Electronic Supplementary Information for: The role of curvature effects in liquid-liquid extraction: Assessing organic phase mesoscopic properties from MD simulations

Magali Duvail,*[a] Steven van Damme,[a], Philippe Guilbaud[b], Yushu Chen[a], Thomas Zemb[a] and Jean-François Dufrêche[a]

S1 MD simulations

S1.1 Ions and water molecules

12-6 Lennard-Jones (LJ) parameters used for La^{3+} and NO_3^- ions are described elsewhere[1]. Water molecules were described by the rigid POL3 model[2,3], which takes into account the polarization. All the parameters for La^{3+}, NO_3^-, and H_2O are given in Table S1.

Table S1 Parameters used for describing La^{3+}, NO_3^- and H_2O by molecular dynamics simulations using explicit polarization.

Atom	ε_{ii}[a]	σ_{ii}[b]	q_i[c]	α_i[d]
La^{3+}	0.272	3.564	+3.000	1.134[e]
O_{H_2O}	0.653	3.204	-0.730	0.528
H_{H_2O}	0.000	0.000	+0.365	0.170
$N_{NO_3^-}$	0.711	3.250	+0.896	0.530
$O_{NO_3^-}$	0.880	3.066	-0.632	0.434

[a] in kJ mol^{-1}. [b] in Å. [c] Partial atomic charge (in e). [d] Atomic polarizability (in Å^3). [e] From Ref.[4].

S1.2 DMDOHEMA and *n*-heptane molecule

The polarizable parm99 AMBER force field[5] was used to model the DMDOHEMA and *n*-heptanemolecules. Atomic partial charges on DMDOHEMA and *n*-heptane have been calculated using the restricted electrostatic potential (RESP) procedure[6,7]. Atom types and atomic partial charges of DMDOHEMA and *n*-heptane are shown in Figure S1 and Figure S2, respectively. 12-6 LJ parameters and atomic polarizabilities are given in Table S2.

[a] *Institut de Chimie Séparative de Marcoule (ICSM), UMR 5257, CEA-CNRS-Université Montpellier-ENSCM, Site de Marcoule, Bâtiment 426, BP 17171, F-30207 Bagnols-sur-Cèze Cedex, France. Fax: +33 (0)4 66 79 76 11; Tel: +33 (0)4 66 79 57 21; E-mail: magali.duvail@icsm.fr*
[b] *CEA, Nuclear Energy Division, Research Department on Mining and Fuel Recycling Processes (SPDS/LILA), BP 17171 F-30207 Bagnols sur Cèze, France.*

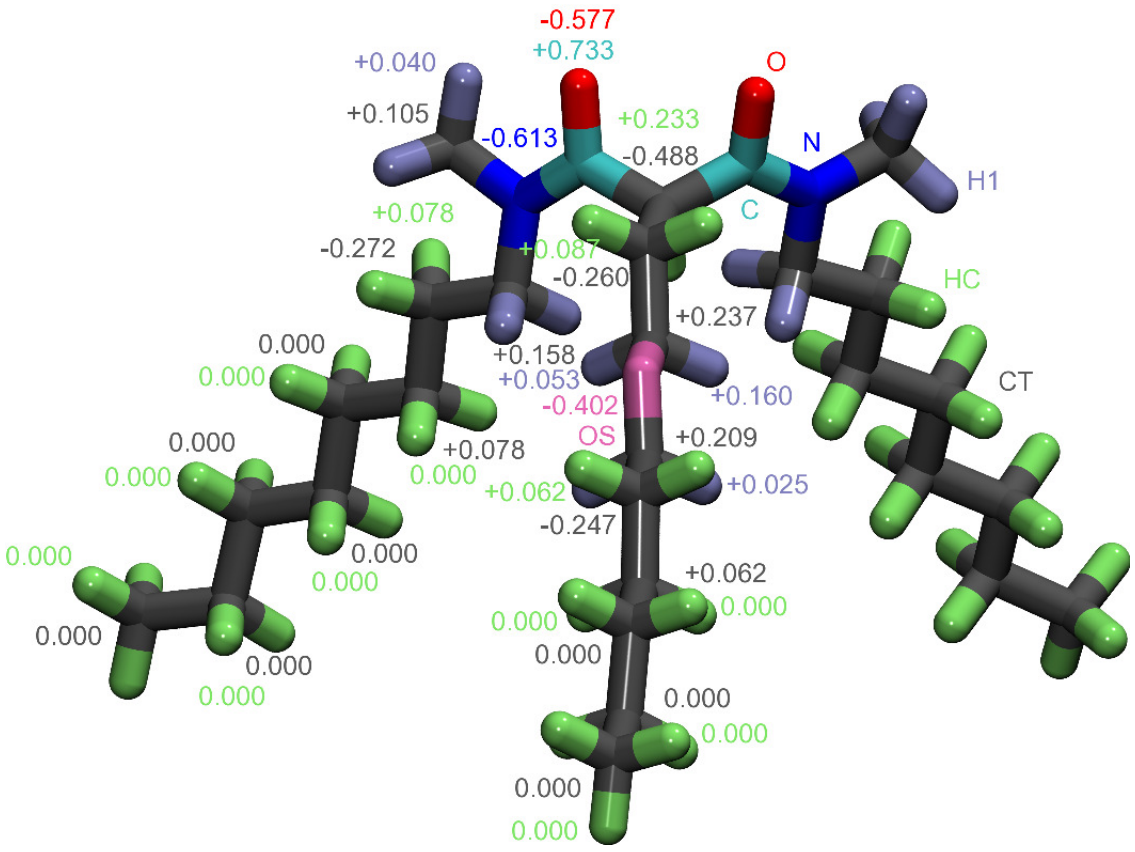

Fig. S1 Atom types and partial atomic charges of the DMDOHEMA molecule. For clarity, partial atomic charges have been written in the same color as the atom type, i.e., C (cyan): sp2 C carbonyl group; CT (gray): sp3 aliphatic C; HC (green): H aliphatic bonded to C without electron-withdrawing group; H1 (purple): H aliphatic bonded to C with 1 electron-withdrawing group; N (blue): sp2 nitrogen in amide groups; O (red): carbonyl group oxygen; OS (pink): ether oxygen.

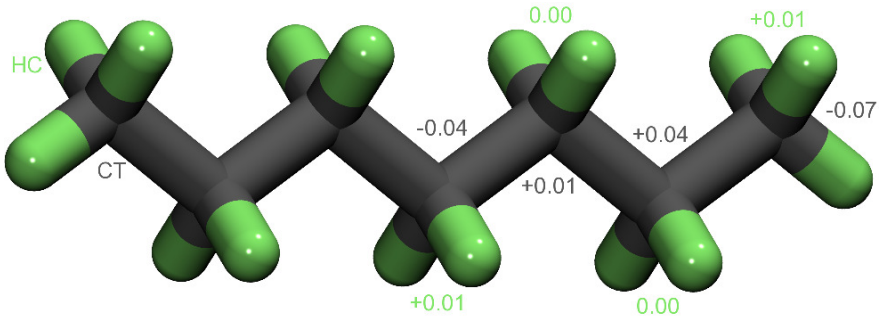

Fig. S2 Atom types and partial atomic charges of the n-heptane molecule. For clarity, partial atomic charges have been written in the same color as the atom type, i.e., CT (gray): sp3 aliphatic C; HC (green): H aliphatic bonded to C without electron-withdrawing group.

Table S2 Parameters used for describing the DMDOHEMA and n-heptane molecules by molecular dynamics simulations using explicit polarization.

Atom type	$\varepsilon_{ii}{}^{a}$	$\sigma_{ii}{}^{b}$	$\alpha_{i}{}^{c}$
C	0.360	3.400	0.616
CT	0.458	3.400	0.878
HC	0.066	2.650	0.135
H1	0.066	2.471	0.135
N	0.711	3.250	0.530
O	0.879	2.960	0.434
OS	0.711	3.000	0.465

[a] in kJ mol^{-1}. [b] in Å. [c] Atomic polarizability (in $Å^3$).

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