Journal of Molecular Liquids 211 (2015) 567–576

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

Interaction studies of methyl acetate in aqueous solutions of quinoxaline derivatives: Effect of temperature and concentration

Gnanapragasam Raphael, Indra Bahadur *, Eno E. Ebenso *

Department of Chemistry, School of Mathematical and Physical Sciences, Materials Science Innovation & Modelling (MaSIM) Research Focus Area, Faculty of Agriculture, Science and Technology, North-West University (Mafikeng Campus), Private Bag X2046, Mmabatho 2735, South Africa

ARTICLE INFO

Article history:
Received 7 June 2015
Received in revised form 26 July 2015
Accepted 27 July 2015
Available online xxxx

Keywords:
Quinoxaline derivatives
Methyl acetate
Apparent molar volume
Apparent molar adiabatic compressibility
Redlich–Mayer type equation

ABSTRACT

The aim of the present work is to examine the effect of temperature and concentration on interactions of methyl acetate with aqueous solutions of quinoxaline derivatives using volumetric and acoustic properties. In addition to this, the density, ρ, and sound velocity, u, of methyl acetate in aqueous solutions of quinoxaline derivatives namely: (N-{−3-[1-methanesulfonyl-5-(quinoxalin-6-yl)-4,5-dihydropyrazol-3-yl] phenyl} methane sulfonamide [MQDPMS]), N-{−2-[1-acetyl-5-(quinoxalin-5-yl)-4, 5-dihydropyrazol-3-yl] phenyl} methane sulfonamide [AQDPMS], N-{−2-[1-propanoyl-5-(quinoxalin-6-yl)-4,5-dihdro-1H-pyrazol-3-yl] phenyl} methane sulfonamide [2PQDPMS] and N-{−3-[1-propanoyl-5-(quinoxalin-6-yl)-4,5-dihydro-1H-pyrazol-3-yl] phenyl} methane sulfonamide [3PQDPMS] have been measured at 293.15, 298.15, 303.15 and 308.15 K and at pressure $p = 0.1$ MPa. These data have been used to calculate the derived properties such as apparent molar volume, V_φ, and apparent molar adiabatic compressibility, k_φ, for the mixtures. The standard partial molar volume, V^0_φ, standard partial molar volume of transfer, ΔV^0_φ, standard partial molar adiabatic compressibility, k^0_φ, and standard partial molar adiabatic compressibility of transfer, Δk^0_φ, have been evaluated using Redlich–Mayer type equation. These results have been interpreted in terms of effect of temperature and concentration on interactions such as solute–solute, solute–solvent and solvent–solvent which exist in the mixtures. Furthermore, apparent molar expansivity, E^0_φ, and Hepler's constant values, $\partial^2 V^0_\varphi/\partial T^2$, have been evaluated to support the conclusions obtained from the volumetric and acoustic studies.

© 2015 Elsevier B.V. All rights reserved.

1. Introduction

Quinoxaline and its derivatives are an important class of heterocyclic compounds, in which N, S and O elements can replace one or more carbon atoms of the ring [1]. Quinoxaline is generally called as benzopyrazine or 1, 4-diazanapthalene and it is described as a bioisoster of quinoline, naphthalene and benzothiophene [2]. They are mostly of synthetic origin with low melting (29–30 °C) solid and weakly basic [3]. These compounds are important in pharmacological industry due to their power to inhibit metal corrosion [4–7], to the preparation of porphyrins, since their structure has chromophores in the natural system, and their utility in the electroluminescent materials [8–10]. Furthermore, they are significant with wide biological properties [4, 11–16] such as antibacterial, antifungal, anticancer, antitubercular, antileishmanial, antimalarial, antidepressant, antimycobacterial, anticandida, and neurological activities, among others.

There are very few reported studies in literature on the solubility of quinoxaline and its derivatives [17]. The knowledge of solubility of quinoxaline in methyl acetate at different temperatures is vital in physical stability studies of liquid dosage forms, in processes where temperature changes are involved and in the preformulation phase of new compounds where only a small quantity of the compounds is present [18]. Thermo-physical properties is required to develop new pharmacologically active compounds and their mechanism of action, in drug's metabolism processes including biological activities of the metabolites, stereochemistry importance in drug design, and to determine space which drug occupies [1]. To characterize the properties of the quinoxalines in pharmaceutically significant solvents assists in finding out correlations among the structure and topology of the molecules with their partitioning, solubility and solvation properties [19].

Thermodynamic and thermo-physical property data are essential in different industries such as oil and gas for flow assurance and oil recovery, in the chemical industry for the design of separation processes; in the pharmaceutical and polymer industry for solvent selection and emission. Thermodynamics/thermo-physical data are also necessary in environmental science for the estimation of the distribution

* Corresponding authors.
E-mail addresses: bahadur.indra@gmail.com (I. Bahadur), Eno.Ebenso@nwu.ac.za (E.E. Ebenso).

http://dx.doi.org/10.1016/j.molliq.2015.07.069
0167-7322/© 2015 Elsevier B.V. All rights reserved.

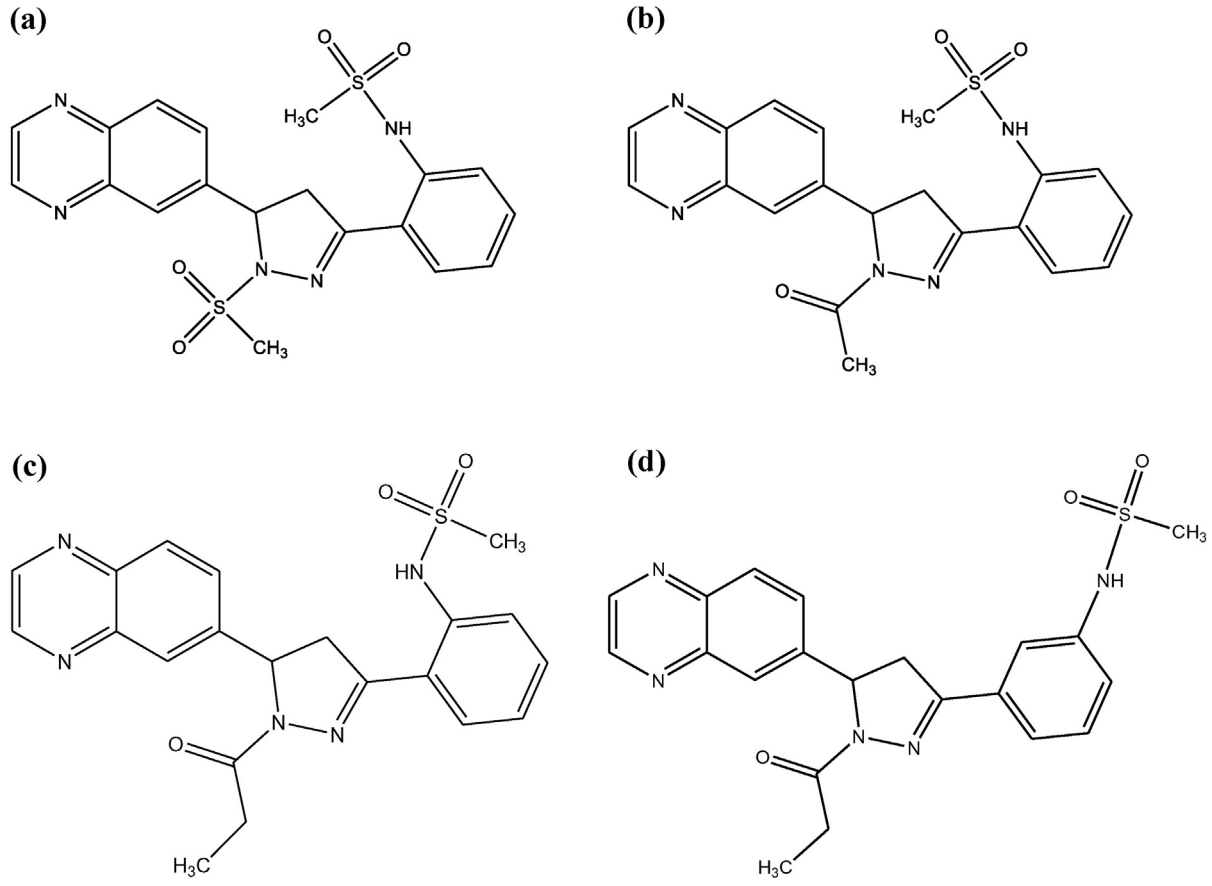

Fig. 1. Chemical structure of (a) [MQDPMS], (b) [AQDPMS], (c) [2PQDPMS] and (d) [3PQDPMS].

of chemicals in various ecosystems, in biotechnology for the origin of many diseases is traced to aggregation of proteins and several protein separations [20]. Furthermore, these data provide information about the interactions such as solute–solute, solute–solvent and solvent–solvent [21–23] and allows for developing new reliable correlations and/or predictive models and to test the solution theories for quinoxaline compounds and their mixtures with methyl acetate.

To the best of our knowledge, no work has been reported in open literature for the studied systems. The increasing uses of these compounds in many industrial processes have greatly stimulated the need for extensive investigation on their thermodynamic and thermo-physical properties and their mixtures with organic solvents. Thus, in the present work, we introduce new comprehensive database for the density, ρ and sound velocity, u, of methyl acetate in aqueous solutions of (N-{−3-[1-methanesulfonyl-5-(quinoxalin-6-yl)-4,5-dihydropyrazol-3-yl] phenyl} methane sulfonamide [MQDPMS]), N-{−2-[1-acetyl-5-(quinoxalin-5-yl)-4, 5-dihydropyrazol-3-yl] phenyl} methane sulfonamide [AQDPMS], N-{−2-[1-propanoyl-5-(quinoxalin-6-yl)-4,5-dihdro-1H-pyrazol-3-yl] phenyl} methane sulfonamide [2PQDPMS] and N-{−3-[1-propanoyl-5-(quinoxalin-6-yl)-4,5-dihydro-1H-pyrazol-3-yl] phenyl} methane sulfonamide [3PQDPMS] at 293.15, 298.15, 303.15 and 308.15 K with pressure $p = 0.1$ MPa. The solute–solute, solute–solvent and solvent–solvent interactions in the mixtures have been evaluated using partial molar properties. Furthermore, the influence of temperature and concentration as well as replacement of group such as methanesulfonyl by acetyl, and acetyl by propanoyl at different position of quinoxaline derivatives has been evaluated. Thus, the results from these studies can be utilized to synthesize the new pharmaceutically active compounds on an industrial scale. The present work is a continuation of our research group's studies on thermo-physical and thermodynamics properties of solutions [24–36]. The structure of the studied quinoxaline derivatives is given in Fig. 1.

2. Experimental

2.1. Chemicals

Quinoxaline derivatives namely: (N-{−3-[1-methanesulfonyl-5-(quinoxalin-6-yl)-4,5-dihydropyrazol-3-yl] phenyl} methane sulfonamide [MQDPMS]), was purchased from Life Chemicals Inc., N-{−2-[1-acetyl-5-(quinoxalin-5-yl)-4, 5-dihydropyrazol-3-yl] phenyl} methane sulfonamide [AQDPMS], N-{−2-[1-propanoyl-5-(quinoxalin-6-yl)-4,5-dihdro-1H-pyrazol-3-yl] phenyl} methane sulfonamide [2PQDPMS] and N-{−3-[1-propanoyl-5-(quinoxalin-6-yl)-4,5-dihydro-1H-pyrazol-3-yl] phenyl} methane sulfonamide [3PQDPMS] were obtained from Vitas-M Laboratory, Ltd., with mole fraction purity of >0.90. Methyl acetate was purchased from Aldrich with mole fraction purity of >0.99. Many suppliers have been checked on the purity of the studied compounds but unfortunately these compounds are fairly new and the

Table 1
Pure component specifications: suppliers, molecular weight, and specified purity.

Chemicals	Supplier	Molecular weight	Mole fraction purity
		($g \cdot mol^{-1}$)	Initial[a]
[MQDPMS]	Life Chemicals Inc.	445.515	>0.90
[AQDPMS]	Vitas-M Laboratory, Ltd.	409.462	>0.90
[2PQDPMS]	Vitas-M Laboratory, Ltd.	423.488	>0.90
[3PQDPMS]	Vitas-M Laboratory, Ltd.	423.488	>0.90
Methyl acetate	Aldrich	74.08	>0.99

[a] Purity values are reported as stated by suppliers.

Download English Version:

https://daneshyari.com/en/article/5410670

Download Persian Version:

https://daneshyari.com/article/5410670

Daneshyari.com