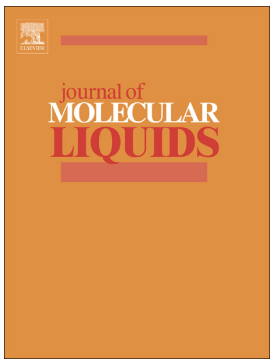

Aqueous solutions of NMA, Na2HPO4, and NaH2PO4 as models for interaction studies in phosphate–protein systems

Karol A. Biernacki, Emilia Kaczkowska, Piotr Bruździak

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Aqueous solutions of NMA, Na_2HPO_4, and NaH_2PO_4 as models for interaction studies in phosphate–protein systems

Karol A. Biernacki, Emilia Kaczkowska, Piotr Bruździak[☆]

Department of Physical Chemistry, Gdańsk University of Technology, Narutowicza 11-12, 80-233 Gdańsk, Poland

Abstract

Phosphate buffers are essential for many areas of studies. However, their influence on buffered systems is often ignored. The phosphate salts can interact with biologically important macromolecules (e.g. proteins) and stabilize or destabilize them. With our research, we want to answer question what kind of interactions, if any, occur between phosphate ions and a protein backbone model – *N*–methylacetamide (NMA). ATR–FTIR spectroscopy in the amide I range and in the regions characteristic for P–O vibrations provides information on direct and indirect (water–mediated) interactions. The analysis is supported by chemometric, DFT, and QTAIM calculations. Our results indicate that direct NMA–phosphate ion interactions are quite rare and indirect. Water molecules seem to play an important role in such systems. The model studies indicate that no preferential interactions between NMA and phosphate ions in solutions are formed, and may imply that such interactions are also unfavorable in protein–based systems.

Keywords: Phosphates, *N*-methylacetamide, Hydration, FTIR, DFT, QTAIM

1. Introduction

The constant pH of a solution is extremely important in many areas of chemistry, biology and physics. A simple way to stabilize it is to use buffers.

[☆]Corresponding author: *piotr.bruzdziak@pg.edu.pl*