*Egypt. J. Phys.* **Vol. 46,** pp. 17- 21(2018)

# Physical and Optical Properties of PbO $Bi_2O_3$ $B_2O_3$ Glasses Dopped With FeO

**Ghada Adel and H.M. Mokhtar***

*Physics Department, Faculty of Science, Al-Azhar University(girls branch), Nasr City, Cairo, Egypt*

THE EFFECT of compositional changes on the physical properties of 40PbO 10$Bi_2O_3$ (50-0.1)$B_2O_3$xFeO glass system has been investigated. The physical properties include , density ,molar volume,optical electronegativity, optical energy gap, linear refractive index, molar refraction , electronic polorizability ,third order nonlinear susceptibility , have been studied theoretically for 40PbO 10$Bi_2O_3$ (50-0.1)$B_2O_3$xFeO glass system where (x= 0.2,0.3,0.4,0.5). An analysis of physical parameters related to these compositions was compared with theoretical predictions. It was found that by increasing FeO content, the glass matrix becomes more dense, and the optical energy gap decrease, but the refractive index increase. The electronic polarizability of oxide ion increase with increasing the optical basicity. The value of optical basicity shows that the glass materials are more basic. It is suggested that the ability of oxide ion to donate electrons to surrounding cations increases. Also, It was found that the values of third order nonlinear susceptibility increase by increasing FeO content and are found to be larger than those of the silica based glasses. The high values of nonlinear refractive index for all the studied samples are advantageous for all optical signal processing and telecommunications. Also, it was found that the values of third order nonlinear susceptibility increase with decreasing the optical energy gap and increasing the refractive index for all the studied samples. Finally, new nonlinear optical materials were suggested.

## Introduction

Nonlinear optics is the study of phenomena that occur as a consequence of the modification of the optical properties of a material system by the presence of light.Dimitrov and Sakka [1] found that the most important factors which govern the nonlinear response of simple oxide are the linear refractive index and the optical energy gap which are related with oxide metallicity. It is suggested that oxides with a high nonlinear refractive index are found to possess a high linear refractive index and a small optical energy gap which has been attributed to the increase of oxide metallicity. The estimation of electronic polarazibility of ions is the subject of the so called polarizability approach in material science. The polarizability approach has shown renewed interest because of the need to design optical functional materials and to search for novel glasses with higher optical performance such as oxide glasses with high third order nonlinearities [2]. It is suggested that oxides with a high nonlinear refractive index are found to possess high values of optical basicity and high values of oxide ion polorizability [3-7]. The optical properties of 40PbO 10$Bi_2O_3$ (50-.1) $B_2O_3$xFeO glass system where (x= 0.2,0.3,0.4,0.5) have been studied [8]. Appropriate amounts (all in mol %) of reagent grades of $Bi_2O_3$, PbO, $H_3BO_3$ and FeO powders were thoroughly mixed in an agate mortar and melted in a platinum crucible in the temperature range 950-1000 $^oC$ in a PID temperature controlled furnace for about 1 h until a bubble free transparent liquid was formed. The resultant melt was then poured in a brass mould and subsequently annealed at 300 $^oC$. The amorphous state of the glasses was confirmed by X- ray diffraction . The optical absorption spectral studies of PbO $Bi_2O_3$ $B_2O_3$FeOglasses [8] indicate the presence of part of iron ions in $Fe^{3+}$ state occupy tetrahedral positions, if FeO is present in lower concentrations; when the concentration of FeO is in higher quantities (> 0.1 %), these ions seems to exist in $Fe^{2+}$ state . The aim of the present work is to calculate theoretically the physical properties of 40PbO 10$Bi_2O_3$ (50-.1)$B_2O_3$xFeO glass system where (x= 0.2,0.3,0.4,0.5) and compare it with the experimental results [8].

## Results and Discussion

*Density*

The density of all the glasses under study can be calculated from the following expression:

*Corresponding author E.mail:hanan.mokhtar72@gmail.com
DOI : 10.21608/ejphysics.2018.3667.1002

$$d = (X_{PbO}\, d_{PbO} + X_{Bi2O3} d_{Bi2O3} + X_{B2O3} d_{B2O3} + X_{FeO} d_{FeO})$$

where, $X_{PbO}$, $X_{Bi2O3}$, $X_{B2O3}$ and $X_{FeO}$ are the molar fraction of PbO,$Bi_2O_3$, $B_2O_3$, FeO and $d_{PbO}$, $d_{Bi2O3}$, $d_{B2O3}$, $d_{FeO}$ are the values of theoretical density of PbO,$Bi_2O_3$, $B_2O_3$, FeO, respectively [9]. The values of theoretical density for all the studied glasses are listed in Table 1. It is clear that, the values of density increase by increasing FeO content. The molecular weight of FeO (71.844 g/mol) is heavier than molecular weight of $B_2O_3$(69.62 g/mol) and hence , the glass matrix becomes more dense.

*The molar volume($V_m$)*

The molar volume of the glass samples can be calculated from the following expression:

$$Vm = \frac{M}{d}$$

Where M is the total molecular weightusually, the density of the glass changes in the inverse direction of the molar volume [5-7]. It was found that, the values of molar volume for all the studied samples which are listed in Table 1 decrease by increasing FeO content.

*The theoretical optical electronegativity ( $\Delta\chi^*$)*

The theoretical optical electronegativity can be calculated [10] as follows:

Where, the values of, $X_{PbO}$ , $X_{Bi2O3}$,$X_{B2O3}$, $X_{FeO}$ are the molar fraction of PbO, $Bi_2O_3$, $B_2O_3$ ,FeO. And $\Delta\chi^*_{PbO}$ , $\Delta\chi^*_{Bi2O3}$, $\Delta\chi^*_{B2O3}$ , $\Delta\chi^*_{FeO}$are the values of theoreticaloptical electronegativity of PbO, $Bi_2O_3$, $B_2O_3$ ,FeO. respectively [10]. The values of optical electronegativity for all the studied samples are listed in Table 2.

*The theoretical optical energy*

The theoretical optical energy gap $\mathbf{E_{opt}}$ can be calculated [11]

$$E_{opt} = \frac{\Delta\chi^*}{0.2688}$$

From Table 2, it is clear that ,the value of therotical optical band gap energy decreased by increasing FeO content . It was suggested [12] that the decrease in $E_{opt}$ may be contributed by the $E_{opt}$of constituent oxides. If constituent oxides are considered to affect $E_{opt}$ of the presently studied glass system, the replacement of $B_2O_3$($E_{opt}$=69.62 eV) with FeO ($E_{opt}$=71.844 ev)[10] contributes to the decrease in $E_{opt}$.of the glass system . Also, it is clear that the theoretical values of $E_{op}$ are larger than the experimental values [8], this is due to amorphous nature of the prepared samples.

*The theoretical optical basicity($A_{th}$)*

The theoretical optical basicity , addresses the ability of oxide glass in contributing the negative charges in the glass matrix. In other words it defines the electron donating power of the oxygen in the oxide glass. The theoretical optical basicity can be calculated [11]

**TABLE 1. Composition , molecular weight, theoretical density, molar volume, for all the Studied samples**

| Sample | Molecular weight (gm/mol) | Density(g/cm$^3$) (theoretical) | Molar volume($V_m$) (cm$^3$/mol) |
|---|---|---|---|
| 40PbO10$Bi_2O_3$49.8$B_2O_3$0.2FeO | 170.690 | 5.291 | 32.260 |
| 40PbO10$Bi_2O_3$49.7$B_2O_3$0.3FeO | 170.693 | 5.295 | 32.237 |
| 40PbO10$Bi_2O_3$49.6$B_2O_3$0.4FeO | 170.695 | 5.298 | 32.219 |
| 40PbO10$Bi_2O_3$49.5$B_2O_3$0.5FeO | 170.697 | 5.301 | 32.201 |

**TABLE 2. Composition , optical electronegativity, theoretical and experimental optical energy gap,for all the Studied samples**

| Sample | Optical electronegativity | Theoretical optical energy gap (eV) | Experimental optical energy gap (eV) |
|---|---|---|---|
| 40PbO10$Bi_2O_3$49.8$B_2O_3$0.2FeO | 1.417 | 5.291 | 1.85 |
| 40PbO10$Bi_2O_3$49.7$B_2O_3$0.3FeO | 1.415 | 5.264 | 1.73 |
| 40PbO10$Bi_2O_3$49.6$B_2O_3$0.4FeO | 1.414 | 5.260 | 1.65 |
| 40PbO10$Bi_2O_3$49.5$B_2O_3$0.5FeO | 1.412 | 5.253 | 1.60 |

**TABLE 3. Composition , optical basicity, oxide ion polorazibility, refractive index, ,for all the Studied samples**

| Sample | Optical basicity($A_{th}$) | Oxide ion polarizability ( $^{02-}$) $(A^0)^3$ | Refractive index |
|---|---|---|---|
| $40PbO10Bi_2O_349.8B_2O_30.2FeO$ | 0.9920 | 2.225 | 1.679 |
| $40PbO10Bi_2O_349.7B_2O_30.3FeO$ | 0.9925 | 2.227 | 1.683 |
| $40PbO10Bi_2O_349.6B_2O_30.4FeO$ | 0.9930 | 2.227 | 1.686 |
| $40PbO10Bi_2O_349.5B_2O_30.5FeO$ | 0.9940 | 2.229 | 1.690 |

$$A^{th} = -0.5\Delta\chi^{*} + 1.7$$

The values of theoretical optical basicity for all the studied samples are listed in Table [3]. The increased optical basicity of the glasses with FeO content indicates that the glass system is basic in nature.

*The electronic polarizability of oxide ions ( $\alpha^{02-}$)*

The electronic polarizability of oxide ions($\boldsymbol{\alpha}^{02-}$) can be calculated [11]

$$\alpha(02-) = -0.9\Delta\chi^{*} + 3.5$$

It is clear that, the electronic polarizability of oxide ion increases with increasing the optical basicity. The values of electronic polarizability of oxide ions are listed in Table 3.

*The linear refractive index*

The linear refractive index, $n_0$, can be calculated [11]

The values of refractive index are listed in Table 3. The refractive index depends on the oxide ion polorazibility of glass material [13]. It is clear, that the values of the refractive index increase by increasing FeO content and increasing the values of oxide ion polorazibility .

*The third order nonlinear susceptibility*

The third order nonlinear susceptibility$\boldsymbol{\chi}^{(3)}$ ( in esu units) is given by the following relation [5],

$$\chi^{(3)} = \frac{(1.4x10^{-11})}{\left(\left(E_{opt} - 1.96\right)\left(E_{opt} - 1.31\right)\left(E_{opt} - 0.65\right)\right)}$$

The values of third order nonlinear susceptibility are listed in Table 4. It is clear that the high values of third order nonlinear optical susceptibility for all the studied samples , were found to be in the range (2.308-2.342) x $10^{-13}$esu, which is larger than that of pure silica glass (2.8x$10^{-14}$ esu) [14] this means that all the studied samples are probably good candidates for nonlinear optical applications [14]. We have plotted the data of the of third order nonlinear susceptibility as a function of optical energy gap and refractive index of all the studied samples in Fig.1 and Fig. 2. It is seen that the third order nonlinear susceptibility increases with decreasing the optical energy gap and increasing the refractive index for all the studied samples.

## Conclusion

From all the above discussion, it was found that, the optical basicity of the glass materials increase by increasing number of oxide ion polarizability. The value of optical basicity shows that the glass materials are more basic. It is suggested that the ability of oxide ion to donate electrons to surrounding cations increases. Also, it was found that the values of third order nonlinear susceptibility increase with decreasing the optical energy gap and increasing the refractive index for all the studied samples. Finally, all the above values are a good basis for predicting new non linear optical materials.

**TABLE 4. Composition , third order nonlinear susceptibility, for all the Studied samples**

| Sample | (Third order nonlinear suceptibility) $\chi^3$x$10^{-13}$esu. |
|---|---|
| $40PbO10Bi_2O_349.8B_2O_30.2FeO$ | 2.308 |
| $40PbO10Bi_2O_349.7B_2O_30.3FeO$ | 2.323 |
| $40PbO10Bi_2O_349.6B_2O_30.4FeO$ | 2.330 |
| $40PbO10Bi_2O_349.5B_2O_30.5FeO$ | 2.342 |

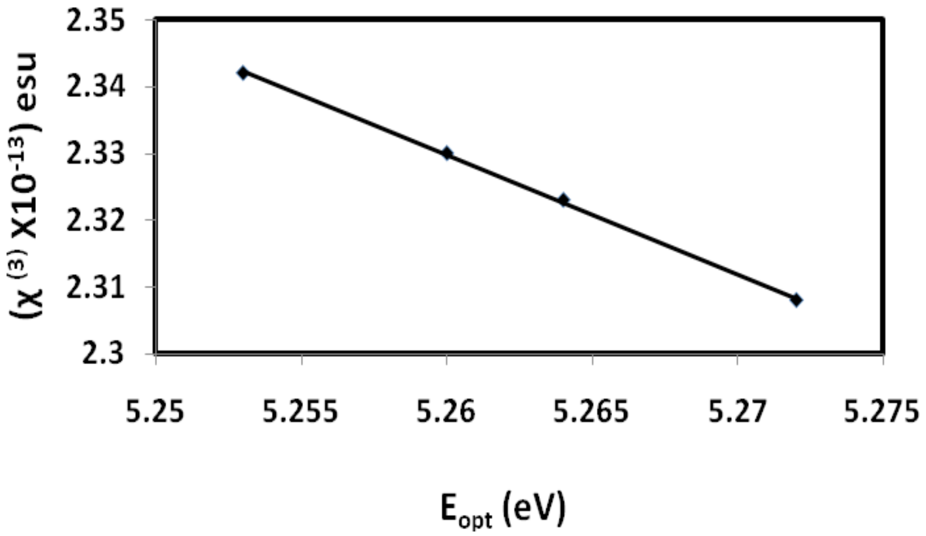


**Fig.1. The third order nonlinear susceptibility as a function of optical energy gap**

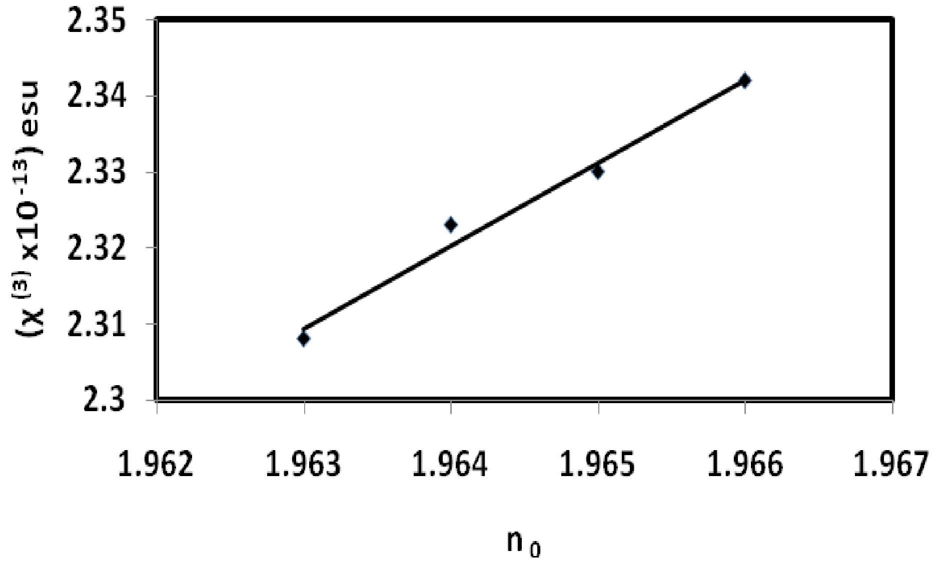


**Fig. 2. The third order nonlinear susceptibility as a function of linear refractive index**


**References**

1. Dimitrov, V. and Sakka, S., Linear and nonlinear optical properties of simple oxide , *J. Appl. Phys*.,**79**,1741(1996).

2. Dimitrov,V. and Komatsu, T. "An interpretation of optical properties of oxide and oxide glasses in terms of the electronic ion polarizability and average single bond strength, *J. of University of Chemical Technology and Metallurgy,* **43**, 2, 19 (2010)

3. Tashera,T. and Dimitrov, V., "Optical properties and structure of $B_2O_3BaOV_2O_5$ Glasses.", *J. Chemical Technology and Metallurgy,* **50,** 441. (2015)

4. Tashva,T. and Dimitrov,V., Optical properties and chemical bonding of $TiO_2BaO$ $V_2O_5$ glasses., *J. Chem. Tech. and Metallargy,* **51**,525 (2016) .

5. Tashva,T. and Dimitrov,V., Synthesis, optical properties and structure of NiOBaO V2O5 glasses., *J. Chem. Tech. and Metallargy,* **52,**369 (2017).

6. Farhan, S.H., Study of some physical and optical properties of Bi2O3 TeO2 V2O5 glasses, Australian *J. of Appl. Sci*., **11**,171 (2017).

7. Saudi, H. and Adel, Gh., The effect of $TiO_2$ on optical and radiation shielding properties of BaO $B_2O_3$ glasses, Optics, **7** (2018)1.

8. Ehasanulla, M., Srikanth,K.,VeerabhadraRao, A. and Emmannel, K.A., Spectroscopic and magnatic properties of PbO $Bi_2O_3$ $B_2O_3$ glasses doped with FeO, *Rasayan J. of Chemistry,* **4,** 343 (2011).

9. Dimitrov,V. and Sakka, S.,Electronic oxide polarizability and optical basicity of simple oxides. , *J. Appl. Phys.* **79,**1736 (1996).

10. Reddy, R.R., Ahamed,Y.N., Gopal, K.R. and Raghuram, D.V., Optical electronegativity and refractive index of materials, *Optical Mat.*,**10**,95 (1998).

11. Zhao , X., Wang,X., Lin , Z. Wang , Anew approach to estimate refractive index, electronic polarizabilty and optical basicity of binary oxide glasses, *Physica,* B,403,2450 (2008)

12. Umair, U.M.,and Yahya, A.K., Effect of $Nb_2O_5$ net work stabilizer on elastic and optical properties of $xNb_2O_5$( 20-x)] $80TeO_2$ tellurite glass system, *Chalcogenide Letters,***12**,287 (2015).

13. Azlan, M.N., Hlimah,M.K., Shafinas, S.Z. and Daud, W.M., "Polarizability and optical basicity of Er3+ ions doped tellurite based glasses", *Chalcogenide letters,* **11**,319 (2014).

14. Haralmpieva, A.,Lozanova, I.S., Dimitrov, V., Optical properties and structure of BaO $V_2O_5$ glasses, *J. Chemical Technology and Metallurgy,* **47**,392 (2012).

(*Received:*25/ 4 /2018;
*accepted:*24/7/2018)

## الخصائص الفيزيائية والضوئية لمركب الزجاج PbO $Bi_2O_3$ $B_2O_3$ المحقون باكسيد الحديد FeO

**غادة عادل وحنان مختار**
قسم الفيزياء – كلية العلوم – جامعة الأزهر - مصر

تم دراسة تأثير التغير الكيميائى على الخصائص الفيزيائية ل 40PbO $10Bi_2O_3$ (50-0.1)$B_2O_3$ xFeO ، و تشتمل الخصائص الفيزيائية على الكثافة ، الحجم المولارى ، السالبية الكهربية ، المنطقة المحرمة ، معامل الانكسار الخطى molar refraction الاستقطاب الالكترونى third order nonlinear susceptibility . تم مقارنة تحليل المعاملات الفيزيائية المتعلقة بالتغير الكيميائي (x= 0.2,0.3,0.4,0.5)، تم دراستها نظريا بالتنبئات النظرية. وقد وجد أنه بزيادة محتوى اكسيد الحديد ، تصبح المصفوفة الزجاجية أكثر كثافة ، وتنخفض فجوة الطاقة الضوئية ، ولكن يزيد مؤشر الانكسار. يزداد الاستقطاب الإلكتروني لأيون أكسيد مع زيادة القاعدية البصرية توضح قيمة الأساس البصري أن المواد الزجاجية أكثر أساسية. ومن المرشح زيادة قدرة أيون الاكسيد على منح الالكترونات للكاتيونات المحيطة ، أيضا ، وجد أن قيم الدرجة الثالثة من الحساسية غير الخطية تزداد بزيادة محتوى اكيد الحديد ووجد أنها أكبر من تلك الموجودة في نظارة السيليكا. تعتبر القيم العالية لمؤشر الانكسار غير الخطي لجميع العينات المدروسة مفيدة لكل معالجة الإشارة البصرية والاتصالات. كذلك ، وجد أن قيم القابلية غير الخطية من الدرجة الثالثة تزداد مع تقليل فجوة الطاقة الضوئية وزيادة معامل الانكسار لجميع العينات المدروسة. وأخيرا ، تم اقتراح مواد بصرية غير خطية جديدة.