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Abstract Book

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Experimental measurements of thermophysical properties and theoretical quantum chemical calculations of alcohol and hydrocarbon binary systems

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Thermophysical properties of alcohol and hydrocarbon systems: experimental and modeling

Insight in different types of mixtures' behavior (such as volumetric and transport properties, and related excess properties) has high importance [1]. These properties depend on the intermolecular interactions between molecules in liquid phase. The theoretical aspect can quantitatively and accurately model the non-covalent interactions using the quantum mechanical methods. In theoretical modeling of interaction energies, a benchmark study of quantum mechanical methods is an essential step [2]. So far, we have studied the interactions of double and single bonds and interactions between two double or two single bonds on a model system of 2-butene and n-butane molecules [3]. The results provide the insights of interactions at molecular level, offering an understanding of experimental measured properties of substances and mixtures with double bonds.
The aim of this work is to investigate experimental volumetric and transport properties and their deviations from ideal mixtures and use the computational modeling for analyzing the same effects on deviations at molecular level for the mixtures containing alcohols and hydrocarbons. The combination of experimental measurement and computational modeling is the future in predicting chemical processes in systems and mixtures, providing better and more complete information on properties and chemical processes.

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DISCLOSING THE INTERACTIONS OF FLUORINATED IONIC LIQUIDS WITH THERAPEUTIC PROTEINS

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Therapeutic proteins are of great importance in the pharmaceutical market as natural biological products to therapy of several diseases. The application of therapeutic proteins has been hindered because they are very instable, dependent of the environmental conditions and poor bioavailability due to the short half-life in the blood stream, among others. Therefore, the necessity of new drug delivery systems (DDSs) capable to solve these drawbacks by time-controlled and site-specific delivery and protection of the protein are of great urgency in the biomedical field.(1)

Fluorinated Ionic Liquids (FILs) have been pointed out as an efficient solution to formulation of new DDSs, because they can be designed to have unique properties such as total miscibility in water; improved surfactant power due to their amphiphilic behaviour, allowing the formation of self-assembled aggregates in aqueous systems; and they can have low acute ecotoxicity in aquatic organisms and negligible cytotoxicity in human cell lines.(1) However, scarce information regarding the interactions of FILs with proteins is known, which is of vital importance in order to demystify the mechanisms related to conformational stability and activity of therapeutic proteins and of the FILs structuration of in aqueous solution.

In this work, the interactions between FILs and two therapeutic proteins, interferon-alpha2b (IFN-α2b) and lysozyme (LYS), will be investigated. The thermophysical and thermodynamic properties, as well as, FILs structural features will be studied experimentally and by soft-SAFT equation of state (2) to select the FILs with the best characteristics for this application. Thus, the cytotoxicity of the selected FILs will be determined in two different human cell lines, underlining the suitability of these FILs in the biomedical field. The conformational stability and the binding affinity of IFN-α2b and/or LYS in the presence of different FILs, will be disclosed by differential scanning fluorimetry (DSF) and isothermal titration calorimetry (ITC), respectively. The interactions between FILs and proteins will be studied through Fourier-transform infrared spectroscopy (FTIR) and circular dichroism (CD) spectroscopy by the determination of possible modifications in the secondary structure of IFN-α2b and/or LYS that can occur in the presence of FILs in different concentrations. Finally, the activity of IFN-α2b and/or LYS will be tested in order to verify that FILs do not affect their biological activity.

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