



## The microscopic structure of cold aqueous methanol mixtures

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Auteur	Pozar, Martina [1], Kerasidou, Ariadni P. [2], Lovrinecic, Bernarda [3], Zoranic, Larisa [4], Mijakovic, Marijana [5], Primorac, Tomislav [6], Sokolic, Franjo [7], Teboul, Victor [8], Perera, Aurélien [9]
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Résumé en anglais	<p>The evolution of the micro-segregated structure of aqueous methanol mixtures, in the temperature range 300 K-120 K, is studied with computer simulations, from the static structural point of view. The structural heterogeneity of water is reinforced at lower temperatures, as witnessed by a pre-peak in the oxygen-oxygen structure factor. Water tends to form predominantly chain-like clusters at lower temperatures and smaller concentrations. Methanol domains have essentially the same chain-like cluster structure as the pure liquid at high concentrations and becomes monomeric at smaller ones. Concentration fluctuations decrease with temperature, leading to quasi-ideal Kirkwood-Bu integrals, despite the enhanced molecular interactions, which we interpret as the signature of non-interacting segregated water and methanol clusters. This study throws a new light on the nature of the micro-heterogeneous structure of this mixture: the domain segregation is essentially based on the appearance of linear water clusters, unlike other alcohol aqueous mixtures, such as with propanol or butanol, where the water domains are more bulky.</p>
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### Liens

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