Title: On the solubility and miscibility of carboxylic acids in water through transferability and torsional potentials

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Abstract:
Torsional interactions are critical in some molecular structures, as they directly influence specific physicochemical properties such as water solubility and dielectric constant, through cis/trans conformational mixtures. The present study examines the effect of the rotational potential on the miscibility and solubility of carboxylic acids. A set of liquid and solid acids (butyric, BA; propionic, PA; succinic, SA; adipic, AdA; and azelaic, AzA), were selected to evaluate their water solubility using molecular dynamics (MD) simulations and the TIP4P/$\ epsilon$ water model. Following the assessment of a typical force field (OPLS-AA-LIGPARGEN), united atom models were generated through the transferability of the interaction parameters from acetic acid, derived from the previously reported 4-Step Systematic Parameterization Procedure (4SSPP). Systematic control of the rotational potential barrier, together with parameter transferability, demonstrates that this methodology accurately reproduces the experimental solubility of these organic acids in good agreement with available data.

Biography:

Dr. Edgar Núñez Rojas is a Researcher for Mexico form SECIHTI at Departamento de Química in the Universidad Autónoma Metropolitana Iztapalapa in Mexico City, Mexico. With expertise in development of force fields of molecules applied in extraction of contaminants, energy storage devices, cocrystals used to transport drugs and solvents used in important applications in industry where molecular dynamics is a key methodology to generate knowledge. Edgar has developed in his research group a re-parameterization methodology capable to generate interaction parameters useful to reproduce mixture properties (the 4SSPP fouth step systematic procedure to parametrize). Such method has been applied in the extraction of N- and S- aromatic compounds, the development of electrolytes of energy storage devices, optimal interaction parameters of cocrystals useful to carry drugs, etc. Actually is interested in the generation of a mexican united atom force field with reliable interaction parameters capable to be applied in complex issues of science and industry. Also, he is involved in the development of a an automated process to apply the 4SSPP and generate optimal interaction parameters for any molecular system.