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Dielectric Spectroscopy in Ibuprofen-Dioxane Mixture

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ABSTRACT

In recent years, the dielectric study of amorphous pharmaceuticals has made a considerable effort towards correlating the molecular mobility with their physical and chemical stability. The molecular mobility of amorphous materials is affected by temperature, additives (such as water) and specific interactions (such as Hydrogen bond). Therefore, to understand the physicochemical instability of amorphous materials, nature of their molecular mobility needs to comprehend. In this order, the Dielectric and Calorimetric measurements were performed on a mixture of ibuprofen and 1,4-dioxane. The αD process is found to be Debye-like (i.e., αHN = 0 and βHN= 1) in nature and α process kinetically freezes at Tg-onset (DSC) implies that α- process indeed corresponds to the glass transition event. Both processes are found to be non-Arrhenius in nature. In addition, two secondary relaxation processes (designated as βJG and β) are observed and are comparable with the literature. The activation energy of β process indicates that its originating from the fluctuations of the side group larger than -OH group. Also, the calculated fragility index demonstrates that ibuprofen is a fragile glass former.

It is known for decades that several monohydroxy alcohols [7-15] and amides [16] hydrogen bonded glass forming systems results in intramolecular and intermolecular hydrogen bonding and behave differently. A study of monohydroxy alcohols reveals that hydrogen-bonded networks aggregate their polar -OH group in the chain or ring-like structures [9-12]. The aggregation of the chain-like structure shows a Debye relaxation, where the strength of Debye process depends on temperature, pressure, dilution, and confinement volume. On the basis of the position of -OH group in molecular structure, monohydroxy alcohols can classify in three different groups; (i) If -OH group is situated at end position (e.g., 2-ethyl-1-hexanol) then observed Debye peak dominates the dielectric loss spectra. (ii) If -OH group is sterically hindered (e.g., 4-methyl-3-heptanol) then observed Debye peak is weaker. Moreover, if a large cyclic group (e.g., phenyl ring) is located in the molecular structure, it can limit the formation of H-bonding. If two or more -OH groups are present in the proximity of the same molecule (e.g., glycerol) then Debye peak vanishes [12] or may be hidden under conductivity contribution in the imaginary part of permittivity [13-16]. It is reported that Debye process could not be detected in calorimetric [17], light scattering [18] and nuclear magnetic resonance [19,20]. Therefore, dielectric spectroscopy is the most useful technique to study the strength of relaxation processes, which can be discussed in terms of Kirkwood correlation factor [7,21]. Recent [1,2] dielectric studies of supercooled pharmaceuticals are revealing the existence of the Debye-like process in complex molecules, and its presence has been reported in ibuprofen. However, the dielectric strength of the Debye process is found to be very low. Moreover, this Debye-like process is reported to be absent in magnetic resonance or shear mechanical experiments [22]. In this work, the detailed dielectric and calorimetric study of supercooled ibuprofen and its liquid mixtures with 1,4-dioxane at test concentrations is reported. The 1,4-dioxane (also known as p-dioxane) is used as a non-polar [23,24] solute in a solution. The measurements can perform up to 3% (weight fraction of 1,4-dioxane) because heterogeneous crystallization intervened for higher concentration. Experimental Section Material characterization The samples studied are: (i) Ibuprofen (IBP) (C13H18O2) (purity ≥ 98%) (Molecular weight (MW) = 206.29 g/mol), also known as α-Methyl-4-(isobutyl) phenylacetic acid, (±)-2-(4-Isobutylphenyl) propanoic acid 1,4-dioxane (DXN) (C4 H8 O2) (purity ≥ 99.5%) (MW=88.11 g/mol). The IBP sample is obtained from Sigma-Aldrich co., and DXN is obtained from Fisher Scientific (ExcelaR). Both the samples were dried to remove absorbed water and used without further purification. Experimental techniques Perkin-Elmer sapphire differential scanning calorimeter (DSC) with *Corresponding author: Manoj K. Saini, School of Physical Sciences, Jawaharlal Nehru University, New Delhi 110067, India, E-mail: manojspsjnu@gmail.com Received November 22, 2017; Accepted December 22, 2017; Published December 29, 2017 Citation: Saini MK (2017) Dielectric Spectroscopy in Ibuprofen-Dioxane Mixture. Pharm Anal Acta 8: 572. doi: 10.4172/2153-2435.1000572 Copyright: © 2017 Saini MK. This is an open-access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited. Dielectric Spectroscopy in Ibuprofen-Dioxane Mixture Manoj K. Saini* School of Physical Sciences, Jawaharlal Nehru University, New Delhi 110067, India Abstract In recent years, the dielectric study of amorphous pharmaceuticals has made a considerable effort towards correlating the molecular mobility with their physical and chemical stability. Both processes are found to be non-Arrhenius in nature. In addition, two secondary relaxation processes (designated as βJG and β) are observed and are comparable with the literature. The activation energy of β process indicates that its originating from the fluctuations of the side group larger than -OH group. Also, the calculated fragility index demonstrates that ibuprofen is a fragile glass former. Pharmaceutica Analytica Acta ISSN: 2153-2435 Pharmaceutical Analytica Acta Page 2 of 5 Citation: Saini MK (2017) Dielectric Spectroscopy in Ibuprofen-Dioxane Mixture. Pharm Anal Acta 8: 572. doi: 10.4172/2153-2435.1000572 Volume 8 • Issue 12 • 1000572 Pharm Anal Acta, an open access journal ISSN: 2153-2435 quench-cooling accessory was used for the calorimetric measurements.

According to Bras et al. [1] the Molecular Dynamics (MD) simulation reveals a strong tendency of IBP to form noncovalent molecular aggregates such as dimer (μ0 = 1.29D to 2.15D) and trimer (μ0 = 1.68D to 2.50D) either cyclic or linear, where cyclic structures were found to have a smaller dipole moment and less gk " value (~0.3 (for cyclic) and ~0.8 (for linear)) at T = 360K. Also, it is suggested that hydrogen bonded cyclic structures might be associated with Debye process in IBP.

Keywords: Debye relaxation; Dielectric spectroscopy; Ibuprofen; Dioxane Introduction The study of vitrification transition phenomena has always been interested in hydrogen-bonded supercooled liquids composed of small molecules.