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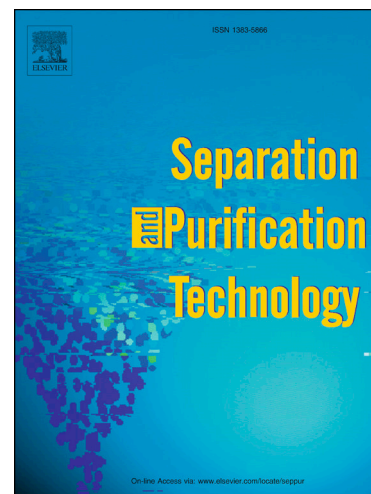
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Emilio J. González, Ismael Díaz, Maria Gonzalez-Miquel, Manuel Rodríguez, Adrián Sueiras

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On the behavior of imidazolium versus pyrrolidinium ionic liquids as extractants of phenolic compounds from water: experimental and computational analysis

Emilio J. González^{a*}, Ismael Díaz^a, Maria Gonzalez-Miquel^{a,b}, Manuel Rodríguez^a, Adrián Sueiras^a,

^a*Departamento de Ingeniería Química Industrial y del Medioambiente, Universidad Politécnica de Madrid, E-28006 Madrid, Spain*

^b*School of Chemical Engineering and Analytical Science, The University of Manchester, Manchester M13 9PL, United Kingdom*

* To whom correspondence should be addressed. Tel.: +34 913 365 341

E-mail address: ej.gonzalez@upm.es (Emilio J. González).

Abstract

The main goal of this work is to compare the ability of aromatic and non-aromatic ionic liquids (ILs) as potential solvents to extract phenolic compounds from aqueous systems. Although these liquid salts have been widely studied in the separation of organic compounds, especially aromatic hydrocarbons such as benzene, toluene, ethylbenzene, and isomer xylenes, their application to separate phenols from wastewater is still much less widespread. For that reason, in this work, the extraction efficiency of phenolic compounds in molecular form (phenol, *o*-cresol, and resorcinol) from water using non-aromatic (1-hexyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide, [HMpyr][NTf₂]) and aromatic (1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, [HMim][NTf₂]) ILs was analyzed and discussed. Firstly, the optimal operating conditions (stirring and settling time, and phase

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