Arabian Journal of Chemistry (2012) **xxx**, xxx–xxx

King Saud University

Arabian Journal of Chemistry

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ORIGINAL ARTICLE

Thermodynamic properties of binary mixtures of 1,3,4-oxadiazole derivative with chloroform, *N*,*N*-dimethyl formamide at 303, 308 and 313 K and atmospheric pressure

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Received 2 March 2012; accepted 4 October 2012

KEYWORDS

Molecular interaction;
Thermodynamic parameter;
Ultrasonic velocity;
1,3,4-Oxadiazole

Abstract The density (ρ), viscosity (η) and ultrasonic velocity (U) of pure solvents (chloroform (CF), *N*,*N*-dimethyl formamide (DMF)) and solutions of 2-((4-acetyl-5-(2-hydroxyphenyl)-5-methyl-4,5-dihydro-1,3,4-oxadiazol-2-yl)methylthio)-3-*o*-tolylquinazolin-4(3*H*)-one ($PD_{I\text{-}C}$) (0.001, 0.002, 0.004, 0.006, 0.008, and 0.010 mol dm^{-3}) in CF and DMF are investigated at 303, 308 and 313 K at atmospheric pressure. Various thermodynamic parameters such as acoustical impedance (Z), adiabatic compressibility (κ_a), inter molecular free path length (L_f), Rao's molar sound function (R_m), Van der Waals constant (b), internal pressure (π), relaxation time (τ), free volume (V_f) and solvation number (S_n) are calculated by using ρ, η and U data. The results obtained are interpreted in terms of solute–solvent and solute–solute interactions. The structure making or structure-breaking abilities of the solute in CF and DMF solvent are also studied.

1. Introduction

The five member 1,3,4-oxadiazole heterocycles are useful intermediates for the development of molecules of pharmaceutical interest where several promising antitumor compounds are found to contain the oxadiazole ring system (Rostom et al., 2003; Kumar et al., 2009). 1,3,4-Oxadiazole heterocycles are good bioisosteres of amides and esters, which can contribute substantially in increasing pharmacological activity by participating in hydrogen bonding interactions with the receptors (Guimaraes et al., 2005). The 2,5-disubstituted-1,3,4-oxadiazole derivatives are known for various pharmacological activities such as antibacterial (El-Emam et al., 2004), anti-inflammatory (Mullican et al., 1993), analgesic (Khan and Akhtar, 2003), antiviral and anticancer (Shah et al., 1998), antihypertensive (Upadhyay and Ram, 1999), anticonvulsant (Khan et al., 2001), antiproliferative (Liszkiewicz et al., 2003; Zahid et al., 2009), herbicidal (Kennedy and summers, 1981),

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Peer review under responsibility of King Saud University.

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http://dx.doi.org/10.1016/j.arabjc.2012.10.002

Nomenclature

C (mol dm^{-3})	concentration
T (K)	absolute temperature
M (kg mol^{-1})	molecular weight of solutions
M_1	molecular weight of solvent
M_2	molecular weight of solute
W_1	weight fraction of solvent
W_2	weight fraction of solute
R (J mol^{-1} K^{-1})	universal gas constant
b (m^3)	Van der Waals constant
m	meter
Pa	pascle
s	second
κ_b	Boltzmann constant
h	Plank's constant

Greek symbol

ρ (kg m^{-3})	density
η (mPa s)	viscosity
U (m s^{-1})	ultrasonic velocity
Z (kg m^{-2} s^{-1})	specific acoustical impedance
$_a$ (Pa–1)	adiabatic compressibility
L_f (m)	intermolecular free length
R_m (m10/3 s^{-1}/3 mol^{-1})	Rao's molar sound function
π (Pa)	internal pressure
V_f (m^3)	free volume

Superscripts

CF	chloroform
DMF	*N,N*-dimethyl formamide
A R	analytical reagent

hypoglycemic (O'Neal et al., 1962), hypnotic and sedative (Adelstein et al., 1976), MAO inhibitor (Mazouz et al., 1990) and insecticidal (Misra, 1983).

The sound velocity is a purely thermodynamic property. Many thermodynamic properties can be elucidated from sound velocity, viscosity and density data. Thermodynamic data are very important tool for understanding molecular interaction; solute–solvent and solute–solute, occurring in the solution. In recent years, the measurements of ultrasonic velocity have been adequately employed in understanding the nature of molecular interaction in pure liquids, binary and ternary mixtures (Srinivasalu and Ramachandra Naidu, 1991; Varadarajalu and Lakshminarayanan Reddy, 1998; Aswar, 1998). A literature survey reveals that ultrasonic velocity of various organic, inorganic and biological compounds in various solvents has been studied (Zhang et al., 2011; Baluja and Oza, 2002; Baluja and Shah, 2004). Our research group has also studied acoustical properties of synthesized compounds in various solvents (Godhani and Parsania, 2002; Godhani et al., 2001).

The choice of 1,3,4-oxadiazole is due to its multi-applicability in the field of medicine. The applications of these compounds attract us to study their behavior in various solvents and also investigate their thermodynamic properties. In the present paper, we have used this technique for the better understanding of the molecular interactions in some solutions. The present work deals with thermodynamic properties of the newly synthesized 1,3,4-oxadiazole derivative of 2-((4-acetyl-5-(2-hydroxyphenyl)-5-methyl-4,5-dihydro-1,3,4-oxadiazol-2-yl) methylthio)-3-*o*-tolylquinazolin-4(3*H*)-one (PD_{I-C}) in chloroform (CF) and *N,N*-dimethyl formamide (DMF) solutions at 303, 308 and 313 K and at atmospheric pressure. The results are interpreted in terms of molecular interaction occurring in the solutions.

2. Experimental

2.1. Materials

The 2-((4-acetyl-5-(2-hydroxyphenyl)-5-methyl-4,5-dihydro-1,3,4-oxadiazol-2-yl)methylthio)-3-*o*-tolylquinazolin-4(3*H*)-one (PD_{I-C}) used in this study was synthesized in our laboratory. The molecular weight of PD_{I-C} is 500.15. The structure of PD_{I-C} was confirmed by IR, ^{1}H NMR and CHN analyses. The structure of the present synthesized new PD_{I-C} is shown in Fig. 1. The solvents: chloroform (CF) and *N,N*-dimethyl formamide (DMF) used in the present study were of A R grade and were purified according to literature methods (Riddick et al., 1986). The estimated purity of solvents was more than 99.8% and was confirmed by HPLC with PDA detector. The schiff-base of (*Z*)-*N*′-(2-hydroxybenzylidene)-2-(4-oxo-3-*o*-tolyl-3,4-dihydroquinazolin-2-ylthio)acetohydrazide was synthesized in our laboratory (Sanghani et al., 2008). The 1,3,4-oxadiazole derivative of 2-((4-acetyl-5-(2-hydroxyphenyl)-5-methyl-4,5-dihydro-1,3,4-oxadiazol-2-yl)methylthio)-3-*o*-tolylquinazolin-4(3*H*)-one (PD_{I-C}) was synthesized by reacting schiff-base with acetic anhydride and was purified three times from chloroform – *n*-hexane prior to its use.

2.2. Synthesis of 2-((4-acetyl-5-(2-hydroxyphenyl)-5-methyl-4,5-dihydro-1,3,4-oxadiazol-2-yl)methylthio)-3-o-tolylquinazolin-4(3H)-one (PD_{I-C})

A mixture of Schiff-base 0.005 mol (2.50 g) and acetic anhydride (10 mL) was taken into a 100 mL round bottomed flask

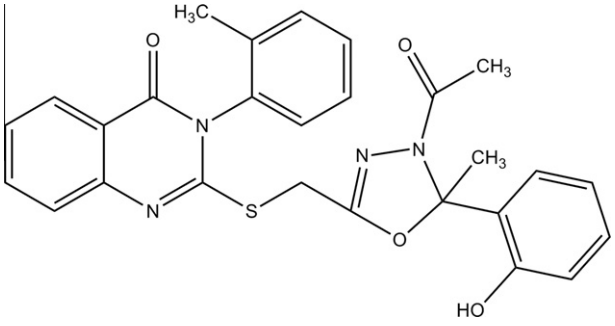

Figure 1 Structure of 2-((4-acetyl-5-(2-hydroxyphenyl)-5-methyl-4,5-dihydro-1,3,4-oxadiazol-2-yl)methylthio)-3-*o*-tolylquinazolin-4(3*H*)-one (PD_{I-C}).

Please cite this article in press as: Godhani, D.R. et al., Thermodynamic properties of binary mixtures of 1,3,4-oxadiazole derivative with chloroform, *N,N*-dimethyl formamide at 303, 308 and 313 K and atmospheric pressure. Arabian Journal of Chemistry (2012), http://dx.doi.org/10.1016/j.arabjc.2012.10.002