass samples $20.0 CaO - 29 Al_2O_3 - 25 B_2O_3 - 25 SiO_2 : 1Pr_2O_3 + xV_2O_5$ with mol% were prepared by melt quenching method. The analytic grade

chemicals of CaO, Al₂O₃, SiO₂, B₂O₃, Pr₂O₃ and V₂O₅ starting materials with 99% purity. These compounds in appropriate amounts were mixed thoroughly in an agate mortar and pestle grinded. A 25ml crucible is used to melt finely mixed powders of chemicals with the use of a programmable furnace. The melting point was estimated to be between 1475 and 1490 degrees Celsius. Final transparent bubble-free melt discharged on brass cast for glass creation was carried out Annealing was then done in the muffle furnace. At 475°C for 12 hours. Samples arrayed in three-dimensional arrays were utilized for a variety of tests. The glass structure was investigated using Fourier transform infrared spectroscopy (FTIR, Mattson 5000 FTIR spectrometer, Madison, USA) in the wavenumber range 400–4000 cm⁻¹.

Table 1 Methods of Investigation are selected for glass preparation, and 'x' changes from 0 to 1 mol percent with a 0.2 mol percent step size.

S. No	Glass Codes	CaO	Al ₂ O ₃	B ₂ O ₃	SiO ₂	Pr ₂ O ₃	V ₂ O ₅
		mol%	mol%	mol%	mol%	mol%	mol%
1	Pr	20	29	25	25	1	--
2	PrV 0.2	20	28.8	25	25	1	0.2
3	PrV 0.4	20	28.6	25	25	1	0.4
4	PrV 0.6	20	28.4	25	25	1	0.6
5	PrV 0.8	20	28.2	25	25	1	0.8
6	PrV 1.0	20	28	25	25	1	1

Results and discussion

FTIR Studies

The host glass network is made up of Al₂O₃ and SiO₂. The borate is part of the glass network with CaO structural units, while SiO₂ is part of the glass network with tetrahedral [SiO₄/2] units and all four oxygen in the SiO₄ tetrahedron are shared. FTIR spectra were taken at room temperature of Pr₂O₃-doped Calcium aluminosilicate glasses with a range of 400 to 1400 cm⁻¹, and they were taken at room temperature. Fig. reports the FT-IR spectra of 20CaO-29Al₂O₃-60SiO₂:Pr₂O₃:xV₂O₅ glasses. The observed spectra exhibited well-resolved following bands due to silicate, calcium, aluminium and vanadium units at different wave number regions are given in Table [2-6].

Table 2 FTIR Assignment on 20CaO-29Al₂O₃-25B₂O₃-25SiO₂:xV₂O₅ glasses.

FTIR (cm ⁻¹)	Assignments
~ 1575	Ca - O Vibrations
~ 415	Al - O Linkage in AlO ₄ .
~ 710 -775	Al - O Linkage in AlO ₆ unit.
~ 1015 to 1023	Si - O - Si Asymmetrical stretching
~ 842 to 851	Si - O - Si symmetrical stretching
~ 461 to 473	Si - O - Si Rocking stretching
~ 415	V - O specific Stretching Vibration

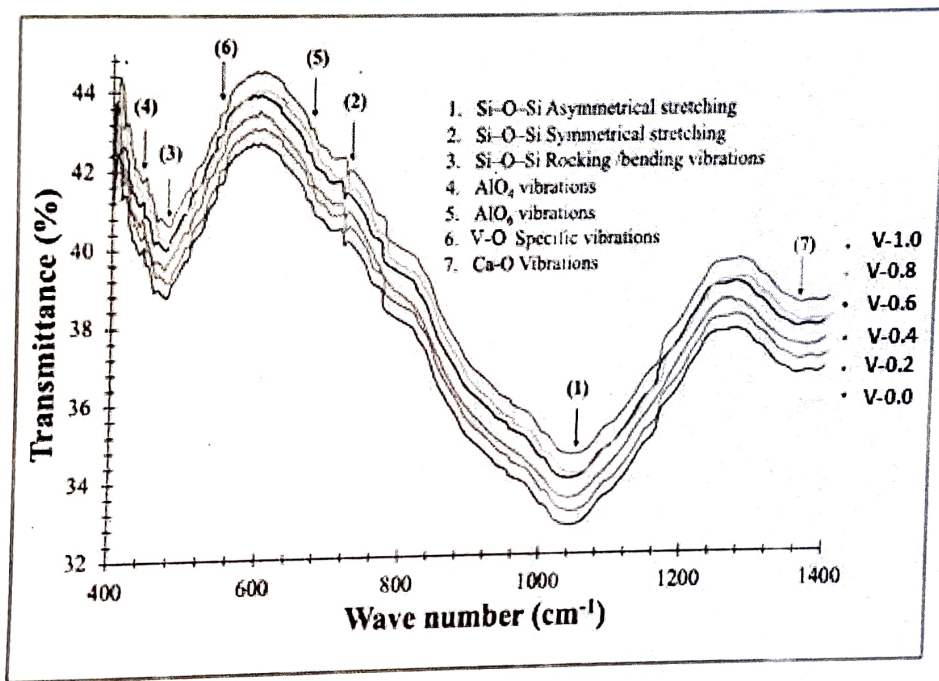


Fig.2 FT-IR spectra of 20CaO-29Al₂O₃-25B₂O₃-25SiO₂:xV₂O₅ glasses are recorded at room temperature.

The glass with a 0.8 mol% V₂O₅ concentration found to be highest in the 20CaO-29Al₂O₃-25B₂O₃-25SiO₂:Pr₂O₃:xV₂O₅ glasses exhibiting the highest shift in wavenumber positions of all the silicate, aluminium, calcium and vanadium structural units. Due to steady inter-ionic forces between V³⁺ ions to Si⁴⁺, Al³⁺, and Ca²⁺ ions.

Specific Physical Characteristics:

Glass	Pr	PrV0.2	PrV0.4	PrV0.6	PrV0.8	PrV1.0
Density (gm/cm ³)	4.06	4.37	4.56	4.69	4.81	4.045
Ionic concentration (x 10 ²⁰)	4.305	4.601	10.574	15.569	22.391	26.762
Ionic radius (Å)	10.86	11.053	8.5244	7.2717	6.4289	6.952
Polaron radius (Å)	2.564	2.377	2.329	1.933	1.8012
Molar volume (x 10 ¹⁴ cm ³ mol ⁻¹)	5.24	6.79	8.0023	9.61	10.44
Field strength (x 10 ¹⁴ cm ⁻²)	20.25	21.06	21.77	21.39	20.66	21.16
Oxygen Packing Density	74.10	75.88	76.13	76.98	77.39	78.08
Electro negativity	7.85	8.99	8.98	8.97	8.96	8.69
Optical Basicity	6.5	6.72	6.73	6.74	6.76	6.70
Refractive index	1.42	1.47	1.48	1.49	1.53	1.51

Glasses composed of 20.0 CaO – 29 Al₂O₃ – 25 B₂O₃ – 25 SiO₂: 1Pr₂O₃ + 0.0 V₂O₅ where 'x' varies 0 to 1 mol% with a step size of 0.2 mol%. have had their physical properties studied. The observed changes in density and molar volume of glasses were explained by understanding the structural changes that happened in the environment of different structural units of polyhedral of silicate, aluminium and borate cations due to calcium and vanadium ions. The decrease in density of glasses is an indication of decreasing structural compactness or rigidity with the increase in the concentration of V₂O₅ due to the depolymerization of glass samples. The magnitude of optical basicity indicates the ionic or covalent nature of glass, because of accumulated basicity suggests diminishing covalence. Accumulation of V₂O₅ interchanges the CaO, which affects in diminishing of magnitude of NBO's, the existing cage average charge around V³⁺ rises, relative molar volume increases, the V-O detachment increases up to 0.8 mol% afterwards decreases. The intensification of the manganese ions generally exists in V³⁺ states, occupy network forming positions with V₂O₅ structural entities rise the rigidity of the glasses. X-ray diffraction reports of the glasses reported [7].

Conclusion

The 20.0 CaO -29 Al₂O₃ - 25 B₂O₃ - 25 SiO₂: 1Pr₂O₃:xV₂O₅ glasses were prepared in this work. X-ray diffraction has been used to investigate the structure of the glasses. The FTIR spectra exhibited the bands due to Al₂O₃, Pr₂O₃, B₂O₃ and V₂O₅ functional groups in all the glasses investigated.

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