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Research Article

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Refractive index, density, molar refraction and polarizability constant of substituted-2,3-dihydroquinazolin-4(1*H*)-ones in different binary mixture

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ABSTRACT

Refractive index measurement for the solutions of four derivatives of 2,3-Dihydroquinazolin-4(1H)-one is done using Abbe's refractometer. From the data of refractive index and density, molar refraction (R_m) and polarizability constant (α) are calculated. The values of these parameters and their variations are used to explain interactions taking place in the solution.

Keywords: 2,3-Dihydroquinazolin-4(1H)-one derivatives, molar refraction and polarizability constant.

INTRODUCTION

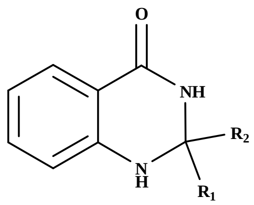
Refractive index is the useful physical characteristic of liquid by means of which pure compounds are identified and with which industrial processes are monitored and controlled[1]. The use of measurements of index of refraction as a quick, convenient, and accurate way to estimate densities of liquid mixtures has been reported[2-4]. The refractive index of liquids is a physical property so easily determined with accuracy that it has become a standard for their characterization[5]. Density and refractive index measurements are expected to shed some light on both solute-solute and solute-solvent interactions[6-8]. The refractometric technique is used to study the miscibility of polymer blend[9]. The use of molar refraction is proposed for the estimation of vapor pressure of pure hydrocarbons from C_1 to C_{100}[10]. Specific refractive index increments have been measured for solutions of neutral water-soluble polymer in binary solvents of formamide/water over the whole range of solvent composition[11]. Density and refraction index are two physical properties easy to measure and can be used to characterize an ionic liquid mixture[12]. Refractometric study is done by many workers[13-17] on different compounds.

The refractive index and the dipole polarizability are fundamental electroptical properties of matter[18]. The refractive index of a liquid can be easily determined to a high degree of accuracy. It is a characteristic property of a liquid. It is one of the important additives properties of liquid[19]. It varies with temperature and wavelength of light used. Generally, the D-line of sodium is used for standard measurement. Instruments used for measuring refractive indices are known as refractometers[20].

2,3-Dihydroquinazolin-4(1*H*)-one derivatives are playing crucial role in the context of drug intermediates, biological and pharmaceutical applications[21-25]. They have drawn much more attention because of their activities such as antibacterial[26], diuretic[27], anticancer[28], antihyperlipidemic[29], antiparkinsonism[30], antimicrobial[31], anti-inflammatory[32], bronchodilator[33], antihypertensive[34], antiproliferative[35] and antimitotic[36] activities.

Absorption, distribution, metabolism, and excretion (ADME) and chemical reactivity-related toxicity are the important factors of drugs[37-39]. Most of the drugs are hydrophobic. This property of hydrophobicity would render drugs difficult to eliminate, since in the absence of metabolism, they would accumulate in fat and cellular phospholipid bilayers[40] in cells. These modern days there is an upsurge in topical formulations such that it can be prepared by varying physico-chemical properties and providing better localized action[41].

The present work deals with the study of molar refraction and polarizability constant of following compounds in non aqueous solvents ethanol and methanol (with different percentage).



L_A : R_1= 4-hydroxy-3-methoxyphenyl
L_B : R_1= 2-hydroxyphenyl
L_C : R_1= 3-hydroxyphenyl
L_D : R_1= 4-hydroxyphenyl
R_2 = H for all

Ligand A (L_A)= *2-(4-hydroxy-3-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one*
Ligand B (L_B)= *2-(2-hydroxyphenyl) -2,3-dihydroquinazolin-4(1H)-one*
Ligand C (L_C)= *2-(3-hydroxyphenyl) -2,3-dihydroquinazolin-4(1H)-one*
Ligand D (L_D)= *2-(4-hydroxyphenyl) -2,3-dihydroquinazolin-4(1H)-one*

EXPERIMENTAL SECTION

The ligands of which physical parameters are to be explored are synthesized by using reported protocol[42]. The analytical grade solvents and freshly prepared doubly distilled water are used. The solutions of compounds under study are prepared in solvent ethanol and methanol by keeping constant ligand concentration system (0.01M). The density measurement is done using a specific gravity bottle. All the weights are taken on one pan digital balance (petit balance AD-50B) with an accuracy of ± 0.001 gm. The refractive indices are measured by Abbe's refractometer at 27± 0.1°C. The accuracy of Abbe's refractometer is within ±0.001 units. The constant temperature of the prism box is maintained by circulating water from thermostat at 27C ± 0.1^0C. Refractometer is calibrated by using glass test piece of known refractive index supplied with the instrument.

RESULTS AND DISCUSSION

It is often desirable to know the refractive index of a solute. This index can be derived from the refractive indices of solution and solvent on using a suitable mixture rule[43]. The molar refraction of solvent, solution can be determined by following equation[44].

$$R_{DMF\text{-}W} = X_1R_1 + X_2R_2 \quad (1)$$

Where, R_1 and R_2 are molar refractions of solvent and water respectively.

The molar refraction[45-47] of solutions of ligand in solvent -water mixtures are determined from-

$$R_{Mix} = \frac{(n^2-1)}{(n^2+2)} + \left\{\frac{[X_1M_1+X_2M_2 + X_3M_3]}{d}\right\} \quad (2)$$

Where,
n is the refractive index of solution, d is the density of solution, X_1 is mole fraction of solvent, X_2 is mole fraction of water and X_3 is mole fraction of solute, M_1, M_2 and M_3 are molecular weights of solvent, water and solute respectively.

The molar refraction of ligand can be calculated as –

$$R_{lig} = R_{Mix} - R_{DMF-w} \quad (3)$$

The polarizability constant (α)[48-49] of ligand can be calculated from following relation-

$$R_{lig} = 4/3\ \pi No\alpha \qquad (4)$$

Where, No is Avogadro's number.

Table 1: Values of molar refraction of different composition of solvents

% of solvent mixture	Molar Refraction [R]	
	Ethanol	Methanol
20	12.5745	7.8523
40	11.6219	6.9111
60	10.1420	5.7181
80	7.9156	4.1420
100	4.2315	7.8523

Table 2: The values of refractive index (n) and density (d) of 0.01M solution of ligand in different composition of Ethanol and Methanol solvent at 300K

Composition in %	Refractive index (n)		Density (d) gm/cm^3	
	Ethanol	Methanol Dioxane	Ethanol	Methanol Dioxane
Ligand (L_A)				
20	1.348	1.346	0.9621	1.0216
40	1.358	1.348	0.9928	1.0227
60	1.362	1.358	0.9909	1.0396
80	1.366	1.361	0.9567	0.9510
100	1.367	1.379	0.9624	0.9161
Ligand (L_B)				
20	1.346	1.340	0.9706	0.9893
40	1.356	1.345	0.9849	1.0081
60	1.362	1.346	1.0065	1.0298
80	1.366	1.347	0.9850	1.0191
100	1.368	1.348	0.9953	0.9261
Ligand (L_C)				
20	1.345	1.341	0.9574	1.0222
40	1.355	1.344	1.0093	1.0317
60	1.366	1.345	0.9950	1.0357
80	1.365	1.347	0.9652	0.9863
100	1.367	1.349	0.9730	0.9373
Ligand (L_D)				
20	1.347	1.343	0.9601	1.0281
40	1.356	1.345	0.9952	1.0309
60	1.362	1.346	0.9866	1.0458
80	1.365	1.348	0.9572	0.9849
100	1.366	1.351	0.9705	0.9203

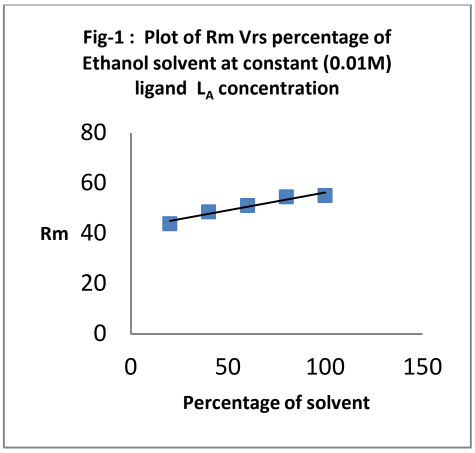
The data of density and refractive index measurement is presented in table no 02. Using equation no 01 to 04 calculations are made to determine the values of molar refraction and polarizability constant and are presented in table no 03. The experimental data of refractive index at the temperature T=300K is presented here. The experimental data shows that generally refractive index increases as the percentage composition of organic solvent component in the binary mixture increase. This is an indication of the fact that refractive index is correlated with the interactions occurring in the solution under study.

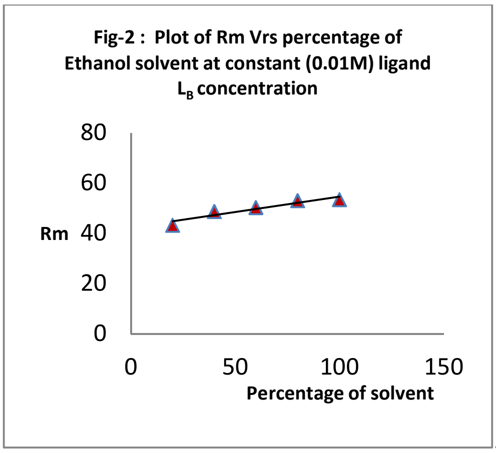
The graphs are plotted using percentage of solvent versus molar refraction (R_m). In all the graphs, it is found that molar refraction increases linearly with the increasing percentage composition of organic solvent component in the binary mixture. Molar refraction is related to the internal forces among the constituents of a liquid mixture. Similarly, polarizability constant increases in the same manner as that of molar refraction suggesting the validity of equation no 04. The polarizability of a molecule can be obtained by summing up the contributions of a variety of atoms and/or functional groups in the molecule. Here is the reasoning: molar refraction (R_m) is found to be an additive property, polarizability is related to molar refraction by the Lorentz-Lorenz equation and therefore polarizability should be an additive property.

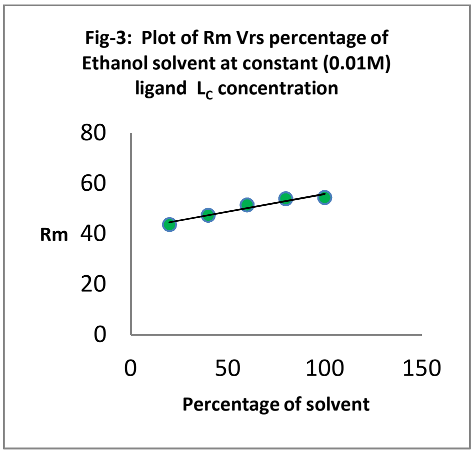
Table 3: The values of molar refraction (Rm), polarizability constant (α) of 0.01M solution of ligand indifferent composition of Ethanol and Methanol solvent at 300K.

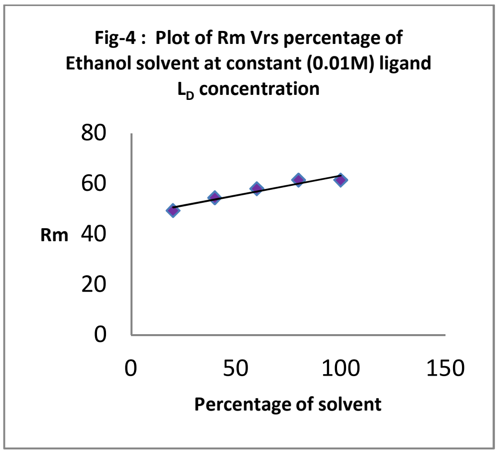
Composition in %	Molar refraction (Rm) x10^3 (cm^3/mol)		Polarizability constant (α) x10^{-23} (cm^3)	
	Ethanol	Methanol	Ethanol	Methanol
Ligand (L_A)				
20	43.8168	40.7415	1.7376	1.6156
40	48.5356	45.5392	1.9247	1.8059
60	51.0888	47.7801	2.0260	1.8948
80	54.5364	53.7012	2.1627	2.1296
100	55.0286	58.9490	2.1822	2.3377
Ligand (L_B)				
20	43.2099	41.4124	1.7135	1.6422
40	48.6780	45.8398	1.9304	1.8178
60	50.2946	46.7768	1.9945	1.8550
80	52.9697	48.3594	2.1006	1.9177
100	53.3430	54.0126	2.1154	2.1419
Ligand (L_C)				
20	43.6931	40.1841	1.7327	1.5935
40	47.3826	44.6718	1.8790	1.7715
60	51.3820	46.3899	2.0376	1.8396
80	53.9233	49.9668	2.1384	1.9815
100	54.4317	53.5093	2.1585	2.1220
Ligand (L_D)				
20	49.3356	45.2465	1.9565	1.7943
40	54.3347	50.5558	2.1547	2.0048
60	57.8931	51.9700	2.2958	2.0609
80	61.3628	56.6125	2.4334	2.2450
100	61.4381	61.8221	2.4364	2.4516

The increase in the value of polarizability constant as well as molar refraction with increase in percent composition of organic solvent part can be attributed to dispersion force. It is the force molecular force which arises from the temporary dipole moment.









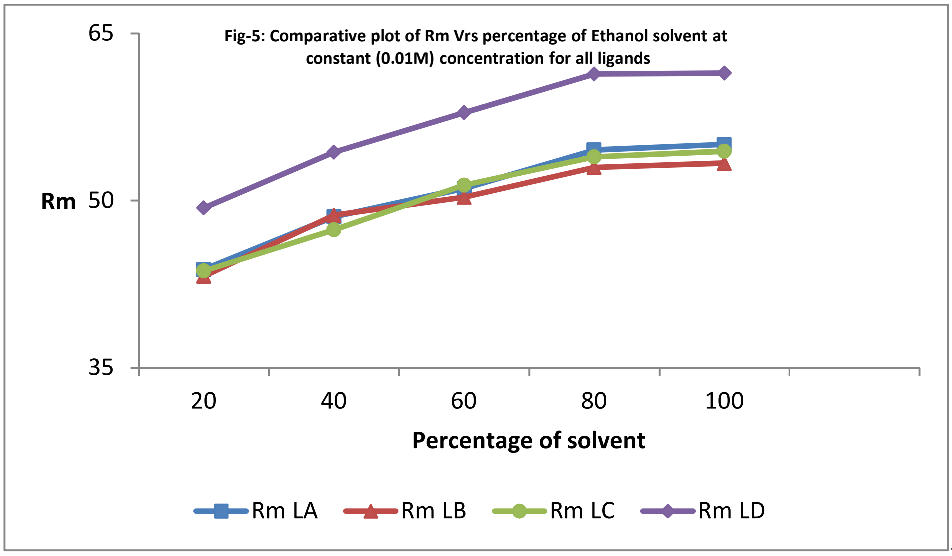
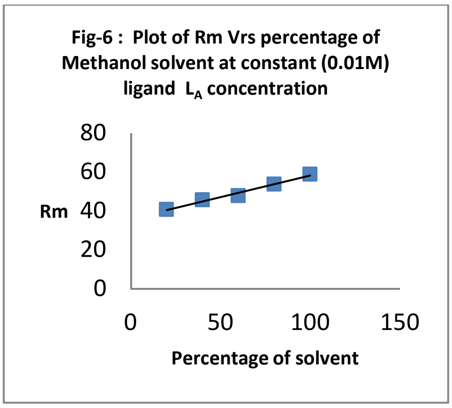
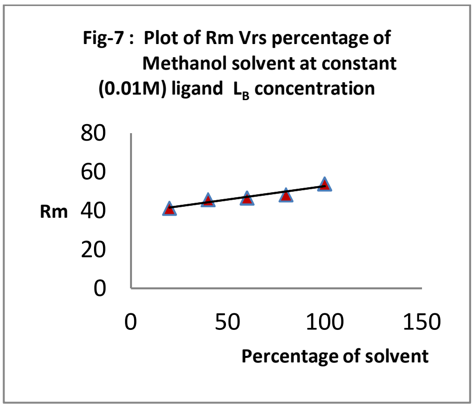
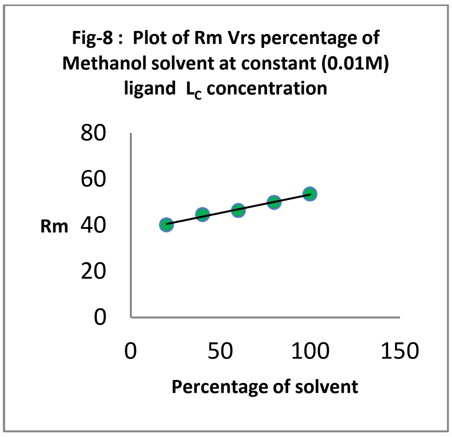
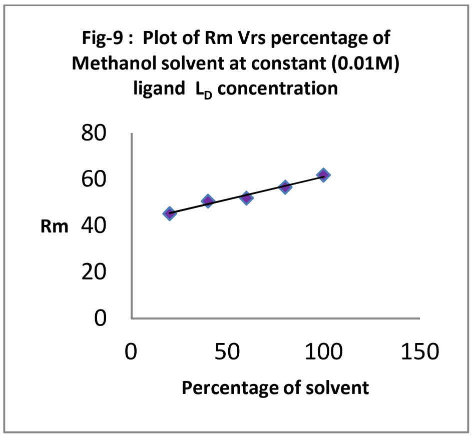


Fig. 1 to 5: Graphical representation of molar refraction (Rm) versus change in Ethanol solvent percentage at constant (0.01M) ligand concentration









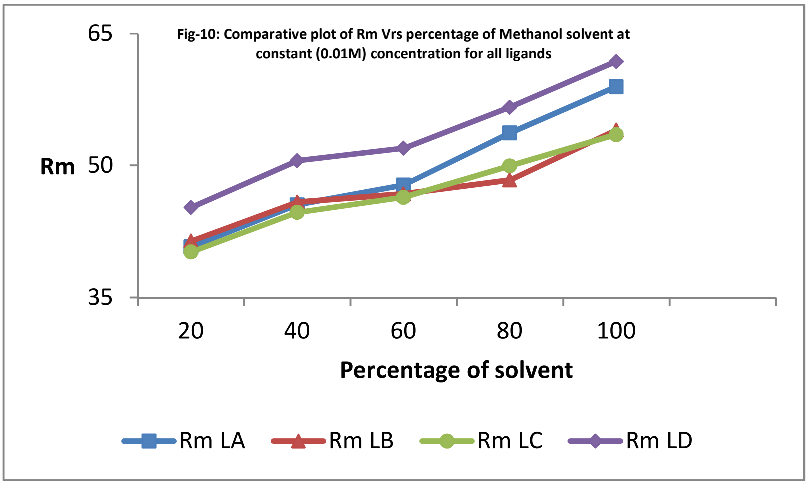


Fig. 6 to 10: Graphical representation of molar refraction (Rm) versus change in Methanol solvent percentage at constant (0.01M) ligand concentration

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REFERENCES

[1] BW Thomas; *Ind. Eng, Chem.*, **1953**, 45(7), 85.
[2] K Fajans; *Physical Methods of Organic Chemistry*, 2nd Edition, Interscience, New York, **1949**, 1159.
[3] S Zamvil; R Pludow; AF Fucaloro; *J. Appl. Crystallogr.*,**1978**, 11, 163.
[4] AF Fucaloro; C Billington; M Varnavas; *J. Chem. Educ.*, **1978**, 55, 793.
[5] JL Lauer; RW King; *Ana. Chem.*, **1956**, 28(11), 1697.
[6] GJ Moody; JDR Thomas; *Dipole Moments in Inorganic Chemistry*; Edward Arnold, London, **1971.**
[7] J Nath; *J. Chem. Thermodyn.*, **2002**, 34, 1857.
[8] SK Mehta; AK Sharma; KK Bhasin; R Prakash; *Fluid Phase Equilib.*, **2002**, 201, 203.
[9] R Varada; A Siddaramaiah; RL Reddy; *J. Appl. Polym. Sci*., **1998**, 70, 1823.
[10] MR Riazi; YS Alqaheem; *Ind. Eng. Chem. Res.*, **2010**, 49, 7104.
[11] SR Gooda; MB Huglin; *Eur. Polym. J.*, **1993**, 29(2), 365.
[12] VH Alvarez; S Mattedi; M Aznar; *Ind. Eng. Chem. Res.*, **2012**, 51, 14543.
[13] DF Charles; PF Medas; *Ana. Chem.*, **1955**, 27(3), 373.
[14] JW Stevens; WE Baier; *Ind. Eng. Chem.*, **1939**, 11(8), 447.
[15] R Talegaonkar; AS Burghate; SA Wadal; *Oriental J. Chem.*, **2011**, 27(3), 1285.

[16] MP Wadekar; AS Shrirao; RR Tayade; *J. Chem. Bio. Phy. Sci.*, **2014**, 5(1), 81.
[17] S Sharma; P Patel; *Fluid Phase Equilib.*, **2015**, 387, 121.
[18] D Goebel; U Hohm; *J. Phys. Chem.*, **1996**, 100, 7710.
[19] GD Tambatkar; MR Gadpayle; *Int. J. Chem. Phy. Sci.*, **2015**, 4, 127.
[20] BR Puri; LR Sharma; MS Pathania; *Principles of Physical Chemistry*, Vishal Publishing Co., Jalandhar, **2011**, 457.
[21] P Yerram; R Chowrasia; S Seeka; J Tangenda; *Eur. J. Chem.*, **2013**, 4 (4), 462.
[22] YS Sadanadam; RM Reddy; A Bhaskar; *Eur. J. Med. Chem.*, **1987**, 22, 169.
[23] G Bonola; E Sianesi; *J. Med. Chem.*, **1970**, 13, 329.
[24] M Hour; L Huang; S Kuo; *J. Med. Chem.*, **2000**, 43, 4479.
[25] RC Gupta; R Nath; K Shanker; *J. Indian Chem. Soc.*, **1979**, 56, 219.
[26] RJ Alaimo; HE Russell; *J. Med. Chem*., **1972**, 15, 335.
[27] HA Parish; RD Gilliom; WP Purcell; *J. Med. Chem.*,**1982**, 25, 98.
[28] MJ Hour; LJ Huang; SC Kuo; *J. Med. Chem.*, **2000**,43, 4479.
[29] KR Saxena; MA Khan; *Indian J. Chem. Sect B*, **1989**, 26, 443.
[30] HB Shivarama; MT Padmaja; MK Shivananda; PM Akbarali; *Indian J. Chem. Sect B*, **1998**, 37, 715.
[31] AN Gangwal; UR Kothawade; AD Galande; DS Pharande; AS Dhake; *Indian J. Heterocycl. Chem*., **2001**, 10, 291.
[32] T Singh; T Singh; VK Srivastava; S Sharma; A Kumar; *Indian J.Chem. Sect B*, **2006**, 45, 2558.
[33] R Tyagi; B Goel; VK Srivastava; A Kumar; *Indian J. Pharm. Sci.*, **1998**, 60, 283.
[34] AR Raghuram; RH Bahekar; *Indian J. Chem. Sect B*, **1999**, 38, 434.
[35] GM Chinigo; M Paige; S Grindrod; *J. Med. Chem.*, **2008**, 51(15), 4620.
[36] T Graening; HG Schmalz; *Angew. Chem.*, **2004**, 43(25), 3230.
[37] G Szakacs; A Varadi; B Sarkadi; *Drug Discovery Today*, **2008**, 13(9), 379.
[38] RL Oostendorp; T Buckle; JH Beijnen; O Tellingen; JH Schellens; *Investigational New Drugs*, **2009**, *27*(1), 31.
[39] S Ekins; Y Nikolsky; T Nikolskaya; *Trends in Pharmacol. Sci.*, **2005**, 26(4), 202.
[40] Y Shai; *Biochim. Biophys. Acta*, **1999**, 1462(1), 55.
[41] S Vats; C Saxena; TS Easwari; VK Shukla; *Int. J. Pharm. Res. Sch.*,**2014**, 3(2), 649.
[42] W Min; JG Jing; GS Zhi; W Lei; *Org. Prep. Proced. Int.*, **2012**, 44, 159.
[43] W Heller; *J. Phys. Chem.*, **1965**, 69(4), 1123.
[44] MP Wadekar; AS Shrirao; RR Tayade; *Der Pharma Chemica*, **2014**, 6(6), 90.
[45] VR Karanth; DK Bhat; *J. Chem. Eng. Data*, **2013**, 58, 271.
[46] SS Dhondge; *J. Chem. Eng. Data*, **2010**, 55, 3962.
[47] BN Solomonov; MA Varfolomeev; RN Nagrimanov; VB Novikov; MA Ziganshin; AV Gerasimov; SP Verevkin; *J. Chem. Eng. Data*, **2015**, 60(3), 748.
[48] J Wang; XQ Xie; T Hou; X Xu; *J. Phys. Chem. A*, **2007**, 111(20), 4443.
[49] AS Burghate; PB Agrawal; SW Quazi; ML Narwade; *Asian J. Chem.*, **2001**, 13(4), 1652.