Supplementary Material for PCCP

MOLECULAR DYNAMICS STUDY OF DICARBOLLIDE ANIONS IN NITROBENZENE SOLUTION AND AT ITS AQUEOUS INTERFACE. SYNERGISTIC EFFECT IN THE Eu(III) ASSISTED EXTRACTION.

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Supplementary Materials

	$Cs^+\cdots N_{NBZ}$	$Cs^+\cdots O_{NBZ}$	$Cs^+\cdots Cl_{CCD}$	$Cs^+\cdots Co_{CCD}$	
30 Cs^+, CCD^- in nitrobenzene					
	6.1	12.7	2.4	1.7	
	4.0 ; 5.8	*3.2 ; 5.9*	*3.7 ; 5.6*	*6.8 ; 10.1*	

	$Cs^+\cdots N_{NBZ}$	$Cs^+\cdots O_{NBZ}$	$Cs^+\cdots Cl_{CCD}$	$Cs^+\cdots Co_{CCD}$	$Cs^+\cdots O_{H2O}$
30 Cs^+, CCD^- in the 50:50 mixture c)					
a)	0.7	0.8	0.5	0.5	7.8
	4.2 ; 5.2	*3.3 ; 4.2*	*3.8 ; 5.2*	*7.4 ; 10.0*	*3.2 ; 4.2*
b)	2.1	2.5	1.4	1.1	5.3
	4.2 ; 5.2	*3.3 ; 4.2*	*3.8 ; 5.5*	*7.4 ; 10.1*	*3.1 ; 4.3*
a)	1.3	1.5	0.5	0.6	7.0
	4.2 ; 5.2	*3.3 ; 4.2*	*3.8 ; 5.2*	*6.9 ; 9.9*	*3.1 ; 4.2*
b)	2.7	3.1	0.9	1.1	4.9
	4.2 ; 5.2	*3.3 ; 4.2*	*3.8 ; 5.2*	*6.9 ; 9.8*	*3.1 ; 4.3*
a)	0.6	0.7	0.2	*id)*	7.8
	4.2 ; 5.1	*3.3 ; 4.2*	*4.0 ; 5.1*		*3.2 ; 4.1*
b)	2.7	3.2	0.3	*id)*	5.8
	4.2 ; 5.1	*3.3 ; 4.2*	*4.0 ; 5.1*		*3.1 ; 4.4*
30 Cs^+, CCD^- in the 90:10 mixture					
a)	1.5	2.0	0.3	*id)*	7.0
	4.2 ; 5.1	*3.3 ; 4.3*	*3.9 ; 5.5*		*3.1 ; 4.2*
10 Eu^{3+}, 30 CCD^- at the nitrobenzene – water interface					
a)	3.7	5.5	*id)*	*id)*	9.0
	5.8 ; 6.8	*5.2 ; 6.0*			*2.5 ; 3.2*
b)	8.7	12.4	*id)*	*id)*	9.0
	5.7 ; 6.9	*5.2 ; 6.0*			*2.5 ; 3.2*

Table S1: Average coordination numbers of M^{n+} cations and CCD^- anions in neat NBZ and in the NBZ – water binary mixtures. They are obtained by integration of the first peaks of the RDF's whose maximum and integration distance are given in italics *(second line)*. a) Averages over all Cs^+ or Eu^{3+} ions. b) Averages over Cs^+ or Eu^{3+} ions in the nitrobenzene phase. *id)* value not reported because the peak is ill-defined.

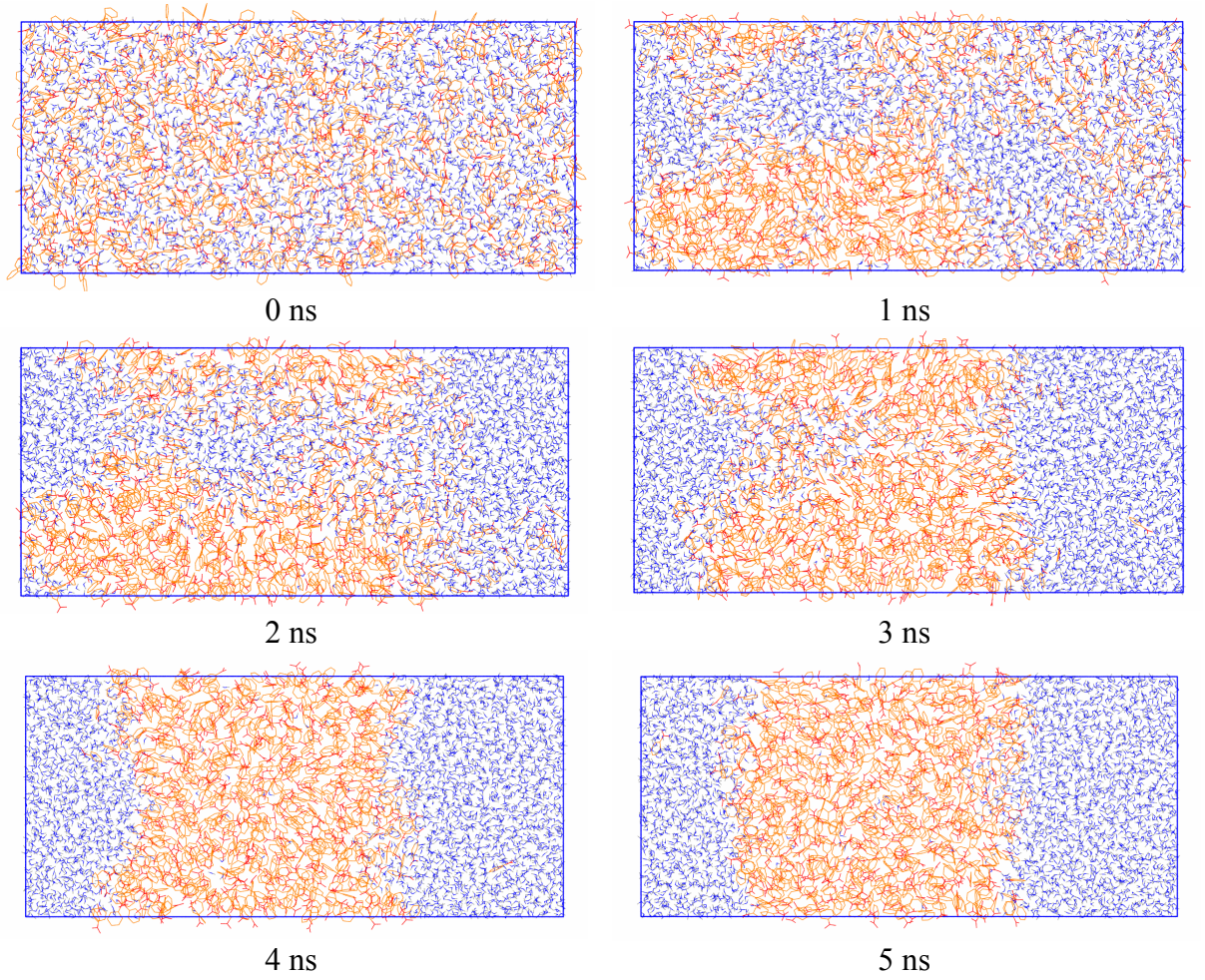


Figure S1: Phase separation of a randomly mixed 50:50 water / NBZ liquids. Snapshots along the dynamics.

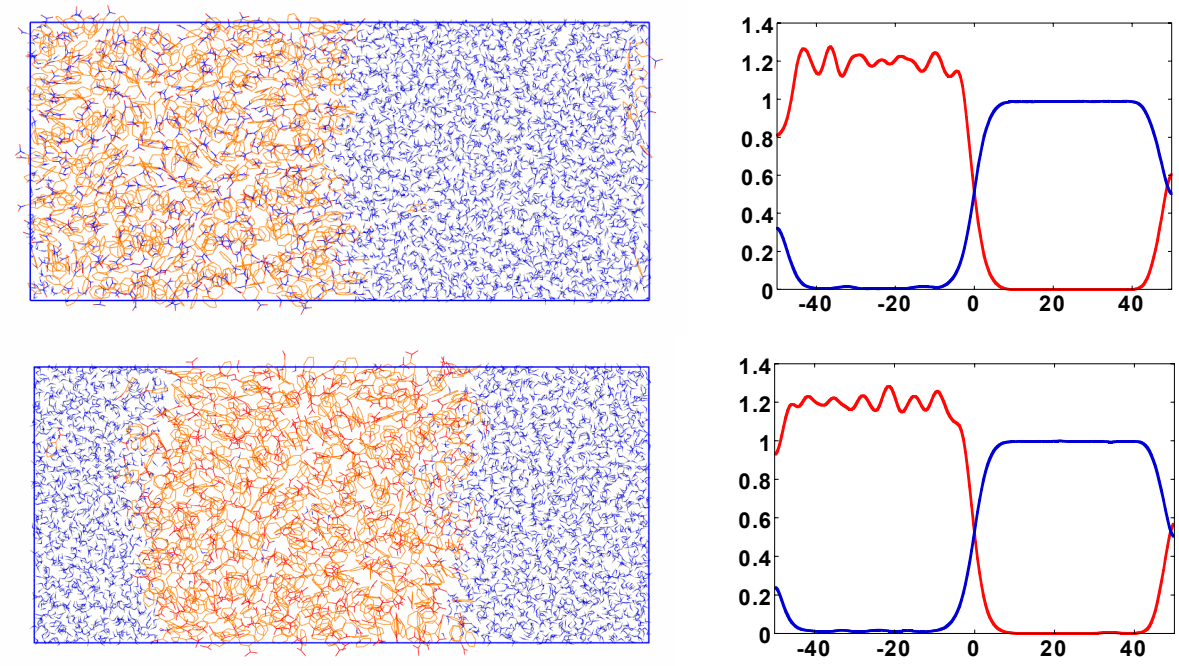


Figure S2 : Final snapshots and density curves of the dynamics that started with juxtaposed (top) and randomly mixed (bottom) 50:50 Water / NBZ liquids.

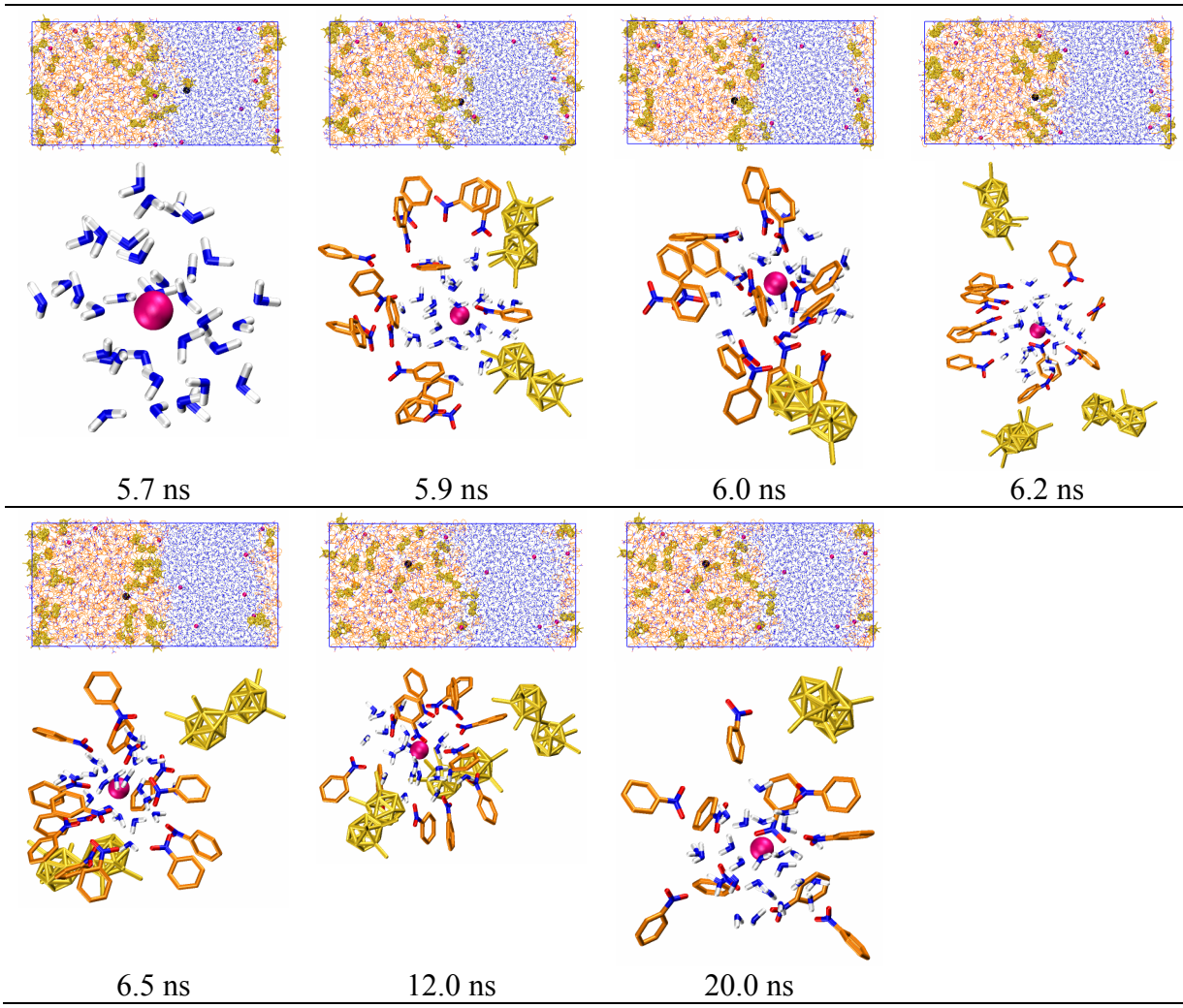
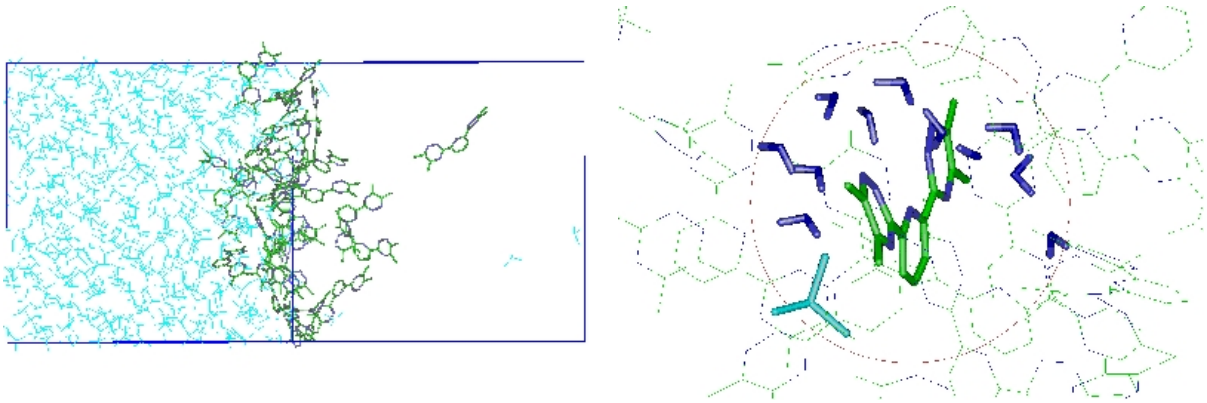
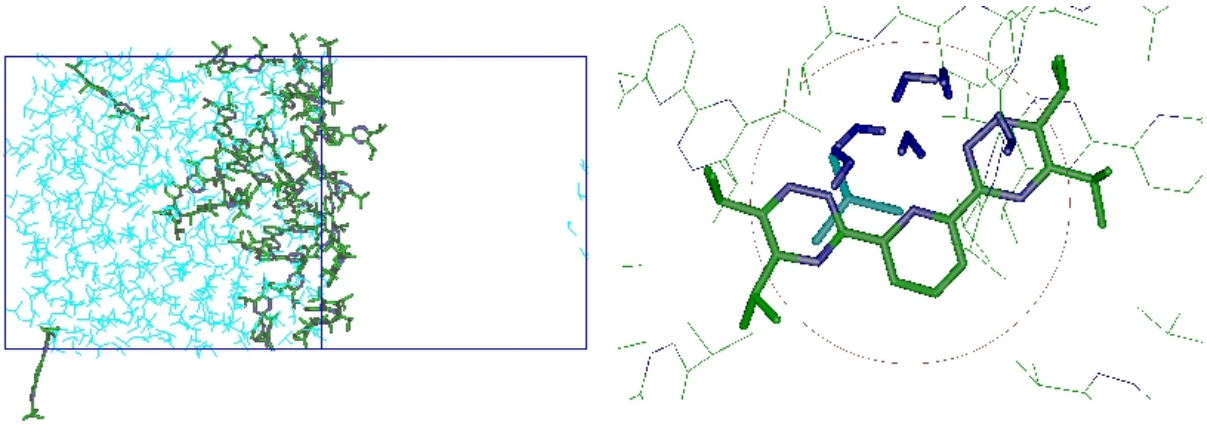


Figure S3 : 30 CCD^-, 10 Eu^{3+} (initially in water) at the NBZ - water interface. Snapshots of an Eu^{3+} cation during his migration from water to nitrobenzene.

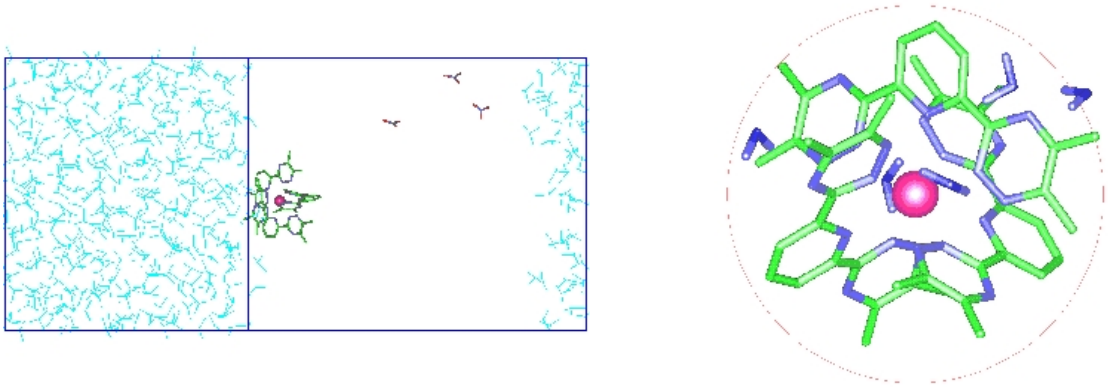


27 Me-BTP ligands

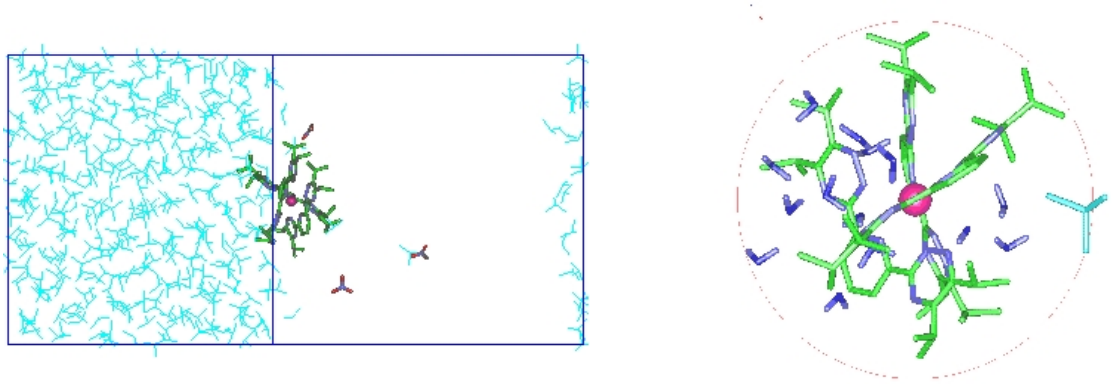


27 iPr-BTP ligands

Figure S4 : MD simulation of BTP ligands at the chloroform – water interface. Comparison of Me-BTP and iPr-BTP. G. Wipff, EUROPART EEC meeting (contract F16W-CT-2003-508-854) in Madrid, June 2004.

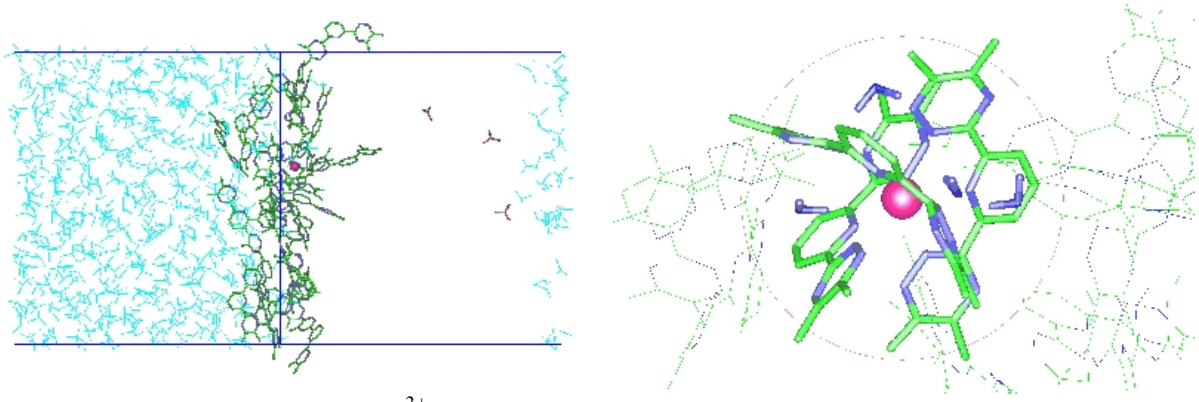


$Eu(Me\text{-}BTP)_3^{3+}$ 3 NO_3^- complex

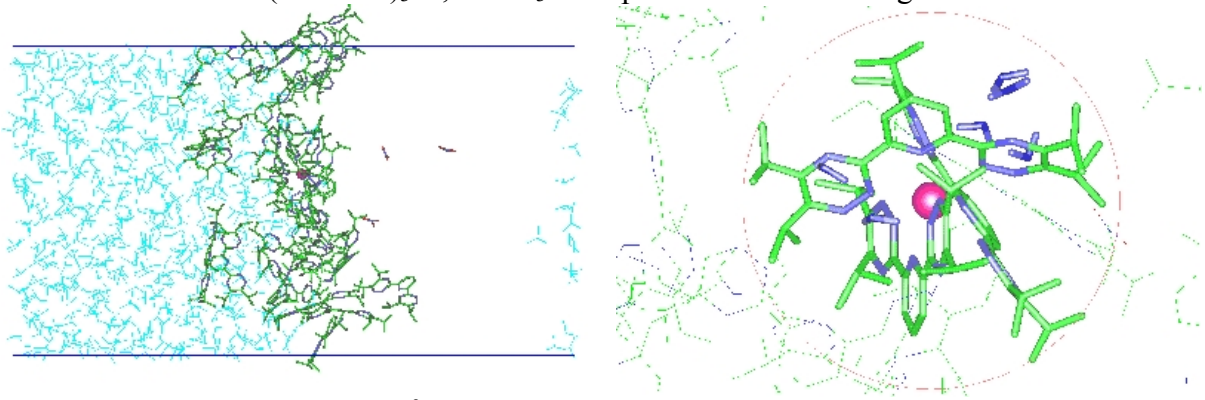


$Eu(iPr\text{-}BTP)_3^{3+}$ 3 NO_3^- complex

Figure S5 : MD simulation of $Eu(BTP)_3^{3+}$ complex at the chloroform – water interface. Comparison of Me-BTP and iPr-BTP. G. Wipff, EUROPART EEC meeting in Madrid, June 2004.



$Eu(Me\text{-}BTP)_3^{3+}$, 3 NO_3^- complex + 24 Me-BTP ligands



$Eu(iPr\text{-}BTP)_3^{3+}$, 3 NO_3^- complex + 24 iPr-BTP ligands

Figure S6 : MD simulation of $Eu(BTP)_3^{3+}$ complexes + 24 BTP ligands at the chloroform – water interface. Comparison of Me-BTP and iPr-BTP. G. Wipff, EUROPART EEC meeting in Madrid, June 2004.

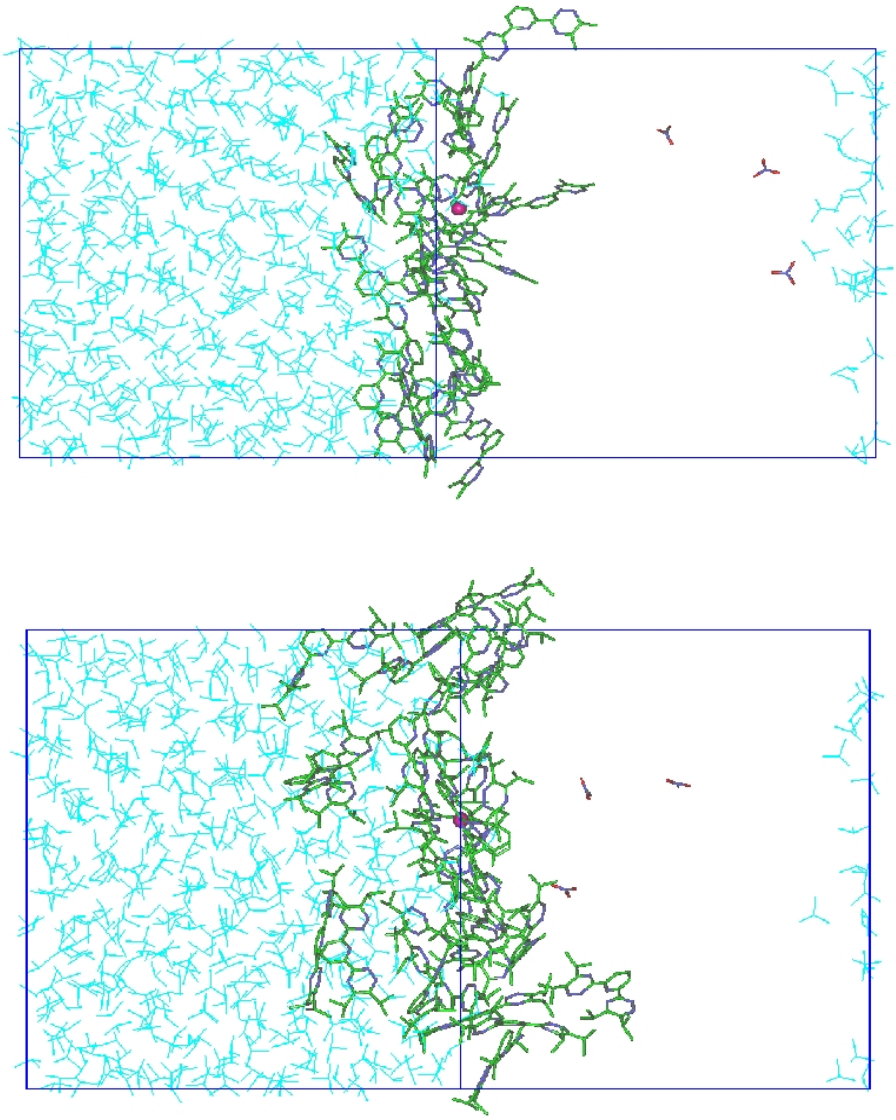


Figure S7 : Zoom on the $Eu(Me\text{-}BTP)_3^{3+}$, 3 NO_3^- complex + 24 Me-BTP ligands (*top*) and $Eu(iPr\text{-}BTP)_3^{3+}$, 3 NO_3^- complex + 24 iPr-BTP ligands (*bottom*) at the chloroform – water interface (water hidden for clarity). G. Wipff, EUROPART EEC meeting in Madrid, June 2004.