

New Approach between the Optical Basicity and the Dielectric Constant through the Molar Polarizability for Some Binary Glasses

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Abstract: Problem statement: In the present study, a new correlation between the optical basicity which describes the electronic charge clouds around the oxide glass and the dielectric constant has been proposed through the molar polarizability of the binary oxide glasses. **Approach:** Two experimental forms have been suggested relating the optical basicity and the molar electronic polarizability. Hence, the dielectric constant and the optical basicity for some binary glass systems can be deduced. **Results:** The molar polarizability and the dielectric constant of these glasses exhibit a linear relation as represented with the optical basicity. We have applied the proposed relation on the binary glasses. **Conclusion:** It was found that a good agreement as the values determined with experimental results determined by previous researchers.

Key words: Dielectric constant, optical basicity, molar polarizability, binary glass systems, linear relation, oxide glasses, optical basicity, binary glasses, electronic charge, experimental results, electronic polarizability

INTRODUCTION

Glasses are very interesting for their potential applications in industry and many applied areas. Recently many researchers studied glasses as switching and memory devices, superior insulators and dielectrics. Thus glass becomes an ordinary electronic material (Khor *et al.*, 2009; Varshneya, 1994).

The dielectric constant of a material is one of the most important factors for the electronic charge carriers and impurities in insulators. The dielectric constant of a solid may be expressed in terms of the polarizability of its constituent atoms α_i (Verma *et al.*, 2009; Nag, 1994; Xue *et al.*, 2000; Marquez and Rinocon, 1995; Moustafa, 2011) as follows Eq. 1:

$$\epsilon_{\infty} = \frac{[1 + \sum_i \frac{N_i \alpha_i}{\epsilon_0}]}{[1 - \sum_i \frac{\gamma N_i \alpha_i}{\epsilon_0}]} \quad (1)$$

where, N_i is the number of atoms of species i per unit volume, ϵ_0 is the free space permittivity and γ is the Lorenz factor. Recently, Xui *et al.* (2000) have proposed a formula as follows Eq. 2:

$$\epsilon_{\infty} = a - bZ_A \quad (2)$$

Where:

a and b = Constants depend on the compounds of material
 Z_A = The atomic number of cation

The prediction of the values of polarizability and the dielectric constant by theoretical methods has made significant contributions and open an active fields for new nonlinear glasses. The molar electronic polarizability is one of the most important properties of materials, which is closely related to its applicability in the field of electronics. In this connection the polarizability approach has been systematically developed in recent researches concerning the origin of molar electronic polarizability and optical basicity for simple oxide glasses (Zhao *et al.*, 2007; Dimitrov and Komatsu, 1999).

In the frequency range of optical phenomena the dielectric constant ϵ_{∞} is due to mainly from the electronic polarizability. In this region the equations of Lorenz-Lorenz and Clousis Mousstti (Chimalawong *et al.*, 2010) are valid as follows Eq. 3:

$$\alpha_m = \frac{(\epsilon_{\infty} - 1)M * 10 - 24}{(\epsilon_{\infty} - 2)\sigma * 2.53} \quad (3)$$

Where:

M = The molecular weight of the glass system
 σ = The density of glass

MATERIALS AND METHODS

Electronic polarizability of ions demonstrates the way of their electronic clouds distributed by applying electric field. It is closely related to many properties of the glass systems such as the optical basicity (Dimitrov and Komatsu, 2010) and refraction, hence the dielectric constant. Recently studies have shown a relationship between refractivity and optical basicity for oxide glasses over a modest range of Λ_{th} (Dimitrov and Komatsu, 1999).

Using electronic polarizability, α_m , is more detectable than the refractivity. It is found that there is a good linearity between the oxide ion polarizability over a very wide range of Λ for oxide materials generally (Dimitrov and Komatsu, 1999).

So it is necessary to know knowledge about the state of polarization of the ions in glassy materials using the optical basicity which describes the electronic charge cloud around these ions. The theoretical optical basicity of the glass is given by Eq. 4 (Vithal *et al.*, 1997):

$$\Lambda = 1 - \sum_i \left(\frac{Z_i r_i}{2} \right) \left(1 - \frac{1}{\gamma_i} \right) \quad (4)$$

Where:

Z_i = The valence of the *i*th cation

r_i = The ratio of the number of the *i*th cations to that of oxide ions

γ_i = The basicity moderating parameter given by Eq. 5:

$$\gamma_i = 1.36(\chi_i - 0.26) \quad (5)$$

where, χ_i is the Pauling, *s* electronegativity of the *i*th atom.

There are four components of contributions of the molar polarizability: electronic, ionic, dipolar and interfacial. The electronic contribution is the movement of negative electrons in the electric field. The ionic contribution is the displacement of charged ions relative to each others. The main contribution is due to the electronic polarizability in the range under test in our work.

Recently many researches has been done (Verma *et al.*, 2009) on the binary glass systems ,which based on the experimental data , The advantage of the empirical forms allow a broad band of works to obtain useful properties and trends become more clear.

The main idea of this study is that the observed linear relation between the molar polarizability and the optical basicity, consequently the dielectric constant for binary glasses. The aim of the present study is to suggest a correlation between the optical basicity and the dielectric constant for binary glasses.

RESULTS

Firstly, the experimental reported data of the molar polarizability have been represented against the value of the theoretical optical basicity.

Figure 1-6 shows the correlation between the optical basicity and the molar electronic polarizability. To obtain a good agreement with the experimental results, we proposed the following form as Eq. 6:

$$\alpha_m = a\Lambda_{th} + c \quad (6)$$

where, *a* and *c* are constants depends on the structure of the glass system, with respect to Fig. 1-6, the relation is a good linear relation for almost binary and simple oxides glasses.

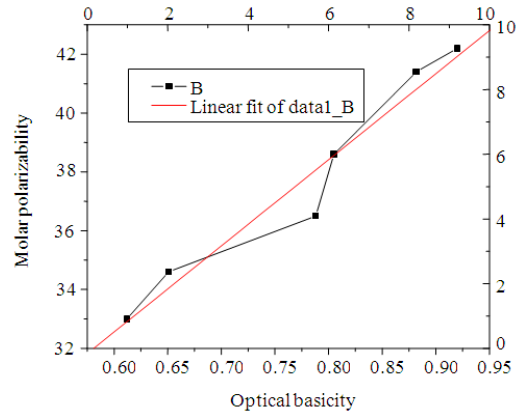


Fig. 1: The relationship between the optical basicity and the molar polarizability in case of $Bi_2O_3-B_2O_3$ glass

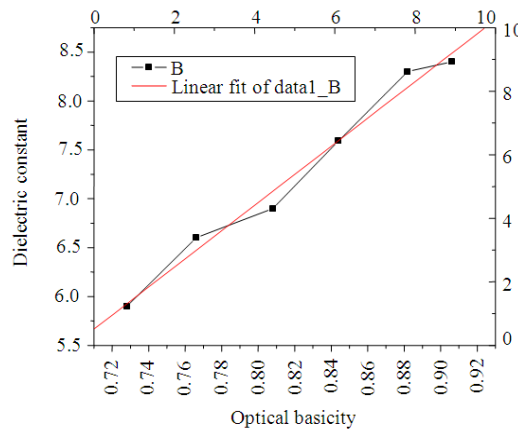


Fig. 2: The relationship between the optical basicity and the dielectric constant in case of $Bi_2O_3-B_2O_3$ glass

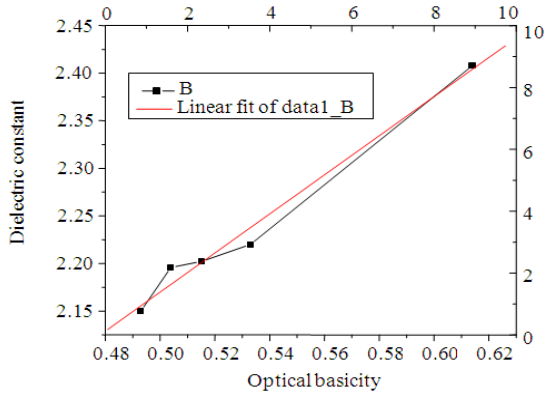


Fig. 3: The relation between the optical basicity and the molar polarizability in case of GeO₂-SiO₂ glass increasing GeO₂

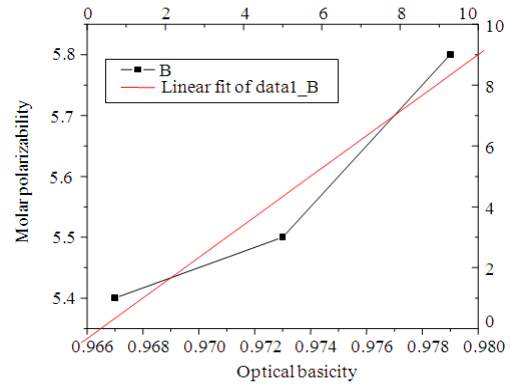


Fig. 6: The relation between the optical basicity and the molar polarizability in case of MgO-TeO₂ glass increasing MO

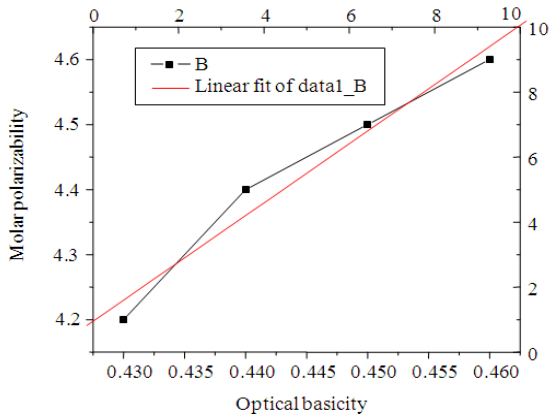


Fig. 4: The relation between the optical basicity and the molar polarizability in case of GeO₂-B₂O₃ glass increasing GeO₂

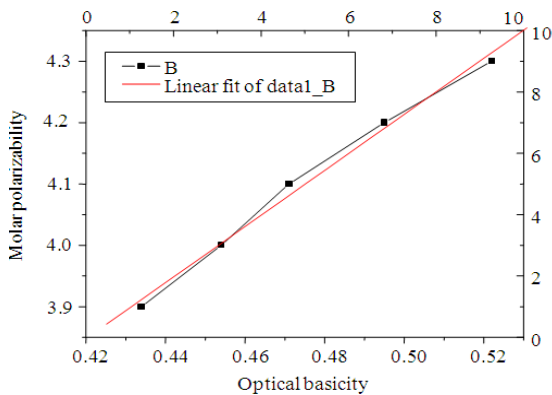


Fig. 5: The relation between the optical basicity and the molar polarizability in case of K₂O-B₂O₂ glass increasing KO₂

Secondly, the experimental reported data of the dielectric constant have been represented against the value of the theoretical optical basicity.

DISCUSSION

Investigating carefully Fig. 7-18, it is easy clear to note that the dielectric constant (ϵ_{∞}) increases with increasing the optical basicity (Λ_{th}).

Comparing the behavior of the dielectric constant and the optical basicity with the behavior of the molar polarizability α_m and Λ_{th} , we can conclude that these above behaviors agree with the Claussis-Mossotti equation, which relates ϵ_{∞} and α_m . It is well known that as the molar polarizability increases the dielectric constant of the glass increases (Verma *et al.*, 2009).

In the present work, a microscopic and analytical vision proposed for almost binary oxide glasses, which correlates the relation between the dielectric constant of these glasses and the optical basicity in the range of optical phenomena.

Dimitrov and Komatsu (1999) had established that there are linear relationship between the optical basicity and the oxide ion polarizability for binary oxide glasses. So it is logically and predicted that there are a linear relation between α_m and Λ_{th} , because the molar polarizability is the sum of cation and oxide ion polarizabilities.

To obtain a good agreement between the theoretical and experimental results for binary oxide glasses, an empirical form was proposed according to the trend of the experimental data between ϵ_{∞} and Λ_{th} as the following Eq. 7:

$$\epsilon_{\infty} = A + B * \Lambda_{th} \tag{7}$$

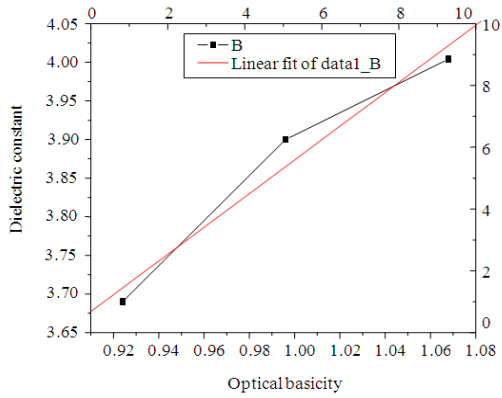


Fig. 7: The relation between the optical basicity and the dielectric constant in case of $SB_2O_3-B_2O_3$ glass increasing SB_2O_3

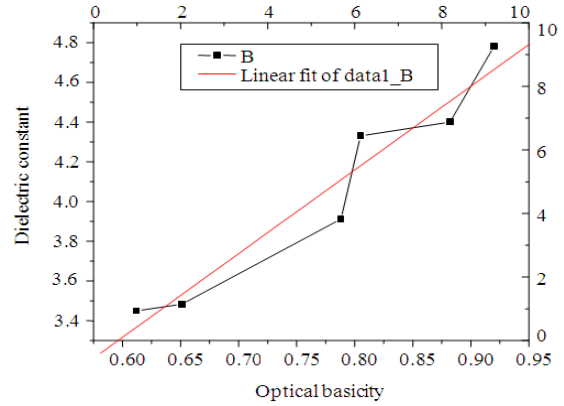


Fig. 10: The relation between the optical basicity and the dielectric polarizability in case of $Bi_2O_3-B_2O_3$ glass increasing Bi_2O_3

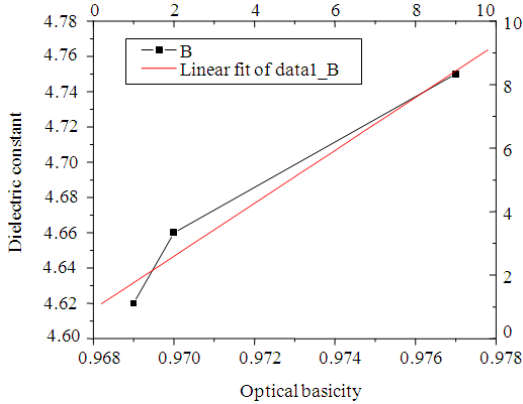


Fig. 8: The relation between the optical basicity and the dielectric constant in case of Ag_2O-TeO_2 glass with increasing Ag_2O

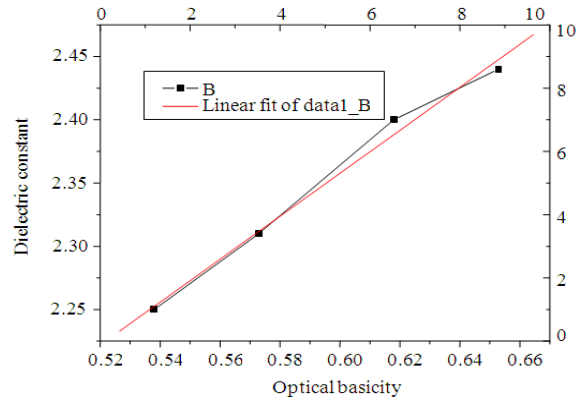


Fig. 11: The relation between the optical basicity and dielectric constant in case of LiO_2-SiO_2 glass increasing LiO_2

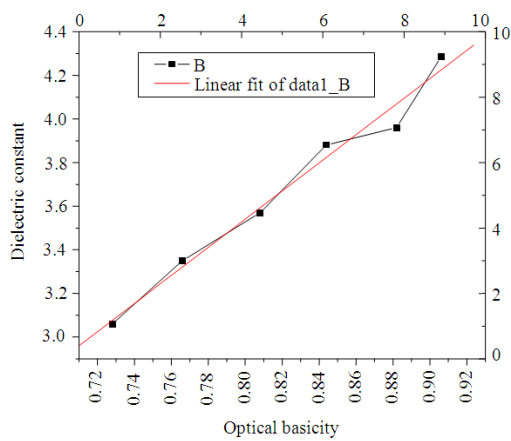


Fig. 9: The relation between the optical basicity and the dielectric polarizability in case of $Bi_2O_3-SiO_2$ glass increasing Bi_2O_3

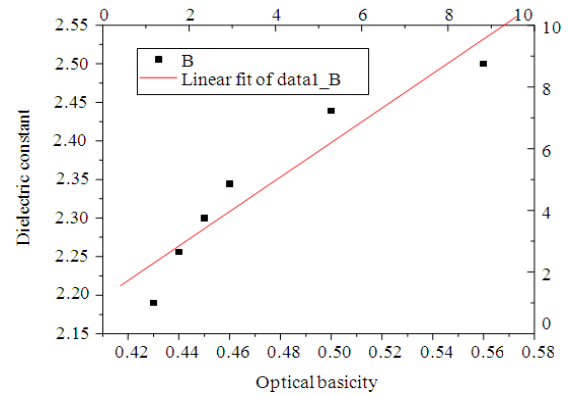


Fig. 12: The relation between the optical basicity and the dielectric constant in case of $GeO_2-B_2O_3$ glass increasing GeO_2

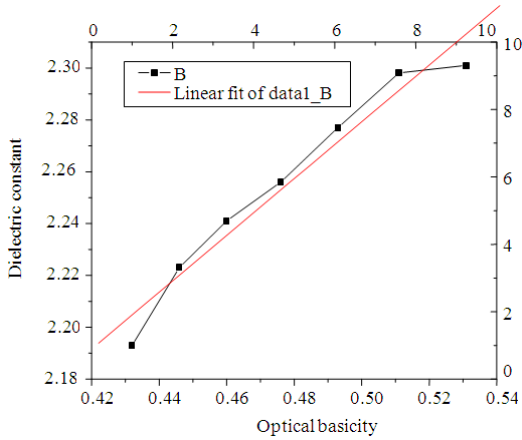


Fig.13: The relation between the optical basicity and the dielectric constant in case of $\text{Na}_2\text{O-B}_2\text{O}_3$ glass increasing Na_2O .

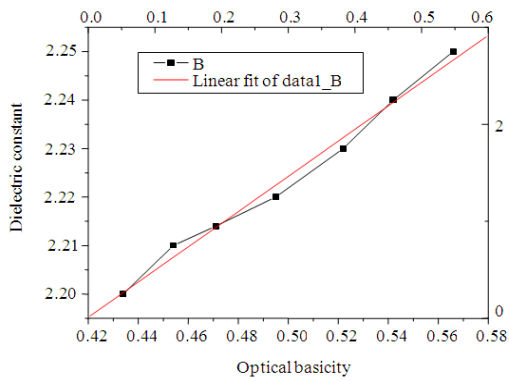


Fig. 14: The relation between the optical basicity and the dielectric constant in case of $\text{K}_2\text{O-B}_2\text{O}_3$ glass increasing K_2O .

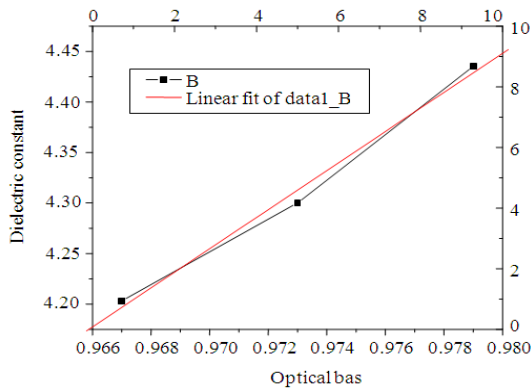


Fig. 15: The relation between the optical basicity and the dielectric constant in case of $\text{MgO-B}_2\text{O}_3$ glass increasing MgO

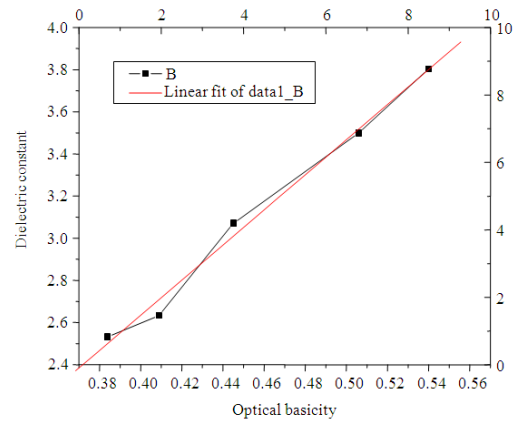


Fig. 16: The relation between the optical basicity and the dielectric constant in case of $\text{Bi}_2\text{O}_3\text{-P}_2\text{O}_5$ glass with increasing Bi_2O_3

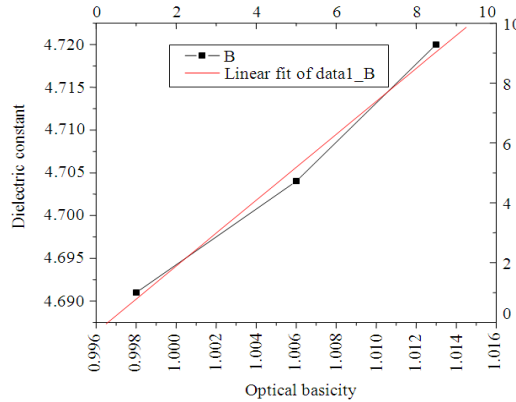


Fig. 17: The relation between the optical basicity and the dielectric constant in case of $\text{Wo}_3\text{-TeO}_2$ glass increasing Wo_3

Table 1: Illustrates the values of constants in the proposed equation of the dielectric constant of the glasses as a function of the optical basicity

Constants	Glass system $\text{A}_p\text{O}_q\text{-B}_r\text{O}_s$
A	0.5-2.5
B	1 - 3

Table 2: Illustrates the values of constants in the proposed formula of the dielectric constant of the glasses as a function of the optical basicity.

Type of glass system	Constants	
	A	B
Borates	2.00	2.50
Silicates	1.33	1.70
Germanates	1.14	2.10
Tellurates	1.60	2.99
Phosphates	1.60	3.00
Titanates	0.50	3.00

Table 3: Comparison between the calculated and experimental reported values of the dielectric constant (ϵ_x) for some binary glass systems

Type of glass system	Theoretical optical basicity Λ_{th}	Calculated values $\epsilon_{x,Cal.}$	Experimental reported values ϵ_x
0.7Sb ₂ O ₃ -0.3B ₂ O ₃	0.924	3.700	3.530
0.65Bi ₂ O ₃ -0.35B ₂ O ₃	0.920	4.990	4.840
0.6GeO ₂ -0.4SiO ₂	0.614	2.410	2.404
0.05Cs ₂ O-0.95SiO ₂	0.511	2.192	2.193
0.1K ₂ O-0.9B ₂ O ₃	0.495	2.220	2.230
0.1Bi ₂ O ₃ -0.9GeO ₂	0.765	2.714	2.940
0.1V ₂ O ₅ -0.9GeO ₂	0.774	2.732	2.822
0.1MoO ₃ -0.9TeO ₂	1.001	4.440	4.473
0.1WO ₃ -0.9 TeO ₂	0.998	4.500	4.660
0.05TaO ₂ -0.95TeO ₂	0.987	4.462	4.682
0.33K ₂ O-0.77TiO ₂	1.047	3.610	3.312
0.20PbO-0.8TiO ₂	0.994	3.500	4.120
0.2Li ₂ O-0.8 SiO ₂	0.538	2.440	2.250
0.1 MgO-0.9TeO ₂	0.979	4.400	4.435
0.10 Bi ₂ O ₃ -0.9P ₂ O ₃	0.384	2.300	2.530
0.05Na ₂ O-0.95 B ₂ O ₃	0.432	2.200	2.193

(Note: $n^2 = \epsilon_\infty$)

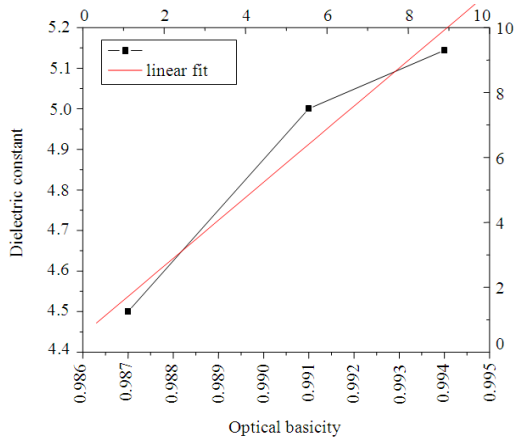


Fig. 18: The relation between the optical basicity and the dielectric constant in case of pbO-TiO₂

A and B are constants depends on the compounds of the glass system i.e., as the weight number of the cations in the glass system increases the values A, B increase such as in system pb₂O-TiO₂ and Wo₃-TeO₂ as illustrated in Table 2. A useful comparison are shown in Table 3, it is obvious that the calculated values of ϵ_x is satisfied relative to the experimental values and this share to predict new binary glasses.

CONCLUSION

Advantage correlation and an empirical form have been proposed for the dielectric constant determination through the theoretical optical basicity for binary oxide glasses. The relation between the molar polarizability and optical basicity has been established as a linear relation in all binary oxide glasses. It was found that for

certain system of glass, the above relation can be represented as linear form. So we can determine unknown value of the molar polarizability by the corresponding value of the theoretical optical basicity simply. Also the dielectric constant of binary glasses can be evaluated in the field of optical frequency phenomena, especially the determination of the dielectric constant that requires more sensitive experimental set-up in that region of that frequency. This can be achieved by applying the proposed form (7). Finally more nonlinear binary glasses can be predicted through the estimated electronic molar polarizability.

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