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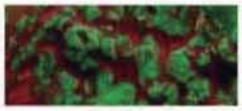

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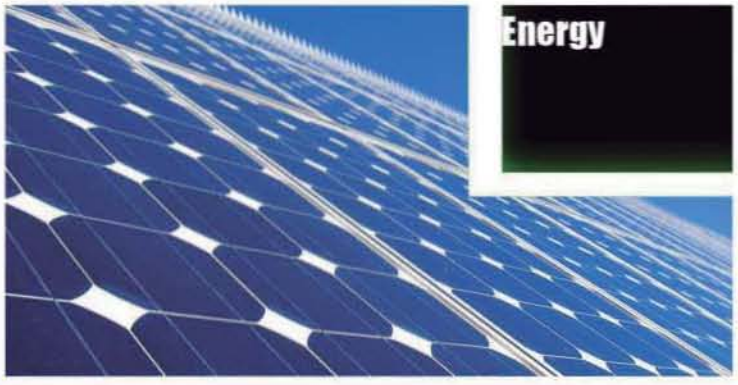

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The cation effect on the aqueous solubility of amino acids in the presence of salts: experimental and molecular dynamics simulation studies

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Aiming at contributing to the understanding the molecular-level mechanisms governing the behavior of biocompounds in aqueous saline environments, experimental solubility measurements and molecular dynamics (MD) simulations were performed for aqueous solutions of three amino acids (alanine, valine and isoleucine) in the presence of a series of inorganic salts.

I. INTRODUCTION

The study of the solubility behavior of amino acids and proteins in aqueous electrolyte solutions is crucial for the development of many areas of biochemistry and life sciences. Although the effect of common salts on the aqueous solubility of amino acids and proteins is phenomenologically well described [1], the underlying molecular-level mechanisms are far from being elucidated. Aiming at further understanding the molecular interactions governing the behavior of these systems, experimental solubility measurements and MD simulation calculations were performed in this work for aqueous solutions of alanine (Ala), valine (Val) and isoleucine (Ile), in the presence of $MgCl_2$, $MgSO_4$, NH_4Cl and $(NH_4)_2SO_4$, at T=298.15 K and different concentrations. By the combined analysis of the thermodynamic data and of the radial distribution functions (RDF) of the various groups and moieties, insight into the interactions established in solution will be provided.

II. METHODS

A. Experimental

The solubility experiments were carried out using the analytical isothermal shake-flask method. The gravimetric method was used for the quantitative analysis.

B. MD Simulations

The isothermal-isobaric NpT (T=298.15 K and p=1 bar) ensemble and the GROMACS 4.0.4 molecular dynamics package [2] were used to carry out the simulations. Potentials available in the literature were used for all the species considered in the simulations.

III. RESULTS AND DISCUSSION

The results obtained for the solubilities of the amino acids are depicted in Tables I and II.

Table I
Amino acid Solubility (g/kg water) in NH_4Cl aqueous solutions at T=298.15K

NH_4Cl Molality	Ala	Val	Ile
0.00	165.44	58.449	34.756
0.25	-	-	36.419
0.50	169.90	60.910	36.722
1.00	172.04	61.010	36.554
2.00	175.88	60.608	35.764

Table II
Valine Solubility (g/kg water) in $(NH_4)_2SO_4$ aqueous solutions at T=298.15K

$(NH_4)_2SO_4$ Molality	Val
0.00	-
0.25	59.629
0.50	57.941
1.00	51.921
2.00	39.947

The RDFs calculated from the MD simulations suggest that: (i) in NH_4Cl solutions, the association of the ammonium ion to the non polar moieties of the amino acids is significant, being the strongest interactions established with the carbon atoms which are closer to the charged groups of the biomolecules; (ii) in $(NH_4)_2SO_4$ aqueous solutions, the interactions of NH_4^+ with the alkyl carbon atoms of the amino acids are strong, but the binding to the least polar groups is less significant and occurs at larger distances; (iii) in $(NH_4)_2SO_4$ aqueous solutions, both SO_4^{2-} and NH_4^+ are surrounding the carbon atoms of the amino acids, but the later is more likely to occur in a second solvation layer, establishing interactions probably mediated by the cation.

REFERENCES

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