

Evidences for complexations of β -cyclodextrin with some amino acids by ^1H NMR, surface tension, volumetric investigations and XRD

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ABSTRACT

Inclusion Composites between β -cyclodextrin and amino acids (viz., L-Methionine, L-Proline and L-Glutamine) are established in aqueous medium. Such complexation of amino acids in aqueous medium without using any organic solvent provides great ideas in different industries. The complexes are characterized by ^1H NMR which proves the formation of inclusion complex. The interactions of β -CD with amino acids are analyzed by means of surface tension and density. Contributions of different groups of the guest molecules to the limiting apparent molar volume are determined. Additionally, the stoichiometry of the inclusion complexes is also determined to be 1:1 in all the three cases. The solid inclusion complex formations of β -CD with amino acids are confirmed by PXRD analysis.

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1. Introduction

Cyclodextrins (CDs) are cyclic oligosaccharide of glucopyranose units that play an important role as a host in inclusion complexes, where non-covalent interactions are involved. They contain six (α -CD), seven (β -CD) and eight (γ -CD) glucopyranose units, which are bound by α -(1–4) linkages forming a truncated conical with a hollow cavity [1,2]. Cyclodextrins (CDs), with hydrophobic inner cavities and hydrophilic outer rims, are capable of interacting with a large variety of guest molecules to form non-covalent inclusion complexes [3]. CDs have been widely employed for encapsulation of several substances which are used in food, pharmaceutical industries, pesticides, toilet articles, textile processing, and other industry [4–7], supramolecular and host-guest chemistry [8,9], models for studying enzyme activity, molecular recognition, studying intermolecular interactions and chemical stabilization [1,3,10]. In the field of agriculture and environmental science huge applications of cyclodextrin have been found as encapsulating agent [11–13].

In this present work, β -CD has been used as host because of its biocompatibility, relatively non-toxicity and relatively low price. The selected biologically active amino acids viz., L-Methionine (L-Met), L-Proline (L-Pro) and L-Glutamine (L-Gln) (Scheme 1) that have been chosen as guest, having a numbers of important roles in the human body

[14–16]. All of them are used in biosynthesis of proteins. L-Met is essential in humans i.e. it must be introduced from outsides and β -CD can be used as good carriers. L-Pro both L-Gln both are non-essential in humans, meaning the body can synthesize it but sometimes body demands glutamine in larger amount then L-Gln must be incorporated from outsides [17]. Moreover, the formation of proline/ β -CD complexation is reported in theoretical background but no such works have been done to propose a model for 1:1 complexation with L-proline [18]. Encapsulation of guest molecules into CD modifies some physicochemical properties such as state, solubility and stability of the guest molecules after formation of inclusion complex. Changes in the physicochemical properties have been used to characterize whether guest molecules are really included in the cyclodextrin cavity.

In this purpose, the surface tension and density have been measured to find out the nature and interactions of host-guest inclusion complex of the selected amino acids in $w = 0.001, 0.004, 0.007$ mass fraction of aqueous β -cyclodextrin (β -CD) solution at 298.15 K. ^1H NMR technique has also been performed to confirm the inclusion phenomenon.

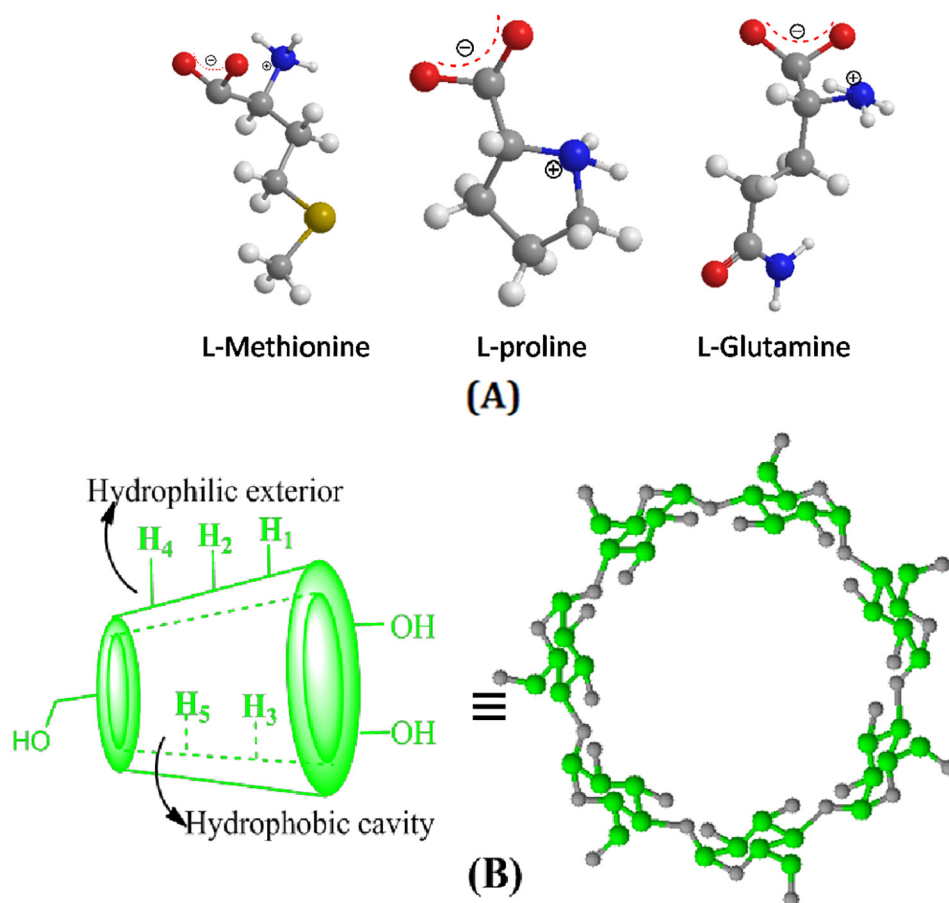
2. Experimental section

2.1. Materials

The titled compounds e.g. amino acids (viz., L-Methionine, L-Proline, L-Glutamine) and β -cyclodextrins of puriss grade, are purchased from Sigma-Aldrich, Germany. The mass fraction purity of L-Met, L-Pro, L-Gln, and β -cyclodextrin are $\geq 0.98, 0.98, 0.99$, and 0.98 , respectively.

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Scheme 1. The molecular structure of the selected amino acids in aqueous solutions (A) and the structure of β -CD (B) (host molecule).

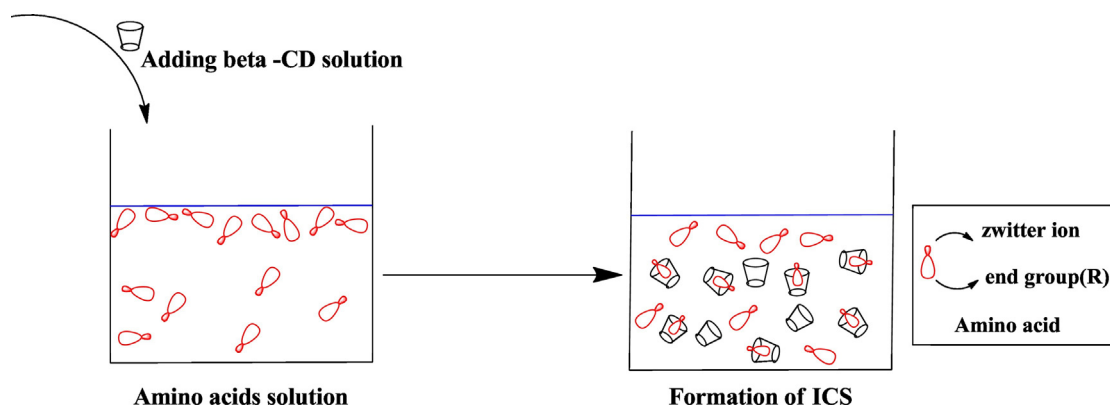
D₂O (deuterium content 99.9%) is purchased from Sigma-Aldrich, Germany.

2.2. Apparatus and methods

Solubility of the β -Cyclodextrin and the chosen amino acids have been precisely checked in triply distilled, deionised and degassed water and it is observed that both β -CD and amino acids are soluble properly. The stock solutions of the amino acids (uncertainty in molality of the solutions $\pm 0.0001 \text{ mol kg}^{-3}$) for physicochemical studies have been prepared by adopting the course mentioned in earlier work [17].

The surface tension experiments ($\pm 0.1 \text{ mN m}^{-1}$) are done by using a Tensiometer (K9, KRÜSS; Germany) at 298.15 K ($\pm 0.01 \text{ K}$) and density (ρ) of the solvent are measured by means of vibrating a U-tube Anton Paar digital density meter (DMA 4500 M) with a uncertainty of $\pm 0.00005 \text{ g cm}^{-3}$ [17]. The surface tension is measured of the sets of solutions of L-Methionine, L-Proline, L-Glutamine having concentration 10 mM with aqueous β -CD solution by dilution method at 298.15 K (Table S2).

NMR spectra are recorded at 300 MHz Bruker ADVANCE at 298.15 K ($\pm 0.01 \text{ K}$) in D₂O. Signals are quoted as δ values in ppm using residual protonated solvent signals as internal standard (D₂O: δ 4.79 ppm). Data are reported as chemical shift.



Scheme 2. Schematic representation of formation of inclusion complexes between amino acid and β -CD in aqueous medium at 298.15 K.

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