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VABILO NA PREDAVANJE
V OKVIRU DOKTORSKEGA ŠTUDIJA
KEMIJSKE ZNANOSTI / INVITATION TO THE
LECTURE WITHIN DOCTORAL PROGRAMME IN
CHEMICAL SCIENCES

Prof. Enrique Lomba

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z naslovom / title:

**Anomalous behaviour of dilute short-chain
alcohol solutions**

v sredo, 19. 1. 2022 ob 15:00 uri /

on Wednesday, 19. 1. 2022 at 15:00

preko spletnega orodja Zoom / via Zoom:

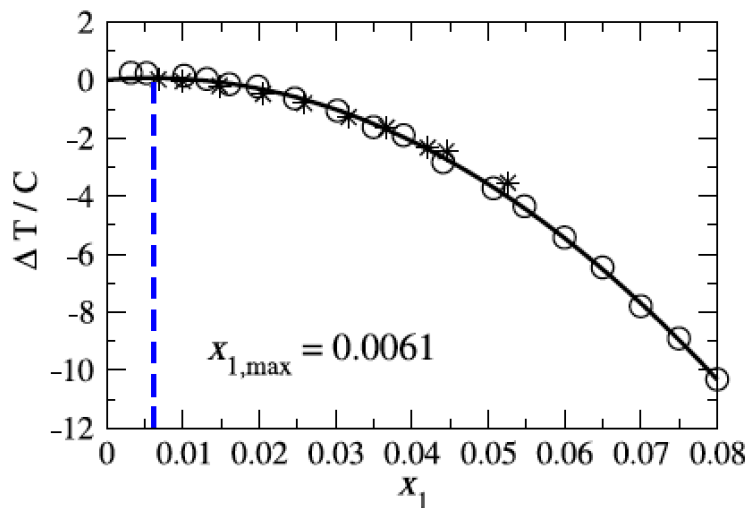
<https://us06web.zoom.us/j/4890013416?pwd=UDl2bTgzM0wvTXREb2lNYlUvOUYvZz09>

(Meeting ID: 489 001 3416, Passcode: gyNg5n)

Vljudno vabljeni! / Kindly invited!

Abstract:

The presence of structural, thermodynamic, and dynamics in water, lies at the core of its importance in biological processes. Among these anomalies, the presence of a temperature of maximum density at constant pressure —4C at 1 bar— is perhaps the most well known, and it is key to the preservation of life in surface frozen lakes and seas. In parallel, dynamic anomalies can be found, such as the counterintuitive increase of self-diffusion when pressure is increased. Interestingly, some of this anomalies can be enhanced in the presence of very small amount of short chain alcohols^{1,2}, a feature unique to these substances that is not shared by other polar or non-polar solutes. For this reason, dilute short-chain alcohols are said to act as ‘structure-builders’ in water. Common sense indicates that the influence of alcohol groups on the hydrogen bond structure of water should be at the core of these behaviour, In this presentation, we will review recent studies³ on this relatively old but unsolved problem, presenting new experimental results, together with computer simulations using both realistic and simplified models, in an attempt to elucidate the different factors at play in the ‘structure-builder’ role of short-chain alcohols.



Wada, G. & Umeda, S., Effects of Nonelectrolytes on the Temperature of the Maximum Density of Water, 1*Bull. Chem. Soc. Jpn.*, **1962**, 35, 646 - 652 Harris, K. R. & Newitt, P. J., Diffusion and Structure in Dilute Aqueous Alcohol Solutions. *J. Phys. Chem. B*, **21998**, 102, 8874 - 8879 M. S. Marques, E. Lomba, E. G. Noya, D. González-Salgado, and M. Barbosa, “Modeling the temperature of 3maximum density of aqueous tert-butanol solutions,” *Physica A*, **2021**, 582, 126243.