

**A high throughput method to determine selectivity of ion phase transfer in multi- component chemical systems: towards predictive modelling of extraction**

Johannes Theisen, Julien Rey, Christophe Penisson, Jean Duhamet, Véronique Dubois, Nicolas Verplanck, Olivier Diat, Stéphane Pellet-Rostaing, Jean-Francois Dufrière, Daniel Meyer, et al.

► **To cite this version:**

Johannes Theisen, Julien Rey, Christophe Penisson, Jean Duhamet, Véronique Dubois, et al. A high throughput method to determine selectivity of ion phase transfer in multi- component chemical systems: towards predictive modelling of extraction. PACIFICHEM, Nov 2015, Honolulu, Hawaii, United States. 2015, <<http://www.pacificchem.org/>>. <cea-01555685>

**HAL Id: cea-01555685**

**<https://hal-cea.archives-ouvertes.fr/cea-01555685>**

Submitted on 4 Jul 2017

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

A high throughput method to determine selectivity of ion phase transfer in multi-component chemical systems: towards predictive modelling of extraction

Johannes Theisen, Julien Rey, Christophe Penisson, Jean Duhamet, Véronique Dubois, Nicolas Verplanck, Olivier Diat, Stéphane Pellet-Rostaing, Jean-Francois Dufrêche, Daniel Meyer, Helmuth Möhwald, Jean-Christophe Gabriel, Thomas Zemb

Institut de Chimie Séparative de Marcoule

ICSM UMR5257 CEA/CNRS/UM/ENSCM

F30207 Bagnols-sur-Cèze Cedex

Liquid-liquid extraction is a crucial process for recycling chemistry. In order to reuse and to avoid mining of rare earths, recycling has often to be performed by separating and purifying the rare earths from iron. This known technology relies on ion equilibria in coexisting phases located between binodal tie-lines in the Winsor II regime of a microemulsion with excess brine. Since the systems contain ten components, the phase diagram in seven dimensions must be projected in tetrahedron.

The selectivity and differences of free energy of transfer can be determined with good reliability and with reasonable time: days instead of months needed by batch methods. Availability of data with variable composition allows to challenge the very few predictive models based on first principles and evaluating the free energy of transfer terms.

We show here first results obtained with a micro-fluidic device allowing continuous exploration of lines in a complex phase diagram. We model the ion and extractant distribution and separation, and compare to expected values from available theories. Finally we discuss how to further speed up the process by electroacoustic fields.