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Theoretical and experimental study on the evolution of xanthan gum inter/intramolecular forces with temperature, around the phase transition point

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Abstract

Here, we investigate experimentally and theoretically the conformational transition of the natural polymer xanthan gum (XG) solution. Densities of dilute aqueous solutions of the xanthan were accurately measured in the temperature range of 20-60 ^{o}C. The plot of densities versus concentrations shows three different behaviors of XG solutions at 20-30, 35-45, and 50-60 ^{o}C, which may be attributed to the order-disorder conformational transition. Fluorescence studies of the interaction of XG solution with the protein human serum albumin (HSA) at 26, 30, 37, and 42 °C show anomalous behavior at 37 °C, implying XG structural change. The molecular realization of these behaviors was appealed by an MD simulation study of the xanthan solvation in water. Wherein, three different conformational variables; one at the backbone of β-1,4-D-glucopyranose glucan linkage and two at the side chain of mannose (β-1,4) and glucuronic acid (β-1,2) linkages were defined, and computed after equilibrium and at the last 60 ns as well. Results corroborate the conformational anomalous changes around 36℃. Also, DFT calculations of standard change of the thermodynamic functions verify a sudden fluctuation in standard heat capacity changes from 36℃. These findings are along with that reported in this work for measured viscosity is evaluated and also in the literature that proposes a conformational change of the xanthan from the same temperature. Finally, the use of conformational temperature tuning, as an effective drug delivery approach, was presented. It was shown that the combination of xanthan in the complex with the anti-diabetic drug metformin is the most stable at normal body temperature.

Keywords: xanthan gum, order-disorder transition, temperature tuning, drug deliver, Fluorescence, polysaccharide