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# Solvation behavior of some nucleic acid bases and nucleosides in water and in aqueous guanidine hydrochloride solutions: Viscometric, calorimetric and spectroscopic approach

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ABSTRACT

Viscosity, $\eta$ and enthalpy of dilution, $q$ of studied nucleic acid bases (uracil, cytosine, thymine) and nucleosides (uridine, cytidine and thymidine) in water and in aqueous solutions of (0.10, 0.25, 0.50, 0.75 and 1.00) mol · kg$^{-1}$ guanidine hydrochloride (GnHCl) have been determined over a temperature range (288.15-318.15) K at (101.3 ± 0.5) kPa. These data have been used to calculate viscosity *B*-coefficients and standard molar enthalpy of dilution, $\Delta_{dil}H^o$ which have further been used to evaluate corresponding transfer parameters $\Delta_{tr}B$ and $\Delta_{tr}\Delta_{dil}H^o$, respectively. Positive $\Delta_{tr}B$ values and negative $\Delta_{tr}\Delta_{dil}H^o$ values indicate the predominance of hydrophilic–ionic interactions in these systems. Temperature dependence of *B*-coefficient and $\Delta_{dil}H^o$ has also been discussed. Spectroscopic studies have been carried out to further investigate the structural changes and the interactions involved in the mixed aqueous solutions.



## 1. Introduction

Nucleic acids (DNA/RNA) consist basically of one or more linear copolymer chains, which are formed by four chemically distinct types of monomer units linked together by sugar–phosphate bonds in a genetically determined sequence [1,2]. The stability, denaturation and annealing of these nucleic acid helices play an integral role in many biomedical diagnostic applications and medicinal chemistry [1,2]. The thermodynamic stability of any biopolymer conformation is the net result of several secondary or non-covalent interactions which occur intramolecularly or with the solvent [3,4]. Owing to the complex structure of the nucleic acids, it is difficult to understand the exact nature of interactions occurring in the aqueous and mixed aqueous systems. Hence the physicochemical investigations of their model compounds can provide an insight into the folding and unfolding mechanism, stabilization and genetic transformations in the cells [5–7]. Most of the physiological processes occur in aqueous media, so the abnormalities in the properties of aqueous solutions may be attributed to the change in the solution structure caused by various additives or the temperature [8,9]. Although some reports are available on the apparent molar volumes, heat capacities and compressibilities of some nucleic acid bases and nucleosides (solutes) in water and in mixed aqueous solutions [10–18], but the studies on the rheological properties are scarce. Therefore, in continuation of our work [19] on solution behavior of nucleic acid bases and nucleosides, in the present study we report the viscosity, enthalpy of dilution and UV–vis spectra for these solutes to further investigate the various types of interactions in water and in aqueous solutions of co-solute i.e. guanidine hydrochloride (GnHCl) as a function of temperature. GnHCl is one of the most powerful denaturing agent for globular proteins and nucleic acids [1]. It is widely used to investigate protein stability and folding kinetics. Therefore, an understanding of the hydration properties of these solutes is essential for the interpretation of structural, transport and energetic properties that describe the solute–solvent interactions in the presence as well as in the absence of GnHCl. To the best of our knowledge, this is the first report on the viscometric, calorimetric and spectroscopic properties of nucleic acid bases and nucleosides in aqueous solutions of GnHCl at various temperatures. The viscosity *B*-coefficient, viscosity *B*-coefficient of transfer, standard molar enthalpy of dilution, $\Delta_{dil}H^o$ and standard molar enthalpy of transfer, $\Delta_{tr}\Delta_{dil}H^o$ have been calculated and discussed in terms of various interactions. The spectroscopic studies have also been carried out to further investigate the structural changes in these solutes.

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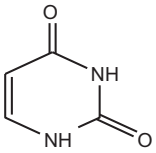
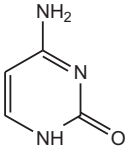
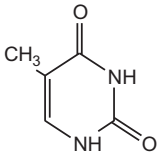
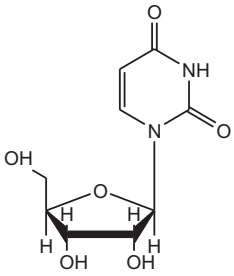
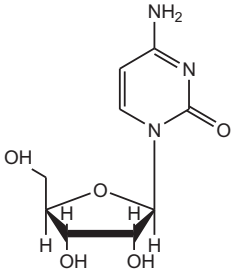
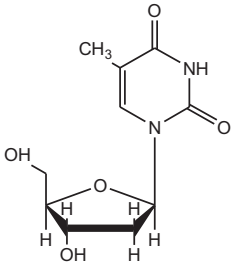
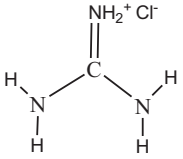
**TABLE 1**
Chemicals used in this study with their molar mass ($M$), source (SRL = Sisco Research Laboratories, India), CAS number, mass fraction moisture content ($w$), and mass fraction purity ($x$).

| Chemical name | Structures | $M$ | Source | CAS no | [a]$w$ | $x$ | Analysis |
|---|---|---|---|---|---|---|---|
| Uracil |  | 112.09 | SRL | 66-22-8 | 0.005 (0.0005) | ⩾0.99 | HPLC [b](0.999) |
| Cytosine |  | 111.10 | SRL | 71-30-7 | 0.01 (0.00045) | ⩾0.99 | HPLC (0.999) |
| Thymine |  | 126.12 | SRL | 65-71-4 | 0.01 (0.0007) | ⩾0.98 | HPLC (0.999) |
| Uridine |  | 244.20 | SRL | 58-96-8 | 0.005 (0.0005) | ⩾0.99 | HPLC (0.999) |
| Cytidine |  | 243.22 | SRL | 65-46-3 | 0.01 (0.0006) | ⩾0.99 | HPLC (0.995) |
| Thymidine |  | 242.23 | SRL | 50-89-5 | 0.01 (0.00075) | ⩾0.99 | HPLC (0.990) |
| Guanidine hydrochloride |  | 95.53 | SRL | 50-01-1 | 0.005 (0.0015) | ⩾0.99 | Used as such |

[a] As reported by the suppliers and in parenthesis are given the mass fraction water content obtained from the Karl-Fisher analysis.
[b] Mass fraction purity as obtained from HPLC analysis.