

## Judd Ofelt Study of Absorption Spectrum for Neodymium Doped Borate Glass

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### Abstract

A series of Neodymium doped borate glass with chemical composition (58-x) B<sub>2</sub>O<sub>3</sub>-xNa<sub>2</sub>O-40ZnO-2Nd<sub>2</sub>O<sub>3</sub> x= 0, 5, 10, 15, 20 and 25mol%. This type of glass has good optical properties due to its applications in laser applications. The glass has fabricated and annealed by the conventional casting method for glass fabrication. The variation between the borate oxide and sodium oxide causes a change of the oscillator strength, which gives us a good optimization for choosing the best chemical composition that gives maximum absorption oscillator strength. Spectroscopic analyses based on Judd-Ofelt theory were performed, beginning with absorption spectrum, oscillator strength and the intensity parameters  $\Omega_2$ ,  $\Omega_4$  and  $\Omega_6$  have been evaluated. These types of glasses have good optical properties which cloud be used for photonics applications like lasing medium or waveguide.

**Keywords:** spectroscopic analysis, Judd-Ofelt, lasing mediums, glass material, photonics

### INTRODUCTION

Glass and glass technology has a various applications in many fields in science like optical absorptions filters, radiation protection, and lasing mediums as in photonic applications [1-10]. The Photonic glass is a part of glass technology with particular applications. The glass doped with rare earth has potential applications in laser mediums, optical fibers, optical amplifiers, and waveguide.

In classical E&M, oscillator strength ( $f_j$ ) is used as a statistical weight indicating the relative number of oscillators bound at each resonant frequency ( $\nu_j$ ). In quantum mechanics, oscillator strength is used as a measure of the relative strength of the electronic transitions within atomic and molecular systems. Oscillator strength is

particularly useful as a method of comparing transition “strengths” between different types of quantum mechanical systems. The oscillator strength is often used as a method for calculating the concentration of impurities in a host from known  $f$  values and measured absorption coefficients or emission. In this paper, we report a spectroscopic study for neodymium doped borate glass with chemical composition  $(58-x) \text{B}_2\text{O}_3-x\text{Na}_2\text{O}-40\text{ZnO}-2\text{Nd}_2\text{O}_3$   $x = 0, 5, 10, 15, 20$  and  $25\text{mol}\%$ .

## EXPERIMENTAL METHOD

### Glass preparation:

Neodymium doped Borate glass system with a chemical composition  $(x-42) \text{B}_2\text{O}_3.(100-x) \text{Na}_2\text{CO}_3.40\text{ZnO}.2\text{Nd}_2\text{O}_3$  (where  $x = 100, 95, 90, 85, 80$  and  $75$ ) were prepared by conventional melting method in a porcelain crucible. The mixed powders were preheated at  $600^\circ\text{C}$  for 1 to 1.5 hours to relive gases, and then heated in  $1150^\circ\text{C}$  for two hours with clockwise shaking to ensure high homogeneity. The casting glass were quenched and annealed in steel mold.

### Physical measurements:

The optical absorption was recorded at room temperature in the region UV/Vis/NIR absorption were obtained for the thin glass samples with two parallel polished faces were measured by using (Lambda-950) spectrophotometer in the wavelength range 320-2800 nm.

### Judd Ofelt and oscillator strength theory:

The random oriented systems it is meant ions in solution, glasses or powders. These systems are usually studied by notarized light. The oscillator strength  $f$  can be estimated experimentally through:

$$f = \frac{8\pi^2 m_e c \nu}{h e^2} \int \epsilon(\nu) d\nu \quad (1)$$

Where

$e = 4.803 \times 10^{-10}$  esu (elementary charge)

$m_e = 9.10904 \times 10^{-28}$  g (electron mass)

$h = 6.6261 \times 10^{-27}$  erg (plank constant)

$c = 2.9979 \times 10^{10}$   $\text{cm s}^{-1}$  (speed of light)

$\nu$  = wave number at the absorption maximum ( $\text{cm}^{-1}$ )

Filling in the constants yields:

$$f = 4.32 \times 10^{-9} \int \epsilon(\nu) d\nu \quad (2)$$

The molar absorptivity  $\epsilon$  values can be calculated from the absorbance  $A$  by use of Lambert Beer Law:

$$A = \epsilon \cdot d \cdot c \quad (3)$$

where  $\epsilon$  is the molar absorptivity [dim:  $\text{L}^2$ , units:  $\text{mol}^{-1}[\text{cm}^{-1}]$ ],  $c$  is the concentration [dim:  $\text{L}^{-3}$ , units:  $\text{mol}^{-1}$ ] and  $d$  is the optical path length [dim:  $\text{L}$ , units:  $\text{cm}$ ].

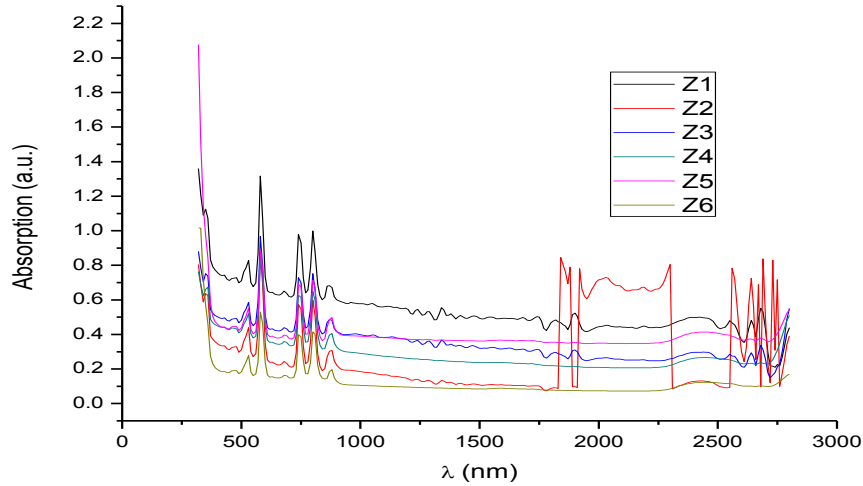
The area under an absorption peak is a better measure of the intensity than the molar absorptivity at the peak maximum, because the area is the same for the resolved and the unresolved band. The area can be determined by integrating the peak which is equivalent to the calculation of the integral

$$\int \varepsilon(\nu) d\nu \quad (4)$$

The spectroscopic parameters for rare earth ions are calculated by the theory that proposed by Judd and Ofelt. The summary of this theory depend on the majority of the intra-configurationally f-f transitions of trivalent rear earths that observed in the absorption spectrum are induced electric dipole transitions [11-12].

## RESULTS AND DISCUSSION

The absorption spectrum of the neodymium doped borate glasses sample are shown in Fig 1, the spectroscopic properties of the glass samples were analyzed by oscillator strength and Judd Ofelt models. The use of this model needs some physical measurement were done to complete the computational calculations.



(Z1)  $58\text{B}_2\text{O}_3.0\text{Na}_2\text{O}.40\text{ZnO}.2\text{Nd}_2\text{O}_3$  (Z2)  $53\text{B}_2\text{O}_3.5\text{Na}_2\text{O}.40\text{ZnO}.2\text{Nd}_2\text{O}_3$   
 (Z3)  $48\text{B}_2\text{O}_3.10\text{Na}_2\text{O}.40\text{ZnO}.2\text{Nd}_2\text{O}_3$  (Z4)  $43\text{B}_2\text{O}_3.15\text{Na}_2\text{O}.40\text{ZnO}.2\text{Nd}_2\text{O}_3$   
 (Z5)  $38\text{B}_2\text{O}_3.20\text{Na}_2\text{O}.40\text{ZnO}.2\text{Nd}_2\text{O}_3$  (Z6)  $33\text{B}_2\text{O}_3.25\text{Na}_2\text{O}.40\text{ZnO}.2\text{Nd}_2\text{O}_3$

The oscillator strength a measure of the strength of a transition and it is the ratio of actual intensity to the intensity radiated by one electron oscillating harmonically in three dimension for trivalent lanthanide ions, the oscillator strength  $f$  of allowed magnetic dipole (MD) and forbidden (induced) electric dipole (ED) transitions is on the same order of  $10^{-6}$ . One has to be cautious when comparing the intensities of transition in different spectral regions, for instance, if an absorption band A in the infrared region one should expect smaller oscillator strength than an absorption band B in UV region [13].

The f-f transitions are considered to be electric dipole in nature, because the magnetic dipole oscillator strength ( $f_{md}$ ) will be relatively small [14]. For that reason in the present work, these magnetic dipole line strengths have not been considered. The table 1 we can see that the low RMS values suggest the good agreement between calculated and experimental oscillator strengths of  $Nd^{3+}$  ions in our glasses samples.

**Table 1:** Shows the oscillator strength for the absorption bands

Sample	Z1								
transitions	max.wavelength nm	energy cm-1	area	concentration	thickness	f exp.	U2	U4	U6
4D5/2	350	28571.42857	1.0261	2	1.13	2.08852E-09	0.0001	0.0567	0.0275
2K13/2	530	18867.92453	7.2564	2	1.13	1.47697E-08	0.0068	0.0002	0.0312
4G5/2	580	17241.37931	9.4628	2	1.13	1.92606E-08	0.8979	0.4093	0.0359
4F7/2	740	13513.51351	19.477	2	1.13	3.96435E-08	0	0.0027	0.2352
4F5/2	800	12500	15.27	2	1.13	3.10805E-08	0.001	0.2371	0.397
4F3/2	870	11494.25287	4.6003	2	1.13	9.36344E-09	0	0.2293	0.0549
Sample	Z2								
transitions	max.wavelength nm	energy cm-1	area	concentration	thickness	f exp.	U2	U4	U6
4D5/2	350	28571.42857	0.68539	2	1.18	1.33593E-09	0.0001	0.0567	0.0275
2K13/2	530	18867.92453	6.028	2	1.18	1.17495E-08	0.0068	0.0002	0.0312
4G5/2	580	17241.37931	7.3365	2	1.18	1.43E-08	0.8979	0.4093	0.0359
4F7/2	740	13513.51351	20.384	2	1.18	3.97315E-08	0	0.0027	0.2352
4F5/2	800	12500	17.839	2	1.18	3.47709E-08	0.001	0.2371	0.397
4F3/2	870	11494.25287	13.193	2	1.18	2.57152E-08	0	0.2293	0.0549
Sample	Z3								
transitions	max.wavelength nm	energy cm-1	area	concentration	thickness	f exp.	U2	U4	U6
4D5/2	350	28571.42857	0.72234	2	1.47	1.13019E-09	0.0001	0.0567	0.0275
2K13/2	530	18867.92453	5.5829	2	1.47	8.73515E-09	0.0068	0.0002	0.0312
4G5/2	580	17241.37931	6.4583	2	1.47	1.01048E-08	0.8979	0.4093	0.0359
4F7/2	740	13513.51351	17.157	2	1.47	2.68443E-08	0	0.0027	0.2352
4F5/2	800	12500	15.006	2	1.47	2.34788E-08	0.001	0.2371	0.397
4F3/2	870	11494.25287	11.71	2	1.47	1.83218E-08	0	0.2293	0.0549
Sample	Z4								
transitions	max.wavelength nm	energy cm-1	area	concentration	thickness	f exp.	U2	U4	U6
4D5/2	350	28571.42857	0.33	2	1.25	6.072E-10	0.0001	0.0567	0.0275
2K13/2	530	18867.92453	4.935	2	1.25	9.0804E-09	0.0068	0.0002	0.0312
4G5/2	580	17241.37931	5.8914	2	1.25	1.08402E-08	0.8979	0.4093	0.0359
4F7/2	740	13513.51351	16.223	2	1.25	2.98503E-08	0	0.0027	0.2352
4F5/2	800	12500	13.339	2	1.25	2.45438E-08	0.001	0.2371	0.397
4F3/2	870	11494.25287	3.7972	2	1.25	6.98685E-09	0	0.2293	0.0549
Sample	Z5								
transitions	max.wavelength nm	energy cm-1	area	concentration	thickness	f exp.	U2	U4	U6
4D5/2	350	28571.42857	1.5086	2	1.38	2.51433E-09	0.0001	0.0567	0.0275
2K13/2	530	18867.92453	3.7972	2	1.38	6.32867E-09	0.0068	0.0002	0.0312
4G5/2	580	17241.37931	6.2527	2	1.38	1.04212E-08	0.8979	0.4093	0.0359
4F7/2	740	13513.51351	17.911	2	1.38	2.98517E-08	0	0.0027	0.2352
4F5/2	800	12500	15.448	2	1.38	2.57467E-08	0.001	0.2371	0.397
4F3/2	870	11494.25287	24.241	2	1.38	4.04017E-08	0	0.2293	0.0549

Sample	Z6								
transations	max.wavelength nm	energy cm-1	area	concentration	thickness	f exp.	U2	U4	U6
4D5/2	350	28571.42857	1.2198	2	2.17	1.29288E-09	0.0001	0.0567	0.0275
2K13/2	530	18867.92453	3.205	2	2.17	3.397E-09	0.0068	0.0002	0.0312
4G5/2	580	17241.37931	4.1399	2	2.17	4.38791E-09	0.8979	0.4093	0.0359
4F7/2	740	13513.51351	14.06	2	2.17	1.49023E-08	0	0.0027	0.2352
4F5/2	800	12500	11.901	2	2.17	1.2614E-08	0.001	0.2371	0.397
4F3/2	870	11494.25287	2.0303	2	2.17	2.15193E-09	0	0.2293	0.0549

The Judd-Ofelt parameters  $\Omega_k$  (k =2, 4, 6) mainly depend on the host glass composition and they can provide versatile information regarding the rare earth containing glass structure. Some empirical correlations of the Judd-Ofelt parameters and the local structure of the rare earth ions have been reported in literature [15-19].

**Table 2:** Shows the Judd Ofelt for the absorption bands

Sample	1								root mean square
transations	U22	U42	U62	Omega2	Omega4	Omega6	Fcalc	f exp.	RMS
4D5/2	0.00000001	0.00321489	0.00075625	3.17264E-07	1.41729E-06	7.04923E-07	5.08953E-09	2.08852E-09	2.12203E-09
2K13/2	0.00004624	0.00000004	0.00097344	3.17264E-07	1.41729E-06	7.04923E-07	7.00928E-10	1.47697E-08	9.9481E-09
4G5/2	0.80622441	0.16752649	0.00128881	3.17264E-07	1.41729E-06	7.04923E-07	4.94128E-07	1.92606E-08	3.35782E-07
4F7/2	0	0.00000729	0.05531904	3.17264E-07	1.41729E-06	7.04923E-07	3.9006E-08	3.96435E-08	4.50732E-10
4F5/2	0.000001	0.05621641	0.157609	3.17264E-07	1.41729E-06	7.04923E-07	1.90777E-07	3.10805E-08	1.12923E-07
Sample	2								
transations	U22	U42	U62	Omega2	Omega4	Omega6	Fcalc	f exp.	RMS
4D5/2	0.00000001	0.00321489	0.00075625	2.99478E-07	1.36133E-06	7.08042E-07	4.91198E-09	1.33593E-09	2.52865E-09
2K13/2	0.00004624	0.00000004	0.00097344	2.99478E-07	1.36133E-06	7.08042E-07	7.03139E-10	1.17495E-08	7.81095E-09
4G5/2	0.80622441	0.16752649	0.00128881	2.99478E-07	1.36133E-06	7.08042E-07	4.70417E-07	1.43E-08	3.22524E-07
4F7/2	0	0.00000729	0.05531904	2.99478E-07	1.36133E-06	7.08042E-07	3.91781E-08	3.97315E-08	3.9131E-10
4F5/2	0.000001	0.05621641	0.157609	2.99478E-07	1.36133E-06	7.08042E-07	1.88123E-07	3.47709E-08	1.08436E-07
Sample	3								
transations	U22	U42	U62	Omega2	Omega4	Omega6	Fcalc	f exp.	RMS
4D5/2	0.00000001	0.00321489	0.00075625	2.02693E-07	9.18821E-07	4.78037E-07	3.31543E-09	1.13019E-09	1.54519E-09
2K13/2	0.00004624	0.00000004	0.00097344	2.02693E-07	9.18821E-07	4.78037E-07	4.7475E-10	8.73515E-09	5.84098E-09

4G5/2	0.80622441	0.16752649	0.00128881	2.02693E-07	9.18821E-07	4.78037E-07	3.17959E-07	1.01048E-08	2.17686E-07
4F7/2	0	0.00000729	0.05531904	2.02693E-07	9.18821E-07	4.78037E-07	2.64513E-08	2.68443E-08	2.77914E-10
4F5/2	0.000001	0.05621641	0.157609	2.02693E-07	9.18821E-07	4.78037E-07	1.26996E-07	2.34788E-08	7.31977E-08
Sample	4								
transations	U22	U42	U62	Omega2	Omega4	Omega6	Fcalc	f exp.	RMS
4D5/2	0.00000001	0.00321489	0.00075625	2.31537E-07	1.05366E-06	5.32843E-07	3.79038E-09	6.072E-10	2.25085E-09
2K13/2	0.00004624	0.00000004	0.00097344	2.31537E-07	1.05366E-06	5.32843E-07	5.29439E-10	9.0804E-09	6.04644E-09
4G5/2	0.80622441	0.16752649	0.00128881	2.31537E-07	1.05366E-06	5.32843E-07	3.63874E-07	1.08402E-08	2.49633E-07
4F7/2	0	0.00000729	0.05531904	2.31537E-07	1.05366E-06	5.32843E-07	2.9484E-08	2.98503E-08	2.59008E-10
4F5/2	0.000001	0.05621641	0.157609	2.31537E-07	1.05366E-06	5.32843E-07	1.43214E-07	2.45438E-08	8.39127E-08
Sample	5								
transations	U22	U42	U62	Omega2	Omega4	Omega6	Fcalc	f exp.	RMS
4D5/2	0.00000001	0.00321489	0.00075625	2.22882E-07	1.01447E-06	5.27146E-07	3.66006E-09	2.51433E-09	8.10154E-10
2K13/2	0.00004624	0.00000004	0.00097344	2.22882E-07	1.01447E-06	5.27146E-07	5.23491E-10	6.32867E-09	4.10488E-09
4G5/2	0.80622441	0.16752649	0.00128881	2.22882E-07	1.01447E-06	5.27146E-07	3.50323E-07	1.04212E-08	2.40347E-07
4F7/2	0	0.00000729	0.05531904	2.22882E-07	1.01447E-06	5.27146E-07	2.91686E-08	2.98517E-08	4.83004E-10
4F5/2	0.000001	0.05621641	0.157609	2.22882E-07	1.01447E-06	5.27146E-07	1.40113E-07	2.57467E-08	8.08692E-08
Sample	6								
transations	U22	U42	U62	Omega2	Omega4	Omega6	Fcalc	f exp.	RMS
4D5/2	0.00000001	0.00321489	0.00075625	1.28032E-07	3.56266E-07	2.64418E-07	1.34532E-09	1.29288E-09	3.70872E-11
2K13/2	0.00004624	0.00000004	0.00097344	1.28032E-07	3.56266E-07	2.64418E-07	2.6333E-10	3.397E-09	2.21584E-09
4G5/2	0.80622441	0.16752649	0.00128881	1.28032E-07	3.56266E-07	2.64418E-07	1.63247E-07	4.38791E-09	1.12331E-07

## CONCLUSION

A new series of rare earth doped borate have been investigated and characterized. The spectroscopic properties of Nd<sup>3+</sup> in these glasses were investigated. The oscillator strength and JuddOfelt intensity parameters  $\Omega_k$  ( $k=2,4$  and  $6$ ) were calculated and produced a good results for photonics applications as in laser mediums or optical amplifiers.

**REFERENCES**

- [1] YahiaH.Elbashar, "Structural and spectroscopic analyses of copper doped P2O5-ZnO-K2O-Bi2O3 glasses", *International Journal: Processing and application of ceramics*, 9 [3] (2015) 169-173
- [2] Y.H.Elbashar, AlySaeed, "Computational spectroscopic analysis by using Clausius-Mossotti method for sodium borate glass doped neodymium oxide", *Research Journal of Pharmaceutical, Biological and Chemical Sciences (RJPBCS)*, volume 6, issue 5, September-October, Pages 320-326
- [3] AlySaeed, Y. H. Elbashar, S. U. El Kameesy, "Study of Gamma Ray Attenuation of High-Density Bismuth Silicate Glass for shielding applications", *Research Journal of Pharmaceutical, Biological and Chemical Sciences (RJPBCS)*, volume 6, issue 4, July-August 2015, pages 1830-1837
- [4] AlySaeed, Y. H. Elbashar, S. U. El Kameesy, "Towards modeling of copper-phosphate glass for optical bandpass absorption filter", *Research Journal of Pharmaceutical, Biological and Chemical Sciences (RJPBCS)*, volume 6, issue 4, July-August 2015, pages 1390-1397
- [5] D.A. Rayan, Y.H. Elbashar, A.B. El Basaty and M.M. Rashad, "Infrared spectroscopy of cupric oxide doped barium phosphate glass", *Research Journal of Pharmaceutical, Biological and Chemical Sciences (RJPBCS)*, volume 6, issue 3, May-June 2015, pages 1026-1030
- [6] H. Elhaes, M. Attallah, Y. Elbashar, M. Ibrahim, M. El-Okr, "Application of Cu2O-doped phosphate glasses for bandpass filter", *Journal of Physica B: Condensed Matter*, Volume 449, 15 September 2014, Pages 251-254
- [7] AlySaeed, R. M. El shazly, Y. H. Elbashar, A. M. Abou El-azm, M. M. El-Okr, M.N.H.Comsan, A. M. Osman, A. M. Abdal-monem, A. R. El-Sersy, "Gamma Ray Attenuation in Developed Borate Glassy", *Journal of Radiation Physics and Chemistry*, Volume 102, September 2014, Pages 167-170
- [8] NehalAboufotoh, YahiaElbashar, Mohamed Ibrahim, Mohamed Elokr, "Characterization of copper doped phosphate glasses for optical applications", *Journal of Ceramics International*, Volume 40, Issue 7, Part B, August 2014, Pages 10395-10399
- [9] HananElhaes, Mohamed Attallah, YahiaElbashar, Ayser Al-Alousi, Mohamed El-Okr, and Medhat Ibrahim, "Modeling and Optical Properties of P2O5-ZnO-CaO-Na2O Glasses Doped with Copper Oxide", *Journal of Computational and Theoretical Nanoscience* 11 (10), 2079-2084
- [10] D. A. Rayan, Y.H.Elbashar, M.M. Rashad, and A. El-Korashy, " Spectroscopic analysis of phosphate barium glass doped cupric oxide for bandpass absorption filter ", *Journal of Non-crystalline solids*, Volume 382, 15 December 2013, Pages 52-56
- [11] B. R. Judd, "Optical Absorption Intensities of Rare-Earth Ions", *Phys. Rev.* 127, 750-Published 1 August 1962
- [12] G.S. Ofelt, "Intensities of Crystal Spectra of Rare-Earth Ions", *J. Chem. Phys.* 37, 511 (1962)

- [13] Karl A.G and L. Eyring "Handbook on the physics and Chemistry of rare earths" Vol 25 (1998)P109-167
- [14] G.F. de Sá, O.L. Malta, C. de MelloDonegá, A.M.Simas, R.L. Longo, P.A. Santa-Cruz, E.F.da Silva Jr., "Spectroscopic properties and design of highly luminescent lanthanide coordination complexes", *Coordination Chemistry Reviews*, Volume 196, Issue 1, January 2000, Pages 165-195
- [15] R. R. Jacobs and M. J. Weber, *IEEE Journal of Quantum Electronics* 12(2), 102(1976)
- [16] K. Binnemans and C. Cörrler-Walrand, *J.Phys. Condens.Matter* 10, 167(1998)
- [17] H. Ebendorff-Heidepriem, D. Ehrt, M. Bettinelli, A. Speghini, *Journal of Non-Crystalline Solids* 240, 66(1998)
- [18] O. L. Malta, L. D. Carlos, *Quim. Nova*, 26(6), 889(2003)
- [19] Aly Saeed, Y. H. Elbashar, R. M. El shazly, "Optical Properties of High Density Barium Borate Glass for Gamma Ray Shielding Applications", *Journal of Optical and Quantum Electronics* (2016) 48:1