

Research Article

Computer Simulation of Amino Acid Oligomerization in Aqueous Solutions Induced by Condensing Agent

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Physical features of the amino acid oligomerization were studied. Growth model of the L-Glu monomer chain induced by the condensing agent in the aqueous solutions with and without metal ions was proposed. Computer simulation of oligomerization process was conducted and from the comparison of the calculated and experimental data attachment energy of the Leuchs anhydride of L-Glu to the oligomer was estimated.

1. Introduction

Protein molecules perform many key functions in living systems, including the catalysis of biochemical reactions, the transport of substances through the cell membrane, and the replication of DNA. From a chemical standpoint, proteins are linear polymers of amino acids linked in a chain via covalent bonds between nitrogen and carbon atoms, called peptide bonds. In 1953, the famous Miller-Urey experiment [1] demonstrated the synthesis of individual amino acid molecules from simple inorganic compounds under conditions simulating the atmosphere of ancient Earth. Since then, one of the main tasks has been the determination of the optimal physical and chemical conditions to ensure the effective formation of biological molecules from individual amino acids [2].

The equilibrium in the chain formation reaction of amino acids in aqueous media is strongly shifted towards individual monomers. However, studies have shown that even a concentrated NaCl solution could act as a dehydrating agent to facilitate the formation of amino acid oligomers [3]. In another model reaction, N,N'-carbonyldiimidazole (CDI) provided a more effective condensation reaction for amino acid synthesis [4]. The polymerization of amino acids could also be attained through COS volcanic gas, and the mechanism of this reaction is similar to CDI [5]. In a carbonyldiimidazole-mediated reaction, individual amino acids (nonactivated

monomers) interact with condensing agents to form an activated monomer (Leuchs anhydride) that reacts readily [4, 6]. Activated monomers are hydrolyzed in aqueous solution, that is, converted from an activated form to a nonactivated form [7].

The formation of oligomers of the amino acid L-Glu in aqueous solutions induced through sodium and potassium salts during the activation of growth with CDI condensing agent has been previously examined [8]. The results showed that dependence of the oligomer chain distribution in length n (n means the number of monomers in the oligomer) depends on the type of solution i (where $i = \text{Na, K, O}$ with sodium and potassium ions and without ions, resp.) and that the longest monomer chains are produced in aqueous solutions containing potassium ions.

The aim of the present study was to examine the oligomerization kinetics, identify the factors affecting the acceleration of chain growth, and calculate the distribution of oligomers in length.

2. Theoretical Methods

2.1. Growth Model. A distinctive feature of oligomers, that is, monomer chains, grown in aqueous solutions containing sodium or potassium ions, is the formation of "ion-nonactivated monomer" complexes ($1i$) and "ion-monomer chain" (ni) complexes, where n is the chain monomer length and i

is the ion index. Considering the excess metal ions observed during the growth of the monomer chains [9], we assumed that all monomer chains form complexes with metal ions.

The growth of a monomer chain occurs via the attachment of an activated monomer to “ion-nonactivated monomer” or “ion-monomer chain” complexes [6], and growth is determined by the probability of such an attachment. The energy of an activated monomer attachment to “ion-nonactivated monomer” or “ion-monomer chain” complexes depends on the type of ion i and does not depend on the length of the chain, as the energy of the dipole-dipole interaction (between the ion and the end of a chain or a monomer) rapidly decreases (as $1/r^6$, where r is the distance [9]), and, therefore, the following adjacent to the end monomers do not interact with sodium or potassium ions; that is,

$$E_{1i} = E_{ni}. \quad (1)$$

The duration of the activation process (when nonactivated monomers interact with the condensing agent) is a few minutes, whereas the duration of the growth of monomer chains is significantly longer (\sim hours) [8]. The hierarchy of various reaction durations suggests that monomer chain formation can be divided into two stages (index s): the activation stage ($s = A$) and the growth stage ($s = G$). This separation facilitates the use of the results obtained during the activation stage as initial conditions for the growth stage.

The monomer chain concentration dependencies on time are calculated by solving a system of balanced kinetic equations. This approach has been successfully and repeatedly used for studying the growth kinetics of various materials and systems [10–14]. Thus, the equations for characterizing each stage of monomer chain formation process are listed below.

Assumptions of the kinetic model are based on the experimental results of works [8, 15].

At the activation stage ($s = A$), the leading kinetic processes involve interactions between the condensing agent (concentration $C_{CA}(t)$), water (concentration $C_{WA}(t)$), and nonactivated monomers (concentration $C_{1A}(t)$), where t is the time. The reactions between condensing agent and nonactivated monomers result in the formation of activated monomers (concentration $\tilde{C}_{1A}(t)$).

During the growth stage ($s = G$), the basic kinetic processes involve the hydrolysis of activated monomers (concentration $\tilde{C}_{1G}(t)$) and the formation and growth of monomer chains in aqueous solutions without ions $i = O$ or “ion-monomer chain” complexes in aqueous solutions with metal ions $i = Na, K$ (concentration $C_{nG}(t)$).

The probability of the attachment of an activated monomer to the monomer chain, “ion-nonactivated monomer” or “ion-monomer chain” complexes (i.e., the probability to overcome the potential barrier), is represented as the following form:

$$\begin{aligned} p_{1i} &= e^{-E_{1i}/kT}, \\ p_{ni} &= e^{-E_{ni}/kT}, \end{aligned} \quad (2)$$

where k is Boltzmann’s constant and T is the temperature. As follows from the equality of the attachment energies (see (1)), the probabilities p_{1i} and p_{ni} are equal.

2.2. System of the Equations. The calculation of the monomer chain growth kinetics requires consideration of the activation stage ($s = A$). Thus, it is necessary to calculate the rates of all reactions occurring in the solution at this stage. Using the theory of reaction rates [10, 16], the frequency of the reaction $R_{jm}(t)$ between the reactants j and k (during stage s) can be represented as follows:

$$R_{jm}(t) = \alpha_{jm} (D_j + D_m) C_{js}(t) C_{ms}(t). \quad (3)$$

Here, α_{jm} is the parameter characterizing the distance and the angle of reactants interaction; D_j and D_m are diffusion coefficients; and $C_{js}(t)$ and $C_{ms}(t)$ are the concentrations of substances j and m , respectively.

Activation Stage ($s = A$). The reactants in this stage are monomers (1), condensing agents (C), and water (W) (indices j and k in (3)). The change (decrease) in the monomer concentration $C_{1A}(t)$ in time t reflects the interaction of these molecules with the condensing agent (concentration $C_{CA}(t)$):

$$\frac{dC_{1A}(t)}{dt} = -\alpha_{1C} (D_1 + D_C) C_{1A}(t) C_{CA}(t). \quad (4)$$

Here, α_{1C} is the parameter characterizing the distance and angle of interaction between the nonactivated monomer and the condensing agent (see above parameter α_{jm} , where $j = 1$ and $m = C$), and D_1 and D_C are the diffusion coefficients for the nonactivated monomers and condensing agents in the aqueous solution, respectively.

The concentration of the condensing agent $C_{CA}(t)$ decreases with time, reflecting interactions with monomers and water (concentration $C_{WA}(t)$) (see (3)):

$$\begin{aligned} \frac{dC_{CA}(t)}{dt} &= -\alpha_{1C} (D_1 + D_C) C_{1A}(t) C_{CA}(t) p_{1A} \\ &\quad - \alpha_{WC} (D_W + D_C) C_{WA}(t) C_{CA}(t). \end{aligned} \quad (5a)$$

Here, α_{WC} is the parameter characterizing the distance and interaction angle between the condensing agent and water molecules, and D_W is the diffusion coefficient of water molecules in the solution. As the water concentration, $C_{WA}(t)$, in the solution is considerably higher than that of the reactants, $C_{WA}(t) = \text{const}$, which means that $\alpha_{WC}(D_W + D_C) C_{WA} \equiv \beta_{WC} = \text{const}$. Introducing parameter β_{WC} into (5a) generates

$$\begin{aligned} \frac{dC_{CA}(t)}{dt} &= -\alpha_{1C} (D_1 + D_C) C_{1A}(t) C_{CA}(t) \\ &\quad - \beta_{WC} C_{CA}(t). \end{aligned} \quad (5b)$$

The rate of activated monomer formation, that is, changes in the concentration $\tilde{C}_{1A}(t)$ with time t , depends on the current concentrations of monomers and condensing agents in the solution:

$$\begin{aligned} \frac{d\tilde{C}_{1A}(t)}{dt} &= \alpha_{1C} (D_1 + D_C) C_{1A}(t) C_{CA}(t) \\ &= -\frac{dC_{1A}(t)}{dt}. \end{aligned} \quad (6)$$

The initial conditions in the activation process are as follows:

$$\begin{aligned} C_{1A}(t=t_0) &= C_1^0, \\ C_{CA}(t=t_0) &= C_C^0, \\ \bar{C}_{1A}(t=t_0) &= 0, \end{aligned} \quad (7)$$

where t_0 is the start of the growth process and C_1^0 and C_C^0 are the initial concentrations of nonactivated monomers and the condensing agent, respectively.

The rate of the attachment $R_{1n}(t)$ of the activated monomer to the “ion-nonactivated monomer” or “ion-monomer chain” complexes depends on probability p_{1i} and can be expressed as

$$R_{1n}(t) = \bar{\alpha}_{1n} (\bar{D}_1 + D_n) \bar{C}_{1G}(t) C_{nG}(t) p_{1i}, \quad (8)$$

where $\bar{\alpha}_{1n}$ is the parameter characterizing the distance and angle of interaction between the activated monomer and a monomer chain of length n , \bar{D}_1 is the diffusion coefficient of the activated monomers, and D_n is the diffusion coefficient of “ion-monomer chain” complex of length n .

The hydrolysis rate I_{1G} of nonactivated monomers can be expressed as [17]

$$I_{1G} = \gamma_G \bar{C}_{1G}(t), \quad (9)$$

where γ_G is the hydrolysis rate, that is, the number of conversions of the activated monomers into the nonactivated form in a unit time.

Growth Stage ($s = G$). In the growth stage, the concentration $C_{1G}(t)$ of monomers ($i = O$)/“ion-nonactivated monomer” complexes ($i = Na, K$) changes with time, reflecting the attachment of the activated monomers with concentration $\bar{C}_{1G}(t)$ and the transition of activated monomers into a nonactivated form (see (8) and (9)):

$$\begin{aligned} \frac{dC_{1G}(t)}{dt} &= -\bar{\alpha}_{11} (D_1 + \bar{D}_1) C_{1G}(t) \bar{C}_{1G}(t) p_{1i} \\ &+ \gamma_G \bar{C}_{1G}(t). \end{aligned} \quad (10)$$

Here, $\bar{\alpha}_{11}$ is the parameter characterizing the distance and the angle of interaction between monomer/“ion-nonactivated monomer” complexes and activated monomers.

The concentration $C_{nG}(t)$ of monomer chains ($i = O$)/“ion-monomer chain” complexes ($i = Na, K$) of length n decreases due to the attachment of the activated monomers and increases due to the attachment of the activated monomers to monomer chains of length $l = n - 1$:

$$\begin{aligned} \frac{dC_{nG}(t)}{dt} &= -\bar{\alpha}_{1n} (\bar{D}_1 + D_n) \bar{C}_{1G}(t) C_{nG}(t) p_{ni} \\ &+ \bar{\alpha}_{1l} (\bar{D}_1 + D_{n-1}) \bar{C}_{1G}(t) C_{lG}(t) p_{li}. \end{aligned} \quad (11)$$

Here, $\bar{\alpha}_{1n}$ is the parameter characterizing the distance and the angle of interaction between activated monomers and monomer chains/“ion-monomer chain” complexes of length n .

The concentration of activated monomers $\bar{C}_{1G}(t)$ in the growth stage decreases, reflecting the hydrolysis and attachment of these activated monomers to monomer/“ion-nonactivated monomer” and monomer chains/“ion-monomer chain” complexes:

$$\begin{aligned} \frac{d\bar{C}_{1G}(t)}{dt} &= -\gamma_G \bar{C}_{1G}(t) \\ &- \bar{\alpha}_{11} (D_1 + \bar{D}_1) C_{1G}(t) \bar{C}_{1G}(t) p_{1i} \\ &- \sum_{n=2}^N \bar{\alpha}_{1n} (\bar{D}_1 + D_n) \bar{C}_{1G}(t) C_{nG}(t) p_{ni}. \end{aligned} \quad (12)$$

The initial conditions at the growth process stage can be represented as follows:

$$\begin{aligned} C_1^0 &= \bar{C}_{1A}(t_A) + C_{1A}(t_A), \\ C_{nG}(t=t_A) &= 0, \quad n = 2, \dots, N, \end{aligned} \quad (13)$$

where t_A is the duration of the activation stage.

Simulation of the monomer chain formation was carried out by numerical solution of the system of the equations. Numerical solution was obtained within the finite difference approach [18]; in particular the Runge-Kutta-Fehlberg method was employed [19].

3. Results and Discussion

3.1. Estimation of Parameters. To calculate the growth kinetics of monomer chain formation, we solved the obtained system of equations for the physical quantities characterizing the activation ((4)–(7)) and growth ((10)–(13)) stages. Here, the solution of the system of kinetics equations for the activation stage represented the initial condition for the system of equations describing the growth stage. To calculate the growth process of monomer chains, it is necessary to estimate the values of the parameters in (4)–(7) and (10)–(13).

To estimate the diffusion coefficients of the condensing agent D_C , activated monomer \bar{D}_1 , and “ion-nonactivated monomer” D_1 and “ion-monomer chain” D_n complexes in the solution, the geometrical shapes of these molecules should be considered, as friction during molecule movement in the solution depends on the molecular surface area [20]. For simplicity, hereafter, we assume that the molecules of the condensing agent, an activated monomer, and “ion-nonactivated monomer” complexes have a spherical shape and that the molecules of monomer chains have a cylindrical shape. According to the results of a previous study [21], the diffusion coefficient of nonactivated monomers (glutamic acid molecules) in dilute aqueous solutions weakly depends on the concentration and the degree of dissociation of the monomers; with a 50-fold concentration change, the magnitude of the diffusion coefficient is changed 7.5%. Based

on this result, we assumed that the diffusion coefficient of nonactivated monomers does not substantially change during growth, and this value is equal to the experimentally measured value $D_1 = 0.6993 \text{ cm}^2 \text{ s}^{-1}$ at a glutamic acid concentration of 0.05 mol/L .

The diffusion coefficients of the condensing agent D_C and the activated monomer \tilde{D}_1 can be estimated using the Stokes-Einstein relation, according to which the diffusion coefficient of a spherical molecule with radius R in an aqueous solution can be represented as follows:

$$D = \frac{kT}{6\pi\mu R}. \quad (14)$$

Here, μ represents the solvent (water) viscosity.

The radius of a spherical molecule is expressed in terms of the volume V of the molecule:

$$R = \left(\frac{3V}{4\pi}\right)^{1/3}. \quad (15)$$

The volume V of the molecule is estimated as the sum of the atom volumes of its components, considering its structural features (the presence of amino and hydroxyl groups, etc.) [22]. The volume of the condensing agent (CDI) molecule in the aqueous solution is equal to 207 \AA^3 , and the volume of the activated monomer (Leuchs anhydride of L-Glu) is equal to 195 \AA^3 . Substituting the values of the molecule volumes of the condensing agent and the activated monomer in (14) and (15) and considering the viscosity of water $\mu = 1.002 \cdot 10^{-3} \text{ Pa}\cdot\text{s}$ at $T = 20^\circ\text{C}$ for the diffusion coefficients, the following equations can be obtained: $D_C = 0.58 \cdot 10^{-5} \text{ cm}^2 \text{ s}^{-1}$ and $\tilde{D}_1 = 0.59 \cdot 10^{-5} \text{ cm}^2 \text{ s}^{-1}$.

As mentioned above, monomer chains have a cylindrical shape, and the length of the chain consisting of n monomers is equal to $l_n = n \cdot l_1$ (where l_1 is the length of a single monomer) and radius $r_1 \approx 1/2l_1$. The diffusion coefficients of a cylindrically shaped molecule can be calculated as the diffusion coefficient of a molecule consisting of beads forming a cylinder [23]. The diffusion coefficient of each bead can be calculated according to the Einstein-Stokes relation (see (14)). Based on the results of a previous study [23], the diffusion D_n coefficient of an “ion-monomer chain” complex can be estimated as follows:

$$D_n = \frac{kT}{6\pi\mu r_1} \frac{\ln n + \gamma}{(2/3)^{1/3} n^{4/3}}. \quad (16)$$

Here, $\gamma(n) = 0.312 + 0.565/n - 0.1/n^2$.

In the first approximation, the parameter $\tilde{\alpha}_{1n}$, characterizing the distance and angle of interaction between the reactants, is estimated using the Smoluchowski approach [10, 16], as the product of the interaction distance between the reacting molecules on the solid angle at which this interaction $\tilde{\alpha}_{1n} \approx \tilde{r}_{1n}\tilde{\Omega}_{1n}$ is possible. Here, \tilde{r}_{1n} is the interaction distance between the activated monomer and an “ion-monomer chain” complex of length n ($n \geq 1$), and $\tilde{\Omega}_{1n}$ is the solid

angle in which the interaction between the molecules of an activated monomer and an “ion-monomer chain” complex is possible. In these equations, the interaction distance \tilde{r}_{1n} is equal to twice the length of the covalent bond formed when the activated monomer attaches to a monomer chain, $\tilde{r}_{1n} = 1.32 \text{ \AA}$ [24]. Assuming that the interactions between molecules are anisotropic and the “ion-monomer chain” complex is reactive over a circular patch lying in the solid angle $\tilde{\Omega}_{1n} = \pi$ for $\tilde{\alpha}_{1n}$, we obtained $\tilde{\alpha}_{1n} = 4.14 \text{ \AA}$. The value of β_{WC} in these calculations is equal to $\beta_{WC} = 4.04 \text{ s}^{-1}$ [25]. The duration t_A of the activation stage is 5 min, and the duration t_G of the growth stage is 1440 min (24 h). The values of γ_G and α_{1C} were estimated from the comparison of the theoretical and experimental chain length dependencies of the oligomer concentrations in the aqueous solution without ions.

3.2. Oligomerization Kinetics. We now turn to the calculation of the polymerization kinetics of the amino acid L-Glu. First, we calculated the oligomer growth kinetics of L-Glu in aqueous solution with condensing agent and without ions. As the growth stage is completed, the relative monomer chain concentrations C_{nG}/C_{2G} were calculated and compared with those obtained in a previous study [15]. The best fits of the experimental and theoretical chain length dependencies of the monomer chain concentrations were obtained for $\gamma_G = 3.3 \cdot 10^{-4} \text{ s}^{-1}$ and $\alpha_{1C} = 1.15 \cdot 10^{-18} \text{ cm}^3 \text{ s}^{-1}$; see Figure 1.

Considering the estimates of the parameters in (4)–(7) and (10)–(13), a simulation of the oligomer growth of L-Glu in aqueous solutions containing sodium or potassium ions was performed. Upon completion of the growth stage, the concentration ratios C_{nG}^K/C_{nG}^{Na} of the “ion-monomer chain” complexes with the identical length n in aqueous solutions with sodium and potassium ions were calculated and compared with the experimental concentration ratios $C_{nG}^{\text{expK}}/C_{nG}^{\text{expNa}}$ of the monomer chains [8]; see Figure 2.

The difference of the attachment energies $\Delta E_{\text{Na-K}} = E_{1\text{Na}} - E_{1\text{K}}$ estimated from the comparison of the theoretical and experimental data was approximately 0.02 eV . As shown in Figure 2, the enhancement of the oligomer formation in solution with potassium ions compared with the solution with sodium ions only occurred for oligomers with a length of $n \geq 4$. This enhancement reflects the competition of two processes: (i) elongation of the monomer chains due to attachment of the activated monomers to the “ion-nonactivated monomer” and “ion-monomer chain” complexes and (ii) elimination of the activated monomers through hydrolysis. The elongation of the monomers depends on the attachment rate $R_{1n}(t)$ (see (8)), which is higher in the solution with potassium ions because $E_{1\text{K}} < E_{1\text{Na}}$, whereas the hydrolysis rate $I_{1G}(t)$ (see (9)) is the same in solutions with potassium or sodium ions. Moreover, the hydrolysis of the activated monomers increases the number of dimers in the solution, as dimer formation occurs between the activated monomer and the “ion-nonactivated monomer” complex. Therefore, in the solution with potassium ions, the number of activated monomers attached to long monomer chains and the concentration of these monomer chains are higher than those in the solution with sodium ions.

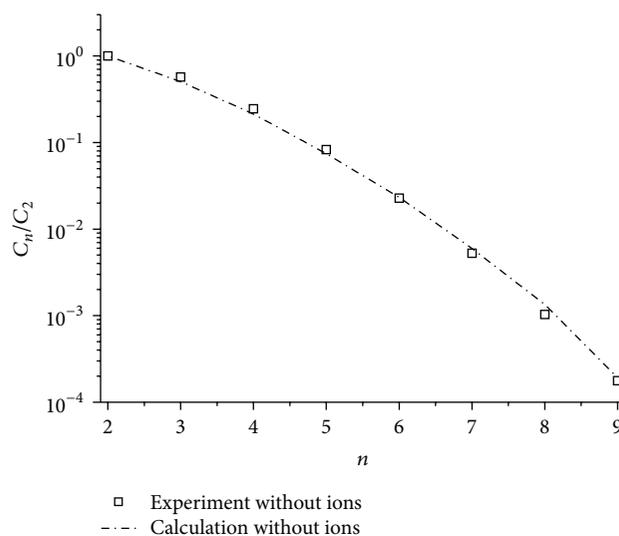


FIGURE 1: Experimental [11] and calculated dependencies of the relative concentrations C_n/C_2 of monomer chains of length n in the aqueous solution without ions.

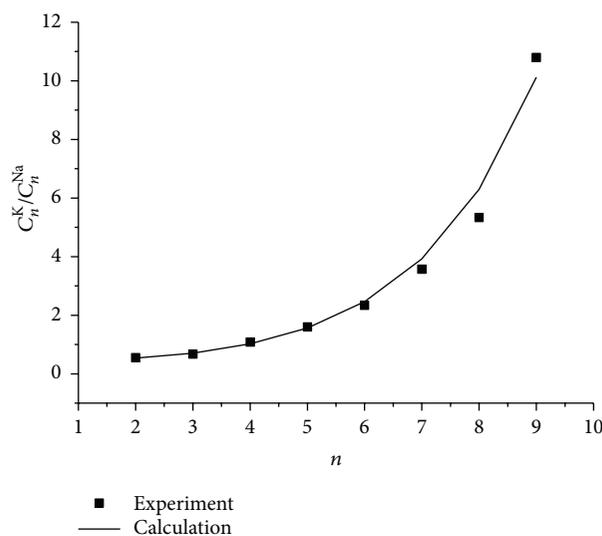


FIGURE 2: Experimental [8] and calculated dependencies of the concentrations ratio C_n^K/C_n^{Na} of monomer chains of length n in aqueous solutions with potassium and sodium ions.

4. Conclusion

A model of carbonyldiimidazole-mediated amino acid oligomer formation in aqueous solution containing sodium or potassium ions was developed. In this kinetic model, oligomer growth rate depends on the energy of the attachment of the activated monomer (Leuchs anhydride) to the monomer/“ion-nonactivated monomer” and monomer chains/“ion-monomer chain” complexes. The oligomer growth kinetics of the amino acid L-Glu in aqueous solutions without metal ions and with sodium or potassium ions was calculated. The values

of γ_G and α_{1C} were estimated through the comparison of experimental and theoretical data. Results of the computer simulation of the monomer chains formation kinetics showed that the longest monomer chains are formed in the solution with the potassium ions.

We showed that the higher rate of monomer chain formation observed in the solution containing potassium ions compared with the solution containing sodium ions reflects the difference ΔE_{Na-K} in the energies of the attachment of the activated monomers to the “ion-nonactivated monomer” and “ion-monomer chain” complexes. The energy difference,

$\Delta E_{\text{Na-K}}$, was estimated from the comparison of the experimental and theoretical data.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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