International Journal of Scientific Research in Physics and Applied Sciences
Research Paper
Vol.6, Issue.6, pp.159-161, December (2018)
E-ISSN: 2348-3423

Refractive Index and Its Thermal Maximum in Water on Two- State Theory

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Available online at: www.isroset.org

Received: 19/Oct/2018, Accepted: 26/Nov/2018, Online: 31/Dec/2018

Abstract- In the present paper, two-state theory of water has been successfully applied in computing the refractive index of it at single wavelength 589.262 nm in the temperature range -5 to 45°C. Further, it is shown that a thermal maximum in refractive index of water also exists near -1° C and agrees well with the experimental result . The present computed results of refractive index of water are also found in excellent agreement with the experimental data.

Keywords- Two-state theory, water, refractive index, thermal maximum

I. INTRODUCTION

Water is an interesting, unique and anomalous liquid in the sense that its physical properties do not exhibit monotonous behavior with temperature as is shown by other similar liquids. For example, density of water exhibits a maximum at 4°C whereas isobaric heat capacity of it exhibits a minimum at 37°C. Similarly, some other physical properties of water also exhibit either a maximum or a minimum with temperature. It is interesting to note that refractive index of water also exhibits a thermal maximum near -1°C [1].

It is of interest to mention here that some of the physical properties of water studied successfully as a function of temperature based on two-state theory are: (i) ultrasonic absorption [2], (ii)NMR shift[3],(iii) dielectric constant[4],viscosity[5] and refractive index [6].

According to two-state theory of Davis and Litovitz [7], the water is considered consisting of two different types of species. One of the specie is called the open-packed specie resembling to ice structure while other is called close-packed specie resembling to un-hydrogen bonded water molecules. The mole fraction of open- packed specie(X_0) decreases whereas that of closed packed specie(X_c) increases with the rise in temperature so that total mole fraction at each temperature is $X_0+X_c= 1$.

In the present paper, we wish to compute the refractive index of water in the temperature range of -5 to 45^0 C and to establish the thermal maximum in the refractive index of water near -1^{0}C with the help of two-state theory of Davis and Litovitz[7].

II. THEORY

The experimental values of refractive index of water [1,8] up to a decimal place of five are available in the temperature range of -5 to 45°C at an interval of 1°C in the temperature range -5 to 15°C[1] and later at an interval of 5°C in the temperature range 20 to 45°C[8]. But, the values of X_0 are available in the temperature range 0 to 100°C at an interval of 10°C [7]. Therefore, to obtain the values of X_0 in the temperature range -5 to 45°C, we make use of the relation given by Kumar et.al [9] and is expressed as

$$X_0(T) = 0.637 - A\ [1-\exp(-Z.T)] \quad (1)$$

Where X_0(T) represents the values of open- packed specie at T° C. Here A and Z are adjustable parameters and the values of these constants are determined by least square fit. The results obtained by eq. (1) are in very good agreement as is evident from the fact that the standard deviation obtained is 0.0016. A comparison of X_0 is shown in Table 1 where the values of A and Z are also reported. Once the values of X_0 become available as a function of temperature, these can be used to compute the refractive index of water.

To determine the refractive index of water as a function of temperature, the relation used here is the one that is given by Dass and co-workers [6] based on two-state theory applied to mixture model where the solute (open-packed specie) is dispersed in the solvent (close-packed specie) and making use of Glaston-Dale [10] relation to represent refractive index for each species. The relation for the refractive of water is expressed as:

$$n_w = [(X_0K_0 + K_cX_c)/V_w] + 1 \quad (2)$$

Where K_0 and K_c are constants corresponding to open-packed and close- packed species, respectively, and are determined by least square fit. n_w and V_w represent the refractive index and volume of liquid water . The values of volume of water are taken from the literature.

The computed results of n_w in water in the temperature range -5 to 45°C are in the excellent agreement with the experimental data as the standard deviation found is $5x\ 10^{-6}$. The computed results of refractive index of water are reported in table 2 along with the values of K_0 and K_c. The calculated results and the experimental data of refractive index of water with temperature are also plotted in fig 1 where the arrow indicates the thermal maximum near -1°C and is in excellent agreement with the experimental result [1].

It is worthwhile to mention here that Dass and Gilra[11] had demonstrated in 1966 based on pre-crystallization theory proposed by Frenkel [12] that a thermal maximum in refractive index of water exists between -3 to -2°C.

III. CONCLUSIONS

It is clearly evident from Table 2 and from Fig.1 that the present computed results of refractive index of water in the temperature range -5 to 45°C from eq.(2) are in excellent agreement with the experimental results and clearly indicates a thermal maximum near -1° C. Present study also strengthen the validity of the two-state theory in studying the physical properties of water as a function of temperature.

ACKNOWLEDGEMENT

The author KK expresses his sincere thanks to Director General and Management of College of Engineering Roorkee, Roorkee for providing all necessary facilities to carry out this research work.

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Table 1 Comparison of X_o as a function of temperature in water along with constants. (Values of A= 0.66678 and Z=$6.83277x10^{-3}$ °C^{-1})

Temp °C	X_o [7]	X_o (calc.)	Temp. °C	X_o [7]	X_o (calc.)
-5	---	0.660	10	0.595	0.593
-4	---	0.655	15	----	0.572
-3	---	0.651	20	0.554	0.552
-2	---	0.646	25	---	0.532
-1	---	0.641	30	0.515	0.513
0	0.637	0.637	35	----	0.495
1	----	0.632	40	0.478	0.477
2	---	0.628	45	----	0.460
3	---	0.623	50	0.443	0.444
4	----	0.619	60	0.411	0.413
5	----	0.615	70	0.382	0.383
6	---	0.610	80	0.355	0.356
7	----	0.606	90	0.331	0.331
8	----	0.601	100	0.309	0.307
9	----	0.597	---		

Table 2 Comparison of refractive index in water as a function of temperature at λ = 589.262 nm.
(Value of K_0 =0.336332 cm^3 and K_c =0.331008 cm^3)

Temp. (^{o} C)	n_w (exptl.)*	n_w (Calc.)	Δn(x10^{-5}) **	Temp. (^{o} C)	n_w (exptl.)*	n_w (Calc.)	Δn (x10^{-5})**
-5	1.33427	1.33427	0	7	1.33420	1.33420	0
-4	1.33430	1.33430	0	8	1.33416	1.33416	0
-3	1.33432	1.33432	0	9	1.33412	1.33411	+1
-2	1.33433	1.33434	-1	10	1.33407	1.33406	+1
-1	1.33434	1.33434	0	15	1.33376	1.33375	+1
0	1.33434	1.33435	-1	20	1.33335	1.33335	0
1	1.33434	1.33434	0	25	1.33286	1.33285	+1
2	1.33433	1.33433	0	30	1.33229	1.33229	0
3	1.33431	1.33431	0	35	1.33165	1.33165	0
4	1.33429	1.33429	0	40	1.33095	1.33095	0
5	1.33427	1.33427	0	45	1.33019	1.33020	-1
6	1.33424	1.33424	0	---	----	----	----

*** Ref. 1 for temperature range -5 to 15^{o}C and Ref. 8 for temperature range 20 to 45^{o}C**
**** $\Delta n = n_w(exptl.) - n_w(Calc.)$**

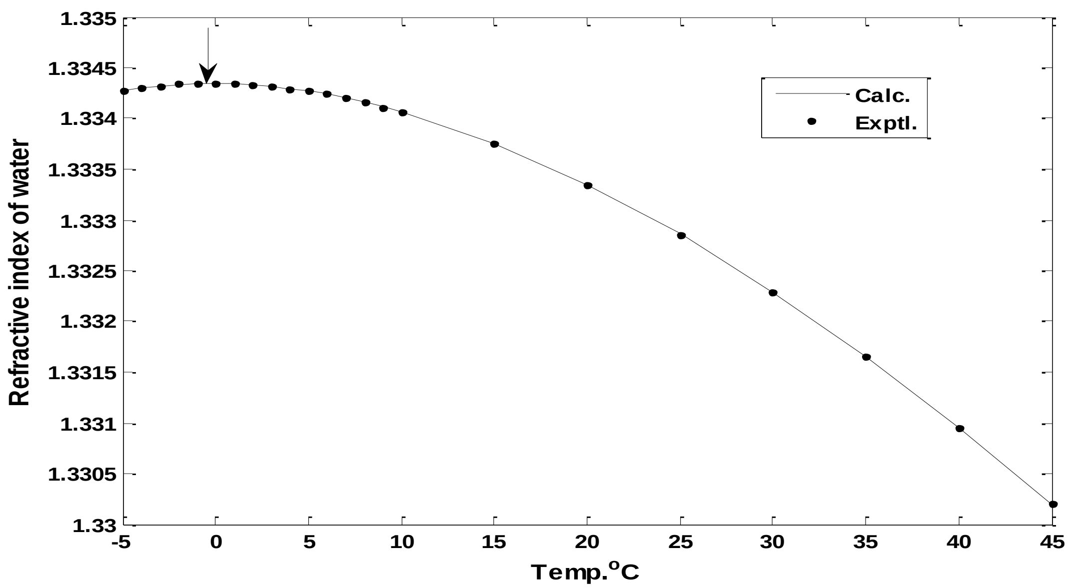

Fig. 1. Temperature dependence of refractive index of water

Author Profile

Mr. N. Dass obtained B.Sc and M.Sc from Birla Science College, Pilani (India) in year 1960 and 1962. He obtained his Ph.D from University of Roorkee (now IIT) in year 1969.He has published more than seventy research papers in International and National Journals. Thirty papers have been accepted for presentation in various International Conferences. He has been the reviewer to some International Journals. After retiring from University of Roorkee, he is presently working in College of Engineering Roorkee, Roorkee (India).

