

# Typical at glance but interesting when analyzed in detail: The story of Tris hydration

V.N. Agieienko, V.V. Nekhlyudov, R. Buchner

<sup>1</sup>Nanotechnology and Biotechnology Department, Nizhny Novgorod State Technical University n.a. R.E. Alekseev, 24 Minina str., 603950 Nizhny Novgorod, Russian Federation

<sup>2</sup>Wolfson Department of Chemical Engineering, Technion - IIT, Haifa 32000, Israel

<sup>3</sup>Institut für Physikalische und Theoretische Chemie, Universität Regensburg, Universitätsstraße 31, D-93040 Regensburg, Germany

vira.agieienko@gmail.com

Tris (2-amino-2-hydroxymethylpropane-1,3-diol), a well-known buffer component, has been recently considered as a promising absorbent in wet-CO<sub>2</sub> absorption technology [1]. A 30% Tris solution in water exhibits a CO<sub>2</sub> absorbing capacity comparable to aqueous monoethanolamine of the same concentration [2]. In addition, Tris is a cheap, non-toxic, non-volatile and non-flammable substance, which allows overcoming significant disadvantages of liquid amines commonly used in the industrial CO<sub>2</sub> sequestration cycles.

In the present work we show the results of dielectric relaxation spectroscopy of aqueous Tris solutions covering concentrations up to its solubility limit ( $c \approx 3.3 \text{ mol dm}^{-3}$ ) and frequencies from 50 MHz to 89 GHz. We show that the dielectric spectra can be best fit by a sum of 1 Cole-Cole and two Debye modes arising from the solute- and solvent-associated relaxations, respectively. The analysis of the amplitudes reveals that a Tris molecule is hydrated by  $\sim 7$  H<sub>2</sub>O molecules over the entire concentration range. Indeed, hydrodynamics friction coefficients extracted from Tris reorientation times indicate rather strong interactions between the solute and its near solvent surrounding. However, according to the size and structure of a Tris molecule and taking into account hydration patterns of previously studied solutes [3-5] it is very unlikely that all 7 H<sub>2</sub>O molecules interact with Tris stronger than with each other. To get more information on the type of solute-solvent and solvent-solvent interactions in the Tris/water system, the dielectric spectra were described by a superposition of 4 Debye relaxations with the slowest mode arising from reorientation of the solute, the second slowest from dynamically retarded hydration water and the two fastest modes assigned to bulk (rather unperturbed) water. Analysis of the data within the framework of this model indicates that although Tris indeed slows down  $\sim 7$ -8 H<sub>2</sub>O molecules their interaction strength with the solute is rather weak compared to their inherent H-bonds. Additionally, the results of quantum chemical calculations performed in the spirit of the step-by-step thermodynamics of hydration strongly support the findings of dielectric spectroscopy.

The present research was funded by the Russian Science Foundation (project no. 22-23-00913).

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