EFFECT OF IONIZATION ON NICOTINE'S HYDRATION BEHAVIOUR

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ABSTRACT

Nicotine is a naturally occurring bicyclic alkaloid, composed of a pyridine ring connected to a pyrrolidine ring. Possessing two heterocyclic nitrogen atoms, it behaves like a dibasic compound in water. The pyrrolidine nitrogen has a pKa of approximately 8.0 while the pyridine nitrogen has a pKa of 3.12-3.41. Therefore, at physiological pH of 7.4 about 69% percent is in a protonated form, while in some extreme regions of the body, such as the stomach (pH≈1,5-3,5), > 99% is in a diprotonated form. As the human body is a water medium, where water interaction is a major driver of molecular behaviour and distribution, understanding the differences in hydration behaviour between non-ionic, mono- and diprotonated forms of nicotine can elucidate it's biological activity within the body.

Nicotine, along with two synthesised nicotinium salts: nicotinium bromide and nicotinium dibromide were examined as water solutions. Measurements of density, sound velocity and viscosity of a series of aqueous solutions with a molality range of 0,02 to 0,25 mol/kg and at temperatures ranging 20-40 °C were performed. The results were interpreted in terms of solute/solute and solute/solvent interactions. The ionisation of nicotine significantly changes it's hydration behaviour, impacting characteristics such as solute/solvent interactions, structure making or breaking behaviour, hydration numbers and even taste. Differences between mono- and diprotonated forms were also observed. These findings underscore the critical role of ionization state in determining molecular behavior in aqueous systems and highlight its importance in evaluating substances for biological applications..

Keywords: Nicotine, ionization, hydration, density, acoustics, viscosity.

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