

# Properties of Vanadium ( $\text{VO}^{2+}$ ) doped $\text{K}_2\text{O}$ - $\text{CdO}$ - $\text{B}_2\text{O}_3$ - $\text{SiO}_2$ (KCdBSi) Glasses

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## ABSTRACT

Glasses of the  $20\text{K}_2\text{O}$  -  $5\text{CdO}$  -  $60\text{B}_2\text{O}_3$  -  $15\text{SiO}_2$  and  $(20-x) \text{K}_2\text{O}$  -  $5\text{CdO}$  -  $60\text{B}_2\text{O}_3$  -  $15\text{SiO}_2$  -  $x\text{V}_2\text{O}_5$  (where  $x = 0.1$  to  $0.5$  mol %) KCBSi systems are prepared by melt quenching technique. Optical and structural properties of undoped glass, and glasses doped with  $\text{VO}^{2+}$  ions are examined. Their structural properties are determined with XRD, Fourier Transform Infrared (FTIR) and Electron Spin Resonance spectra (ESR) and Optical absorption spectra. The ESR spectra of all the glass samples exhibit resonance signals characteristic of  $\text{VO}^{2+}$  ions. The values of spin-Hamiltonian parameters indicated that the  $\text{VO}^{2+}$  ion in KCdBSi glasses are present in octahedral sites with tetrahedral compression and belong to  $\text{C}_{4v}$  symmetry. Spin-Hamiltonian parameters 'g' and 'A' are calculated from their Ultra Violet edges. IR spectra of these glasses are analysed in order of each component to the local structure. The physical parameters are also evaluated.

**Keywords:** Borosilicate glass, Vanadium, Optical Properties, XRD, FTIR, ESR, and spin-Hamiltonian.

## INTRODUCTION

In recent years there has been a considerable interest in the study of glasses doped with transition metal ions because of their technological applications. Borosilicate glasses constitute a subject of wide spread interest in number of fields from the earth science to glass industry in particular for special glasses i.e., Pyrex. The early research is of great importance because it is the first attempt to study symmetrically the relationships between the composition of glass and its physical and chemical properties [1]. Borosilicate glasses are widely used in optical glasses, heat resistant glasses and electronic glass industry for its excellent properties [2]. The structural role of  $\text{CdO}$  and  $\text{K}_2\text{O}$  is unique since they occupy both modifying and glass forming positions. They are glass modifiers and enter the glass network, by breaking up the B-O-B bonds and introduce co-ordinate defects along with non-bridging oxygen's (NBO). On the other hand, potassium Borosilicate glasses have been widely used in the ceramic industry for the fabrication of glaze glass coatings intended for the application on faience porcelain and other types of ceramics [3]. Semiconducting transition metal oxide such as  $\text{V}_2\text{O}_5$  based glasses have gained much interest in solid state chemistry and materials science with regard to their possible applications as memory and switching devices [4]. Vanadium belongs to the unfilled 3d elements and possesses many valence states. The  $\text{V}^{2+}$ ,  $\text{V}^{3+}$ ,  $\text{V}^{4+}$  and  $\text{V}^{5+}$  states are the most well-known valence states of vanadium in oxide glasses. Vanadium containing oxide glasses are known to be semiconductors and the transport mechanism involves the exchange of electrons between vanadium (IV) and vanadium (V) centers [5].



Vanadate glasses are identified as n-type semiconductors for low  $V^{4+} / V^{5+}$  ratio [6]. It is also known that  $V^{5+}$  in low ratios enter the amorphous structure as an impurity whereas  $V^{5+}$  in high ratios are present in the structure as glass formers [7]. Some authors studied the effect of single [8] and multiple [9] (TM) transition metal ions as dopant in alkali and alkaline earth oxide glasses [10]. Binary and ternary  $V_2O_5$  glasses can exhibit a semiconducting behavior which arises from an unpaired  $3d^1$  electron hopping between the transition metal (TM) ions when the TM ions exist in two or more valence states, i.e., an electron hopping from a  $V^4$  site to a  $V^5$  [11]. Glasses doped with TM ions came into prominence because of their notable spectroscopic properties and their suitability for electronic, fiber optic communications, luminescent solar energy concentrators (LSCs) [12].

In the present study, the absorption and transmission of  $20K_2O - 5CdO - 60B_2O_3 - 15SiO_2$  and  $(20-x) K_2O - 5CdO - 60B_2O_3 - 15SiO_2 - xV_2O_5$  (where  $x=0.1$  to  $0.5$ mol %) glasses (KCBSi systems) are of particular interest because these are transparent from the ultra violet to middle infrared region and the addition of  $V_2O_5$  the transition metal ion permits the possibility of glass to exhibit semiconducting behavior. Defects of the surfaces and their structural properties are determined by XRD, ESR, FT-IR

### Experimental:

Glass samples are prepared in the composition  $20K_2O - 5CdO - 60B_2O_3 - 15SiO_2$  for pure sample and  $(20-x) K_2O - 5CdO - 60B_2O_3 - 15SiO_2 - xV_2O_5$  for vanadium doped samples where  $x = 0.1$  to  $0.5$ mol%  $V_2O_5$ . The composition of glass samples are given in Table 1. Using digital balance of sensitivity  $\pm 0.0001$ gms, appropriate amount of chemicals in powder form are weighed and grounded into fine powder and mixed thoroughly. The samples are melted in silica crucibles in an electrical furnace at temperature range of  $1100^\circ C - 1200^\circ C$  for 12 minutes. The melted samples are poured on a clean polished brass plate and carefully pressed with another brass plate to get uniform thickness of the glass. The glasses obtained are transparent and are light greenish in colour. The obtained glasses are polished finely to obtain optical measurements.

X-ray diffraction pattern of glass samples are recorded using Copper target on Philips PW (1710) Diffractometer at room temperature. ESR readings are made at room temp on JEOL-JM FE3 with 100 KHz field modulation EPR spectrometer.

The density of glass samples is determined by using Archimedes's principle with Xylene as an inert buoyant liquid.

## RESULTS

### Physical parameters:

Based on the density ( $d$ ) and calculated average molecular weight ( $M$ ), various physical parameters such as the vanadium ion concentration ( $N_i$ ), mean vanadium ion separation ( $r_i$ ) and the polaron radius ( $r_p$ ) are evaluated using conventional formulae [13] and presented in Table 2.

The density of glass is undoubtedly one of the most important properties in industrial glass production and is important for calculating various physical parameters such as the vanadium ion concentration ( $N_i$ ), mean vanadium ion separation ( $r_i$ ) and the polaron radius ( $r_p$ ) using conventional formulae [13]. Refractive indices for all the glass samples are also found using Abbe's Refractometer. The values are tabulated in Table 2 along with average molecular weight ( $M$ ). There is a small variation in the density of the glass samples from  $V_0$  to  $V_5$  samples and error in the density measurements is estimated to be  $\pm 0.0001$ . The Inter ionic distance and the polaron radius are observed to be decreasing and the optical basicity remains almost equal for all the samples.

## XRD:

The X-Ray diffraction pattern of the (20-x) K<sub>2</sub>O - 5CdO - 60B<sub>2</sub>O<sub>3</sub> - 15SiO<sub>2</sub> - xV<sub>2</sub>O<sub>5</sub> (where x = 0, 0.1 to 0.5mol %) glasses reveals no sharp peaks which confirms the presence of amorphous nature in the present glassy matrix shown in Fig. 1 and Fig 2.

The X-ray diffraction is a useful method to detect readily the presence of crystals in a glassy matrix if their dimensions are greater than typically 100nm. The X-ray diffraction pattern of an amorphous material is distinctly different from that of crystalline material. The XRD patterns of the present glass system reveal no sharp peaks which is the characteristic of the amorphous materials. Fig.1, Fig.2 shows the typical X-ray diffraction patterns for the KCBSi glass system.

## ESR Study:

The ESR spectra recorded at room temperature for (20-x) K<sub>2</sub>O - 5CdO - 60B<sub>2</sub>O<sub>3</sub> - 15SiO<sub>2</sub> - xV<sub>2</sub>O<sub>5</sub> (where x=0, 0.1 to 0.5mol %) glasses under investigation are shown in Fig 7. Spectra are observed to be complex made up of resolved hyperfine components raised from 3d<sup>1</sup> electron of VO<sup>2+</sup> ion in association with <sup>51</sup>V (I=7/2). As the concentration of V<sub>2</sub>O<sub>5</sub> is increased up to 0.5mol% an increasing degree of resolution and the intensity of signal have been observed. Further at low V<sub>2</sub>O<sub>5</sub> content, the ESR spectra observed to be asymmetrical. The values of g<sub>||</sub> and g<sub>⊥</sub> (obtained from these spectra) along with the other pertinent data are furnished in Table 5.

No ESR signal is observed in undoped glasses confirming that the starting material used in the present work is free from transition metal impurities or other paramagnetic centers (defects). The ESR spectra of all the investigated samples from V<sub>1</sub> to V<sub>5</sub> exhibit resonance signals and are shown in Fig. 7. Because of the low content of V<sub>2</sub>O<sub>5</sub> (i.e., x=0.1mol %) these spectra shows a well-resolved hyperfine structure (hfs) typical for vanadyl ions in a C<sub>4v</sub> symmetry. The 16- line feature with eight parallel and eight perpendicular lines is typical of the unpaired (3d<sup>1</sup>) electron of VO<sup>+</sup> ion in association with <sup>51</sup>V (I=7/2) is an axially symmetric crystal field [23]. The analysis of well resolved hyperfine structure of the ESR spectra was made using an axial spin-Hamiltonian.

$$H = g_{||} \beta B_z S_z + g_{\perp} \beta (B_x S_x + B_y S_y) + A_{||} S_z I_z + A_{\perp} (S_x I_x + S_y I_y) \quad (7)$$

where  $\beta$ -Bohr magneton.  $g_{||}$  and  $g_{\perp}$  are the parallel and perpendicular principle components of g tensor.  $B_x$ ,  $B_y$ ,  $B_z$  – components of the magnetic field.  $S_x$ ,  $S_y$ ,  $S_z$ ,  $I_x$ ,  $I_y$ ,  $I_z$  – components of the electron and nucleus spin operator.  $A_{||}$  and  $A_{\perp}$  are principal components of the hyperfine coupling tensor. The values of the magnetic field for the hyperfine peaks from the parallel and perpendicular absorption [24] bands are given by

$$B_{||}(m_l) = B_{||}(0) - A_{||}(m_l) - (63/4 - m_l^2) A_{\perp}^2 / 2 B_{||}(0) \quad (8)$$

$$B_{\perp}(m_l) = B_{\perp}(0) - A_{\perp}(m_l) - (63/4 - m_l^2) (A_{||}^2 - A_{\perp}^2) / 4 B_{\perp}(0) \quad (9)$$

where  $m_l$  is the magnetic quantum number of the vanadium nucleus, which takes the values  $\pm 7/2$ ,  $\pm 5/2$ ,  $\pm 3/2$ ,  $\pm 1/2$ .

$$B_{||}(0) = h\nu / g_{||} \beta \quad \text{and} \quad B_{\perp}(0) = h\nu / g_{\perp} \beta$$

where the symbols have their usual meaning and  $\nu$  is the microwave frequency. EPR parameters in studied glasses are given in Table 4. The values obtained are in good agreement with the other reports given in literature [23, 25-27]. The data shows that  $g_{||} < g_{\perp} < g_e$  and

$A_{\parallel} > A_{\perp}$ , the relation that corresponds to vanadyl ions in KCBSi glasses exist as  $VO^{2+}$  ions in octahedral coordination with a tetragonal compression and have a  $C_{4v}$  symmetry. The vanadyl oxygen is attached axially above the  $V^{4+}$  site along the Z-axis ( $V=O$  bond) while the sixth oxygen forming the  $O-VO_4-O$  unit lies axially below the  $V^{4+}$  site in opposition with “yl” Oxygen. The predominant axial distortion of the  $VO^{2+}$  octahedral oxygen complex along  $V=O$  direction may be the reason for nearly equal  $g$  and  $A$  values for all the glass samples [25]. Fermi contact interaction term ( $K$ ) and dipolar hyperfine coupling parameter ( $P$ ) are evaluated using the expressions developed by Kivelson and Lee [28].

$$A_{\parallel} = -P [(K-4/7) - \Delta g_{\parallel} - 3/7 - \Delta g_{\perp}] \quad (10)$$

$$A_{\perp} = -P [(K-2/7) - 11 / 14 \Delta g_{\perp}] \quad (11)$$

where  $\Delta g_{\parallel} = g_{\parallel} - g_e$ ,  $\Delta g_{\perp} = g_{\perp} - g_e$  and  $g_e = 2.0023$  is the  $g$  factor of the free electrons [29]. The values of  $(\Delta g_{\parallel} / \Delta g_{\perp})$  which measure the tetragonality of the  $V^{4+}$  site are also calculated and are presented in Table 4. A decrease in  $(\Delta g_{\parallel} / \Delta g_{\perp})$  shows that the octahedral symmetry around  $V^{4+}$  ions is improved [30]. When the concentration of  $V_2O_5$  is increased beyond 0.5mol%, suppression in the hyperfine structure has been observed. Such suppression may be due to various interactions of electronic spins with their surroundings. In electronically conducting vanadate glasses, one such interaction occurs via a so-called super exchange of an electron, i.e, hopping of a mobile electron along a  $V^{4+}-O-V^{5+}$  bond. Thus the analysis of ESR with optical absorption makes an impression that there is an increasing possibility of electronic conduction in the glasses containing  $V_2O_5$  beyond 0.5mol%. From data  $V_1$  sample value of  $A_{\parallel}$  and  $P$  is very high compared to other samples.

#### FT-IR Studies:

The Fourier transform infrared (FT-IR) spectra of  $(20-x) K_2O - 5CdO - 60B_2O_3 - 15SiO_2 - xV_2O_5$  (where  $x = 0, 0.1$  to  $0.5$  mol %) glasses recorded at room temperature have exhibited prominent bands in the region  $400-1000cm^{-1}$  are shown in Fig 8, these bands are identified due to the characteristic vibrational bands of Boron Oxygen-Boron, combined stretching vibrations of Silicate-Oxygen-Silicate and B-O-B, B-O stretching vibrations of  $BO_4/V = 0$ , stretching vibrations of B-O bands in  $BO_3$  units, vibrations of  $BO_4$  structural units and due to the bending vibrations of B-O-B linkages respectively. stretching vibrations of B-O attached to large segments of borate network. Close examination of IR spectra reveals that the vibrational intensity increases gradually as  $x$  takes the values as 0.1 to 0.5 mol% of vanadium. A summary of  $(20-x) K_2O - 5CdO - 60B_2O_3 - 15SiO_2 - xV_2O_5$  (where  $x = 0, 0.1$  to  $0.5$  mol %) glasses doped with different concentrations of  $V_2O_5$  is presented in Table 6.

#### FT-IR Studies:

The FT-IR study provides structural information when a thorough analysis of the data is carried out. Fourier Transformation infrared spectroscopy (FT-IR) absorption spectra of  $(20-x) K_2O - 5CdO - 60B_2O_3 - 15SiO_2 - xV_2O_5$  for Vanadium doped samples where  $x = 0, 0.1$  to  $0.5\%$   $V_2O_5$  ( KCBSi ) glass systems are recorded at room temperature and the spectra are presented in Fig.8.

The infrared spectra of these glasses show absorption peaks. The peaks are sharp, medium and broad in nature. The broad bands are exhibited in the oxide spectra are most probably due to the combination of high degeneracy of vibration states, thermal broadening of the lattice dispersion band and mechanical scattering from powder sample. The IR spectra of these glasses consist of broad and sharp bands in different regions ( $400-4000cm^{-1}$ ) are shown in Fig.8 and are tabulated in Table 5. These bands are strongly influenced by increasing substitution of vanadium. The position of the bands is shifted with the variation of transition metal ion composition [31]. The vibrational spectra can readily used to identify the presence of defect groups or

radiation-induced defects, within a glass. Infrared spectroscopy has also been used to identify low concentration impurities such as water, hydroxyl ions etc in a glass [32].

The FT-IR spectrum of the glass system contains nine major bands presenting the wave number range of  $715\text{ cm}^{-1}$ ,  $835\text{ cm}^{-1}$ ,  $922\text{ cm}^{-1}$ ,  $1005\text{ cm}^{-1}$ ,  $1097\text{ cm}^{-1}$ ,  $1092\text{ cm}^{-1}$ ,  $1242\text{ cm}^{-1}$ ,  $1352\text{ cm}^{-1}$ ,  $1471\text{ cm}^{-1}$ . These bands are characteristic vibrational bands of Boron-Oxygen-Boron, combined stretching vibrations of Silicate-Oxygen Silicate and B-O-B, B-O stretching vibrations of  $\text{BO}_4/\text{V} = 0$ , stretching vibrations of B-O bands in  $\text{BO}_3$  units, from pyro-orthoborate groups, B-O stretching vibrations attached to large segments of borate network, stretching vibrations of B-O attached to large segments of borate network. Close examination of IR spectra reveals that the vibrational intensity increases gradually as x takes the values as 0.1 to 0.5 mol% of vanadium. At  $x = 0$ , in the absence of vanadium asymmetric vibrations Si-O-Si is observed. Thus the analysis of IR spectra also supports the view point that as the concentration of  $\text{V}_2\text{O}_5$  is raised up to 0.5mol%, there is a growing degree of disorder in the glass network. Hence there is a possibility for the formation of single Boron – Oxygen – Vanadium frame work to the present glass system.

## DISCUSSION

## CONCLUSION

1. XRD confirms that all glass samples are amorphous in nature. The physical parameter, density shows a small increase in its value by the introduction of  $\text{V}_2\text{O}_5$  into a KCBSi glasses.
2. The optical absorption study indicates the presence of vanadium predominantly in  $\text{VO}^{2+}$  state which takes modifier positions, if  $\text{V}_2\text{O}_5$  is present in lower Concentrations (up to 0.5mol %).
3. The ESR and Optical absorption spectra of  $\text{V}_2\text{O}_5$  doped in KCBSi glasses have been successfully interpreted as the presence of six coordinate tetravalent vanadium existing as a vanadyl complex with a tetragonally compressed octahedral site.
4. The optical band gap energies slightly decrease with the addition of vanadium content; It's due to non-bridging oxygens.
5. The spin-Hamiltonian parameters g and A are found to be independent of  $\text{V}_2\text{O}_5$  content. The increase in  $\Delta g_{\parallel} / \Delta g_{\perp}$  value indicates the improved octahedral symmetry around  $\text{VO}^{2+}$  ion.
6. The Infrared (IR) spectra of glasses in the present system reveals sharp and diffuse absorption peaks.

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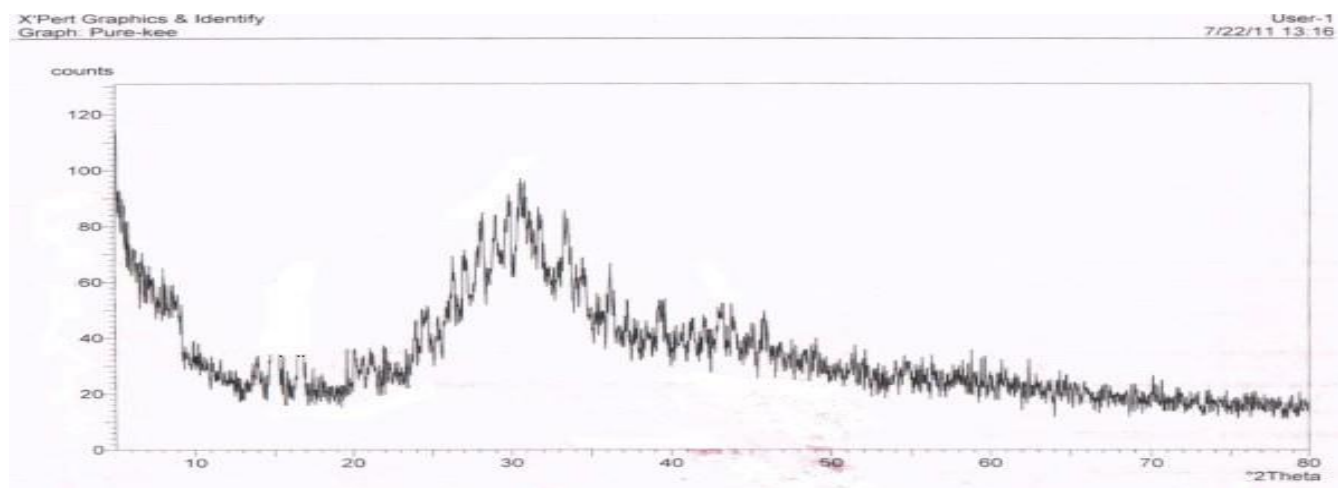
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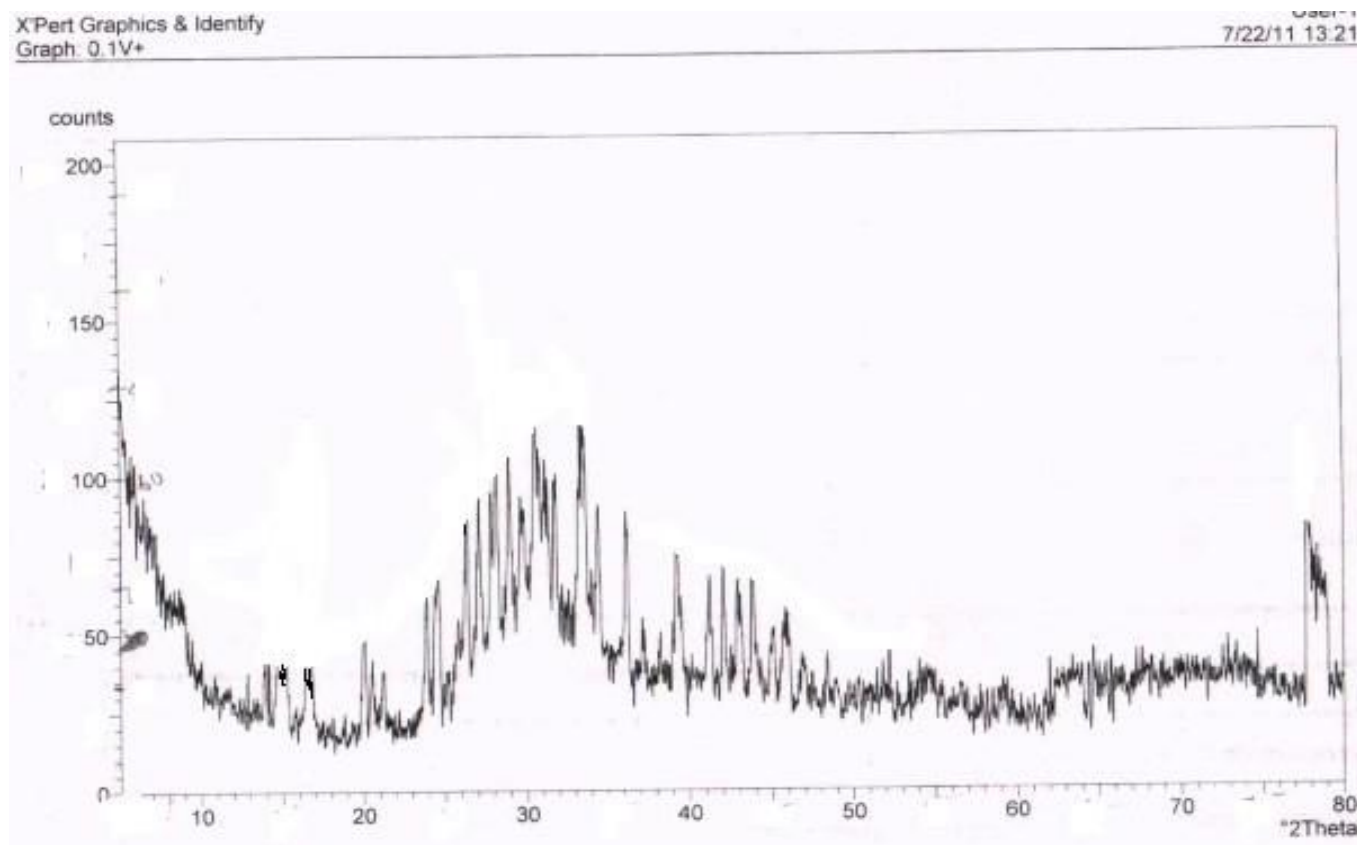


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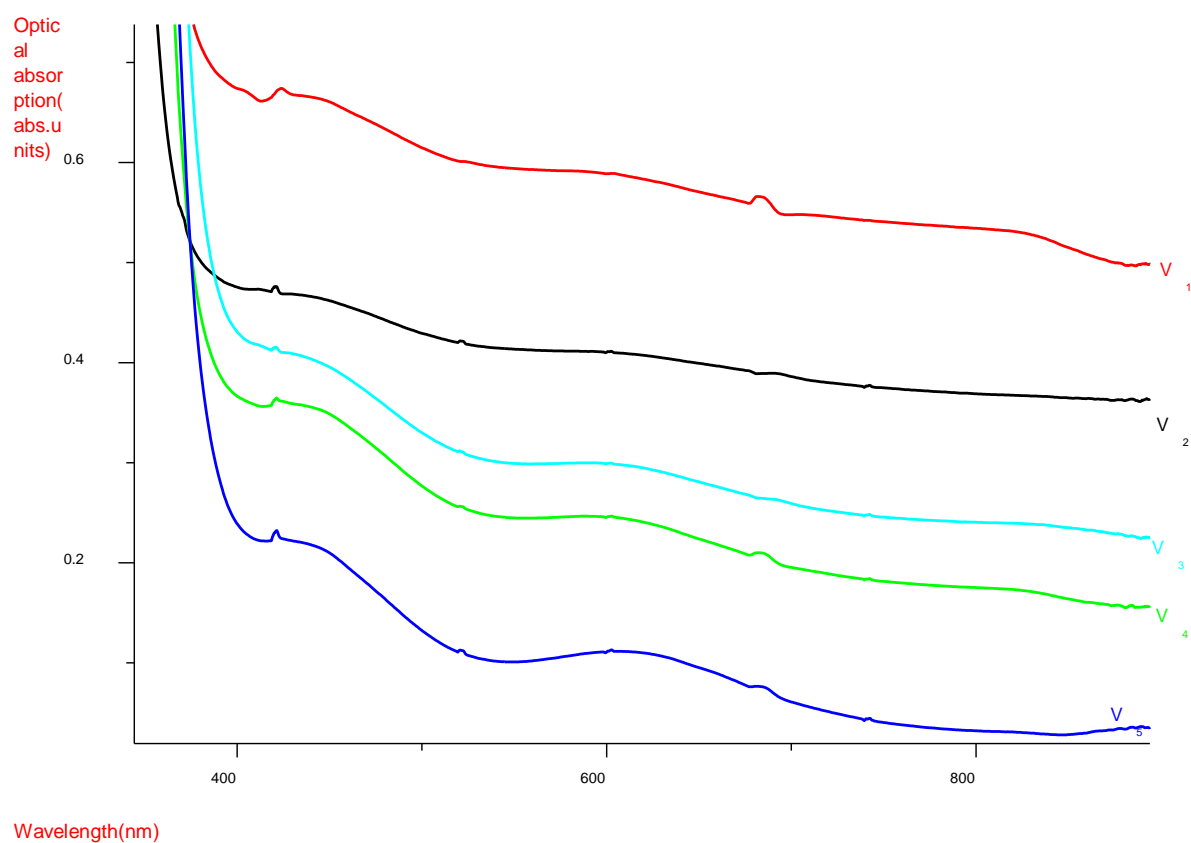
## FIGURES



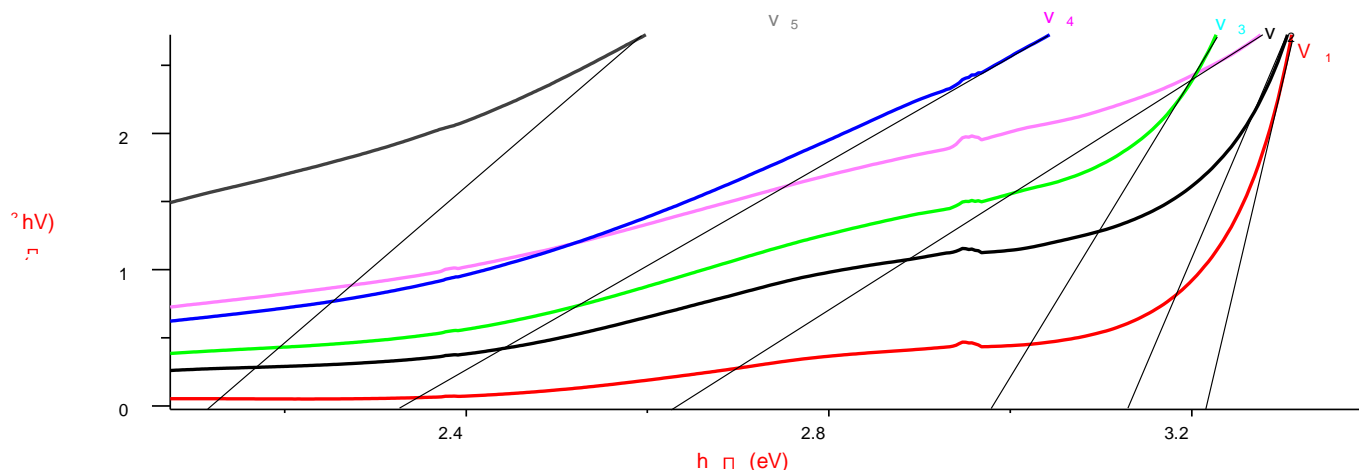
**Fig 1: XRD pattern of pure sample of KCBSi glass system.**



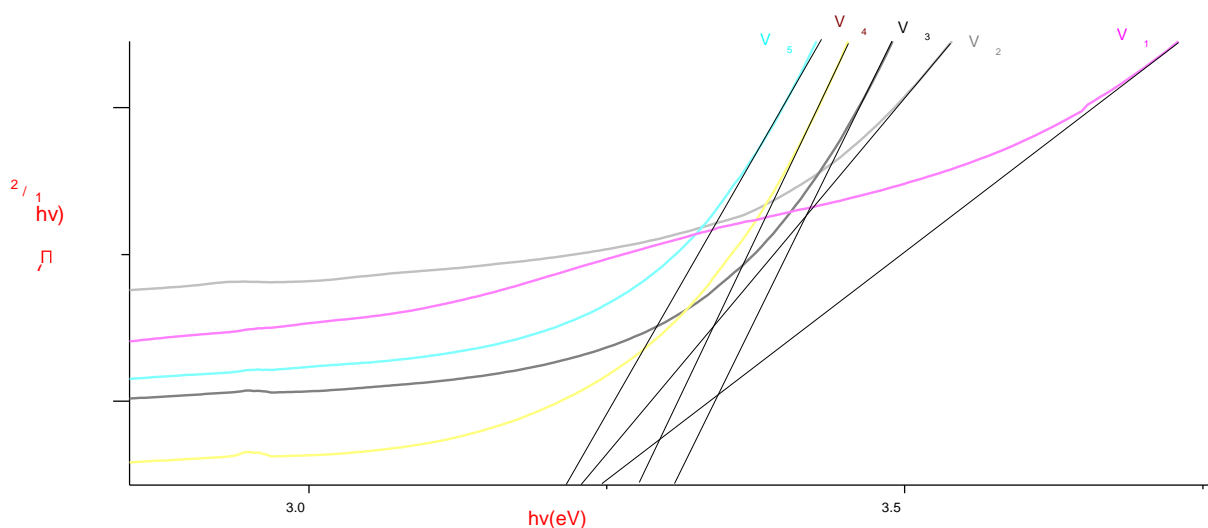
**Fig 2: XRD pattern of 0.1mol%  $\text{VO}^{2+}$  ion doped sample of KCBSi glass system.**



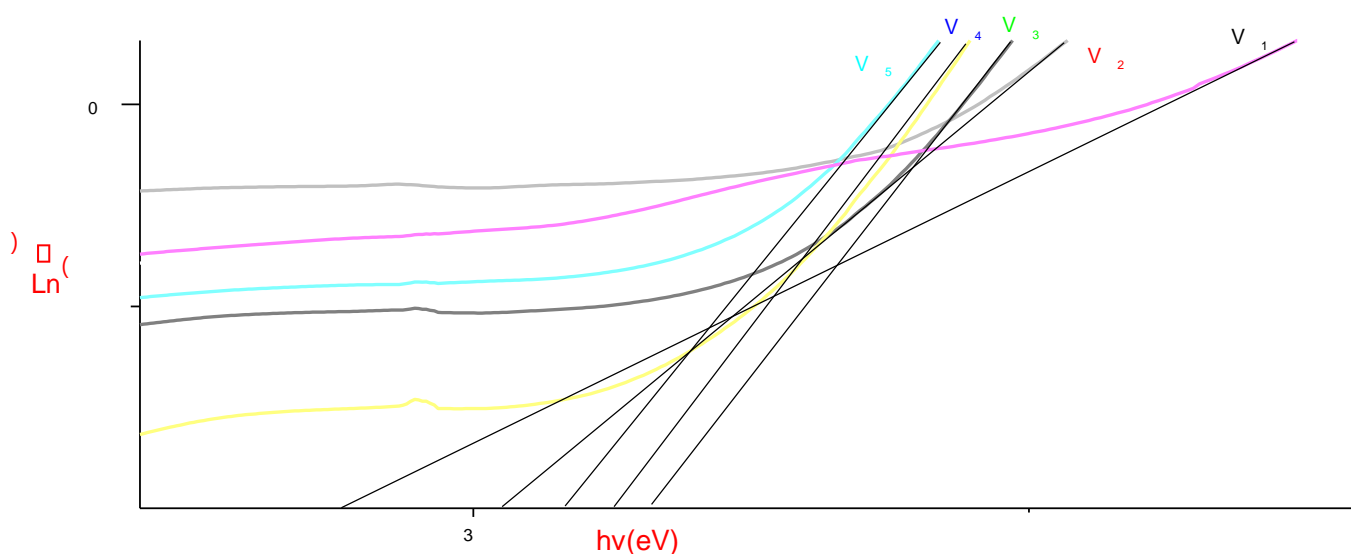
**Fig 3: Optical absorption band spectrum of  $\text{VO}^{2+}$  ion doped KCBSi glass system.**



**Fig 4: Direct bands of  $\text{VO}^{2+}$  ion doped KCBSi glass system.**

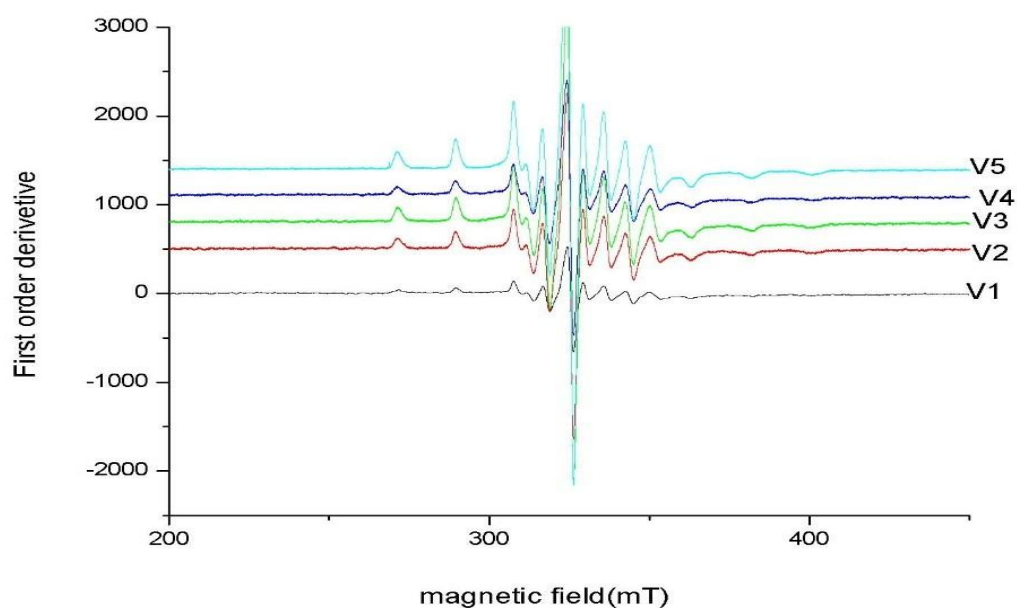


**Fig 5: Indirect bands of  $\text{VO}^{2+}$  ion doped KCBSi glass system.**

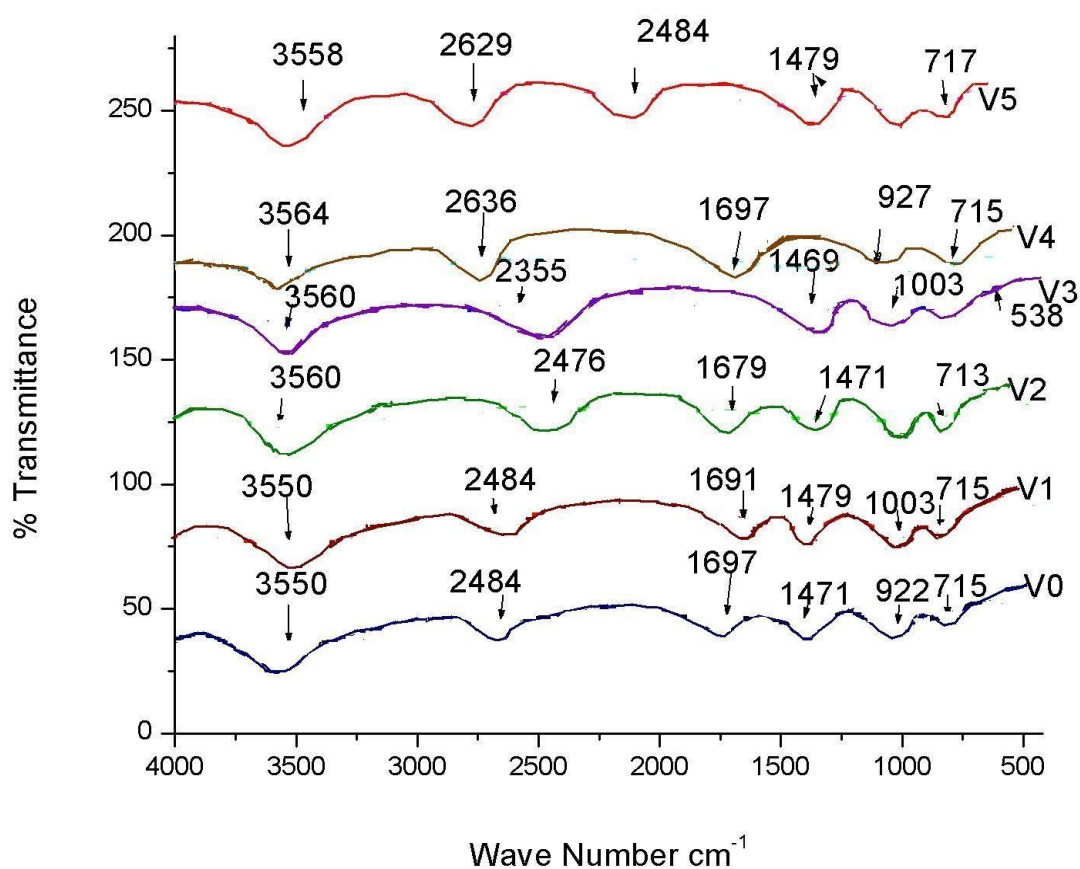


**Fig 6: Urbach plots of  $\text{VO}^{2+}$  ion doped KCBSi glass system.**





**Fig 7: ESR Spectrum of  $\text{VO}^{2+}$  ion doped KCBSi glass system.**



**Fig 8: FT-IR Spectrum of  $\text{VO}^{2+}$  ion doped KCBSi glass system.**

## TABLES

| Glass          | K <sub>2</sub> O mol% | CdO mol% | B <sub>2</sub> O <sub>3</sub> mol% | SiO <sub>2</sub> mol% | V <sub>2</sub> O <sub>5</sub> mol% |
|----------------|-----------------------|----------|------------------------------------|-----------------------|------------------------------------|
| V <sub>0</sub> | 20                    | 5        | 60                                 | 15                    | -                                  |
| V <sub>1</sub> | 19.9                  | 5        | 60                                 | 15                    | 0.1                                |
| V <sub>2</sub> | 19.8                  | 5        | 60                                 | 15                    | 0.2                                |
| V <sub>3</sub> | 19.7                  | 5        | 60                                 | 15                    | 0.3                                |
| V <sub>4</sub> | 19.6                  | 5        | 60                                 | 15                    | 0.4                                |
| V <sub>5</sub> | 19.5                  | 5        | 60                                 | 15                    | 0.5                                |

**Table1: Glass compositions of VO<sup>2+</sup> ion doped KCBSi glass system.**

| Glass sample   | Density d gm/cm <sup>3</sup> (±0.004) | Avg.mol Wt.(M) | Transition metal ion conc. N <sub>i</sub> (10 <sup>19</sup> ions/cm <sup>3</sup> ) ±0.005 | Inter ionic distance r <sub>i</sub> (Å°) ±0.005 | Polaron radius r <sub>p</sub> (Å°) ±0.005 | Optical basicity |
|----------------|---------------------------------------|----------------|---|---|---|------------------|
| V <sub>0</sub> | 2.4788                                | 80.17          | -   | -   | -   | 0.4325           |
| V <sub>1</sub> | 2.5571                                | 80.44          | 1.91  | 37.38   | 15.06                                     | 0.4328           |
| V <sub>2</sub> | 2.5006                                | 80.26          | 3.75  | 29.86   | 12.034                                    | 0.4327           |
| V <sub>3</sub> | 2.5244                                | 80.304         | 5.68  | 26.01   | 10.48                                     | 0.4325           |
| V <sub>4</sub> | 2.5637                                | 80.35          | 7.68  | 23.51   | 9.47                                      | 0.4326           |
| V <sub>5</sub> | 2.5551                                | 80.3 9         | 9.57  | 21.86   | 8.81                                      | 0.4326           |

**Table 2: Data of the Physical parameters of VO<sup>2+</sup> ion doped KCBSi glass system.**

| Glass sample                  | Cut off wave length (nm) | $2B_{2g} \rightarrow 2B_{1g}$ (nm) | $2B_{2g} \rightarrow 2E_g$ (nm) |
|-------------------------------|--------------------------|------------------------------------|---------------------------------|
| V <sub>1</sub> V <sub>2</sub> | 321 330                  | 456 431                            | 627 605                         |
| V <sub>3</sub>                | 342                      | 450                                | 607                             |
| V <sub>4</sub>                | 348                      | 430                                | 604                             |
| V <sub>5</sub>                | 349                      | 458                                | 633                             |

**Table 3: Summary of the data on optical absorption spectra of VO<sup>2+</sup> ion doped KCBSi glass system.**

| Glass sample | Direct (E <sub>opt</sub> ) eV | Indirect (E <sub>opt</sub> ) eV | Urbach Energy (E <sub>U</sub> ) eV |
|--------------|-------------------------------|---------------------------------|------------------------------------|
| V1           | 3.328                         | 3.864                           | 0.266                              |
| V2           | 3.320                         | 3.640                           | 0.273                              |
| V3           | 3.155                         | 3.558                           | 0.280                              |
| V4           | 2.904                         | 3.508                           | 0.284                              |
| V5           | 2.455                         | 3.472                           | 0.289                              |

**Table 4: Summary of data on direct, indirect, Urbach energy of VO<sup>2+</sup> ion doped KCBSi glass system.**

| Glass sample   | g <sub>  </sub> | g <sub>⊥</sub> | A <sub>  </sub> 10 <sup>-4</sup> cm <sup>-1</sup> | A <sub>⊥</sub> 10 <sup>-4</sup> cm <sup>-1</sup> | Δg <sub>  </sub> / Δg <sub>⊥</sub> | k     | P    |
|----------------|-----------------|----------------|---|--|------------------------------------|-------|------|
| pure           | -               | -              | -   | -  | -                                  | -     | -    |
| V <sub>1</sub> | 1.948           | 1.992          | 241.9   | 72.6   | 5.71                               | 0.637 | -168 |
| V <sub>2</sub> | 1.972           | 1.999          | 197.2   | 58.2   | 11.1                               | 0.633 | -154 |
| V <sub>3</sub> | 1.964           | 1.976          | 172.0   | 66   | 0.3                                | 0.83  | -123 |
| V <sub>4</sub> | 1.991           | 1.997          | 182.0   | 72   | 0.67                               | 0.85  | -129 |
| V <sub>5</sub> | 1.931           | 1.969          | 175.9   | 52.9   | 2.02                               | 0.66  | -152 |

**Table 5: Summary of the spin Hamiltonian parameters, molecular orbital coefficients of VO<sup>2+</sup> ion doped KCBSi glass system.**

| V <sub>0</sub> | V <sub>1</sub> | V <sub>2</sub> | V <sub>3</sub> | V <sub>4</sub> | V <sub>5</sub> | Assignment   |
|----------------|----------------|----------------|----------------|----------------|----------------|--|
| 1471           | 1479           | 1471           | 1469           | 1469           | 1479           | B—O stretched vibrations attached to large to large segments of borate network. B-O stretched vibrations attached to large segments of borate network. Stretching vibrations of B(III)-O-B(IV) units |
| 1352           | 1350           | 1354           | 1352           | 1352           | 1352           |  |
| 1242           | 1242           | 1244           | 1242           | 1244           | 1240           |  |
| 1097           | 1003           | 1099           | 1099           | 1003           | 1003           |  |
| 1005           | 833            | 1003           | 920            | 827            | 922            |  |
| 922            | 922            | 929            | 920            | 927            | 831            |  |

|                   |                   |                   |                   |                   |            |  |
|-------------------|-------------------|-------------------|-------------------|-------------------|------------|--|
| 835<br>715<br>457 | 833<br>715<br>493 | 835<br>713<br>484 | 833<br>713<br>489 | 827<br>715<br>489 | 715<br>455 | Stretching vibrations B-O Bands<br>in BO <sub>3</sub> units from<br>pyroorthoborate groups.<br>B-O stretching vibrations of BO <sub>4</sub><br>units/V= 0<br>Combined stretching vibrations<br>of Si-O-Si and B-O-B V-O-V<br>units bending B-O stretching<br>vibrations Asymmetric<br>vibrations.<br>Si-O-Si |
|-------------------|-------------------|-------------------|-------------------|-------------------|------------|--|

**Table 6: Summary of the FT-IR study of VO<sup>2+</sup> ion doped KCBSi glass systems.**

| Glass sample   | g <sub>  </sub> | g <sub>⊥</sub> | A <sub>  </sub><br>10 <sup>-4</sup> cm <sup>-1</sup> | A <sub>⊥</sub><br>10 <sup>-4</sup> cm <sup>-1</sup> | Δg <sub>  </sub> / Δg <sub>⊥</sub> | k     | P         |
|----------------|-----------------|----------------|--|---|------------------------------------|-------|-----------|
| pure           | -               | -              | -  | -   | -                                  | -     | -         |
| V <sub>1</sub> | 1.948           | 1.992          | 241.9  | 72.6  | 5.71                               | 0.637 | -168      |
| V <sub>2</sub> | 1.972           | 1.999          | 197.2  | 58.2  | 11.1                               | 0.633 | -154      |
| V <sub>3</sub> | 1.964           | 1.976          | 172.0  | 66  | 0.3                                | 0.83  | -123      |
| V <sub>4</sub> | 1.991           | 1.997          | 182.0 175.9  | 72  | 0.67                               | 0.85  | -129 -152 |
| V <sub>5</sub> | 1.931           | 1.969          |  | 52.9  | 2.02                               | 0.66  |           |