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Designing new green alternatives to petroleum-based solvents using COSMO-RS 3D-mapping

AUTHORS

Théophile GAUDIN / DASSAULT SYSTÈMES BIOVIA, 334, 335 CAMBRIDGE SCIENCE PARK RD, IMPINGTON, MILTON, CAMBRIDGE
Corresponding author : Jean-Marie AUBRY / jean-marie.aubry@univ-lille.fr

PURPOSE OF THE ABSTRACT

Finding a suitable solvent to dissolve, extract, disperse or precipitate various solutes is a key step in broad areas of industrial chemistry. In the context of improving the sustainability of chemical processes, the replacement of hazardous petro-based solvents (halogenated, aromatics, glycol ethers, DMF, NMP ...) by safer solvents derived from renewable raw materials has become a major challenge in recent years.

In 1967, Hansen designed the most popular method to select solvents as an extension of Hildebrand's theory of regular solutions to polar compounds. It is based on the old principle of alchemists "like dissolves like" which is still well accepted by most contemporary chemists. According to Hansen, any solvent may be positioned in a 3D space by a point whose coordinates correspond to the 3 partial solubility parameters (delta_d, delta_p, delta_h) which respectively express the ability of a solvent to interact with solutes through dispersive, polar and hydrogen-bond interactions. Solutes are in turn defined by a sphere including most of the "good" solvents and excluding others. According to Hansen's approach, any solvent, pure or in mixture, located inside the sphere is supposed to effectively dissolve (or disperse) the solute (or the particle) [1]. Because of its simplicity and relative efficiency, this 3D representation of solvents and solutes is often used in industry as a qualitative guide to find solvents capable of dissolving or dispersing the compound under study. Unfortunately, the hydrogen-bond parameter delta_h does not differentiate between the hydrogen-bond donor and acceptor abilities of organic compounds, which can create an "opposites attract" solute-solvent interaction.

The more sophisticated COnductor-like Screening MOdel of Realistic Solvation (COSMO-RS) model combines quantum chemistry and statistical thermodynamics allowing the estimation of a wide range of molecular properties in the liquid state from knowledge of the molecular structure [2], thus making a priori description of the solvent behaviour [3]. In particular, it is able to handle the two main mechanisms of solubilisation (similarity and complementarity) to quantitatively predict the solubility of any molecular compound in a given solvent. Unfortunately, COSMO-RS in its current form does not provide a graphical representation that would easily show whether a given solvent (or solvent mixture) has solubilizing properties close to a target solvent. To fill that gap, we performed a COSMO-mapping of organic solvents in a 3D-space while striving to reflect their main characteristics. In this space, each solvent is positioned according to its dispersive energy density (Z axis) and its ability to donate or accept hydrogen bonds (X and Y axes). In this contribution, we show how COSMO-mapping makes it possible to effectively find green solvents as substitutes for banned or controversial petro-based solvents.

FIGURES

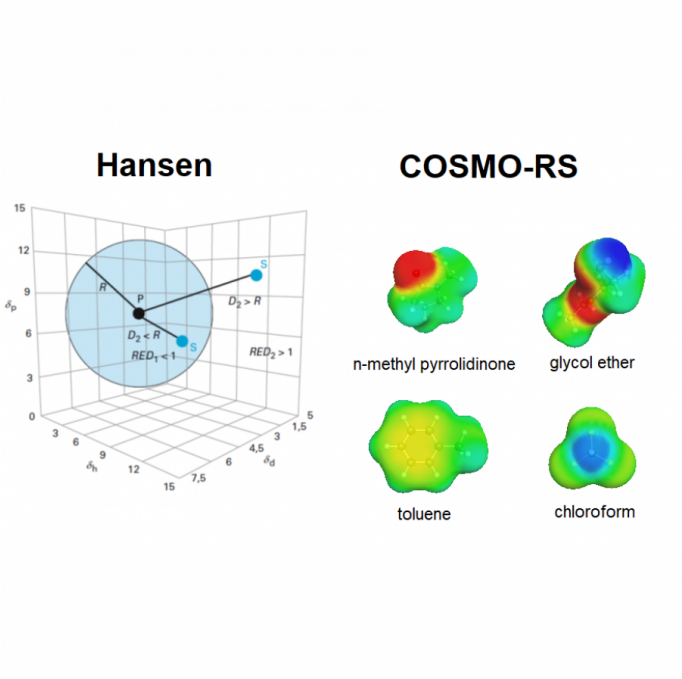

FIGURE 1

Hansen / COSMO-RS

left: Hansen solubility parameters space; right: COSMO surfaces of a few solvents.

FIGURE 2

KEYWORDS

sustainable solvents | COSMO-RS | Hansen Solubility Parameters | substitution

BIBLIOGRAPHY

[1] Hansen C. M., Hansen Solubility Parameters: A User Handbook (2007), Taylor & Francis, 2nd ed.

[2] Klamt, A. COSMO-RS: From Quantum Chemistry to Fluid Phase Thermodynamics and Drug Design (2005), Elsevier.

[3] Moity L., Durand M., Benazzouz A., Pierlot C., Molinier V., and Aubry J.-M., Panorama of Sustainable Solvents using the COSMO-RS approach, Green Chem. (2012), 14, 1132-1145.