



NOTE

Dynamics of Water Molecules in Concentrated Aqueous Solution of D-Glucose

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The diffusion coefficient and dipole auto-correlation function of aqueous solution of α -D-glucose and β -D-glucose were investigated in the temperature range of 283-313 K. The results indicate that diffusion coefficient tended to be slightly different with each other between α -D-glucose and β -D-glucose aqueous solution, especially β -D-glucose aqueous solution, which due to different hydrogen bond distribution. Diffusion coefficients were reasonable proportional to the temperature. A clear description about dipole auto-correlation function was given to reveal the diffusion effect of hydrogen bond contribution.

Key Words: Diffusion coefficient, Hydrogen bond, Dipole auto-correlation function, Mutual diffusion.

The effects of simple sugars solute on living systems are quite important. It is useful and helpful to characterize the dynamics of water and simple sugars in understanding the biological solutes on water¹. In particular as a basic monomeric component of more complex sugars exist in life metabolism, D-glucose as one of the three well-known glass-forming sugars has attracted a wide attention, As a small monomeric which is smaller than biological macromolecules and larger than water molecule can protect living cell from cold or dry²⁻⁴. However, the understanding of various dynamic properties of aqueous solutions of D-glucose is yet not complete.

Mutual diffusion simulation can provide more direct information on molecule motions and has already been used in studying the dielectric properties of saccharide solutions and protein solutions. Smith *et al.*⁴ excellent work provide the evidence that response of the dynamics of glucose and water molecules to changes in sugar concentration and temperature with quasielastic neutron scattering QENS⁴. While Hochtl *et al.*⁵ have quantified the effect of glucose on the water relaxation process and scales directly connected to the H-bonding dynamics. Furthermore Ribeiro *et al.*⁶ and others^{7,8} gave a better understanding of transport properties by simulating binary mutual diffusion coefficients of sugar aqueous solutions.

In the present work we extend the studies by means of MD simulations to microcosmic aspect. Particular attention is addressed to characterization of dielectric dependent transport property and molecules of sugar aqueous solution.

Theory and methods: The simulations have been performed on the NVT ensemble with aqueous solution of D-

glucose in cubic boxes with periodic boundary conditions at temperature range from 283 to 313 K. The number of D-glucose (α -D-glucose and β -D-glucose) water molecules corresponding to Table-1.

TABLE-1
SOLUTE AND SOLVENT CONCENTRATION

Concentration	D-Glucose number	H ₂ O number
α -D-Glucose-H ₂ O	551	491
α -D-Glucose- H ₂ O	539	255
β -D-Glucose- H ₂ O	551	491
β -D-Glucose- H ₂ O	539	255

In each concentration, the box dimensions were chosen to match the simulation environment. Considering different concentrations of sugar aqueous solution have different properties can effect on aqueous solution.

Mean square displacement (MSD): According to Ito's model⁹, the high-frequency relaxation time τ_h in semi-dilute solution is given by

$$\tau_h \approx \frac{\xi^2}{6D}$$

where D is the diffusion coefficient of the counterions in solution in molecular simulation, mean square displacement (MSD) of molecules is thought as the second moment of their distribution when $t > 0$. MSD is related to the diffusion coefficient by the Einstein relation under long time simulation:

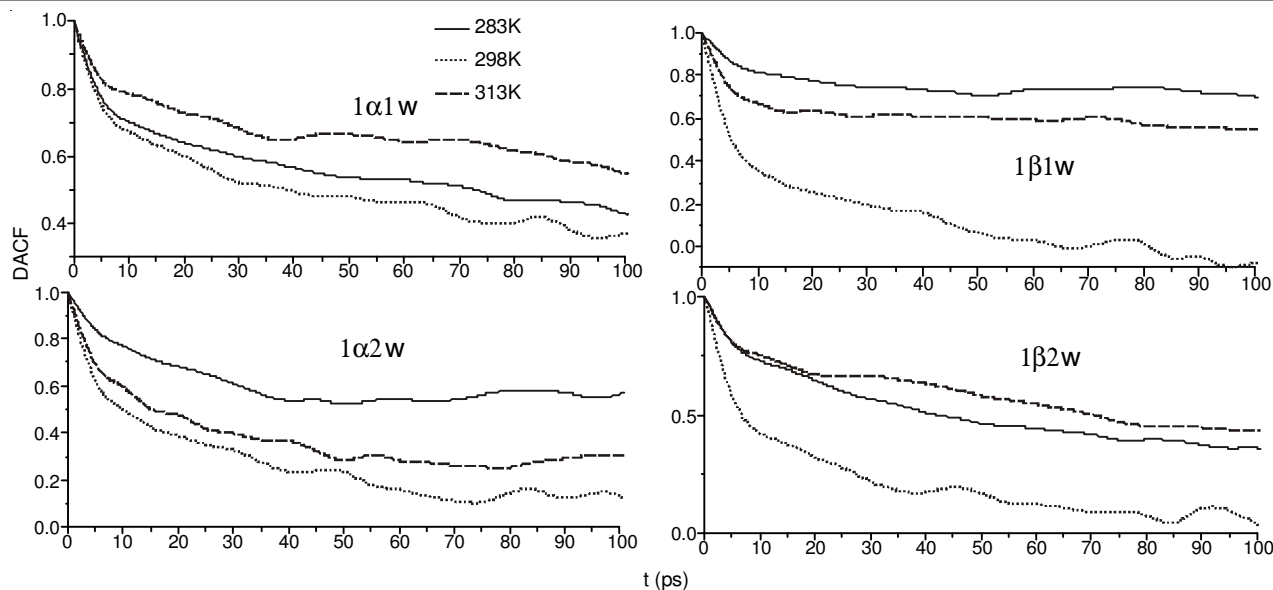


Fig. 1. D-Glucose dipole ACF

Concentration (K)	1 α 1w	1 α 2w	1 β 1w	1 β 2w
283 K	1.081	0.627	1.149	1.7518
298 K	1.420	0.973	1.300	1.1037
313 K	1.748	2.188	1.609	0.7277

$$D_i = \frac{1}{6} \lim_{t \rightarrow \infty} \frac{d}{dt} \left\langle \sum_{i=1}^N [r_i(t) - r_i(0)]^2 \right\rangle$$

where $r_i(t)$ is the location of the center of mass of particle i at time i . While

$$\text{MSD} = \frac{1}{N} \left\langle \sum_{i=1}^N [r_i(t) - r_i(0)]^2 \right\rangle = \Delta + r(t)l^2$$

We can get diffusion coefficient by calculating the slope of the MSD and divided by six. The diffusion coefficient was also calculated using the velocity autocorrelation function.

$$D = \int_0^{\infty} \frac{1}{3N} \sum_{i=1}^N \langle \vec{V}_i(t) - \vec{V}_i(0) \rangle dt$$

where $V_i(t)$ denotes the velocity of particle i at time t .

Diffusion coefficient: It can be seen that most of simulated diffusion coefficient of molecules increases slowly with the temperature increasing in D-glucose aqueous solution and some distributes irregularly especially at molecule ration 1 to 2 in β -D-glucose aqueous solution, which provide transport data necessary to model the diffusion for various chemical and pharmaceutical applications.

Dipole autocorrelation function: A comparison of the molecules dipole ACF at different concentrations and temperature is considered, as seen in Fig. 1. We can see from the two figures glucose molecules dipole ACF line styles are not relatively smooth. This indicated the hydrogen bond net structure enhance interaction between water and glucose molecules, which make behave differently compared to waters further

away "bulk water" and concentration dependent dielectric relaxation time change obviously with temperature, which shows the evidence that relaxation time, is strongly effected by hydrogen bond in ps scale.

Conclusion

This work is based on different concentrated D-glucose aqueous solutions to reveal the microcosmic structure and dynamic features. The results indicate that diffusion coefficient tended to be slightly different with each other between α -D-glucose and β -D-glucose aqueous solution, especially β -D-glucose aqueous solution, which is due to different hydrogen bond distribution induce the irregular dielectric relaxation. So MD simulation gives a better understanding of the thermodynamic and dielectric dependent transport properties of the important carbohydrates in aqueous solutions.

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