DRY $[BMI][PF_6]$					
SOLUTE	**BMI^+**	**PF_6^-**	**Box Size (Å)**	**Temp (K)**	**Time (ns)**
***Cis* - CMPO**	200	200	41.7 x 41.7 x 41.7	300 / 400	2 / 2
***Trans* - CMPO**	200	200	41.6 x 41.6 x 41.6	300 / 400	2 / 2
$[UO_2(NO_3)(CMPO)_{bi}]^+$	300	301	47.7 x 47.7 x 47.7	300 / 400	2 / 2
$[UO_2(NO_3)(CMPO)_{mono}]^+$	300	301	47.7 x 47.7 x 47.7	300 / 400	2 / 2
$[UO_2(NO_3)(CMPO)_{mono}]^+ + NO_3^- + CMPO$	200	200	42.0 x 42.0 x 42.0	300 / 400	2 / 2
$[UO_2(NO_3)_2(CMPO)_2]$	200	200	41.9 x 41.9 x 41.9	300 / 400	2 / 2
$[UO_2(NO_3)_2(CMPO)_2]$ (NO_3^- cst)[a)]	200	200	41.8 x 41.8 x 41.8	300 / 400	2 / 2

HUMID $[BMI][PF_6]$						
SOLUTE	**BMI^+**	**PF_6^-**	**H_2O**	**Box Size (Å)**	**Temp (K)**	**Time (ns)**
***Cis* - CMPO**	200	200	200	42.7 x 42.7 x 42.7	300	2
***Trans* - CMPO**	200	200	200	42.6 x 42.6 x 42.6	300	2
$[UO_2(NO_3)(CMPO)_{bi}]^+$	200	201	200	42.8 x 42.8 x 42.8	300	2
$[UO_2(NO_3)(CMPO)_{bi}]^+$ (NO_3^- cst)[a)]	200	201	200	42.8 x 42.8 x 42.8	300	2
$[UO_2(NO_3)(CMPO)_{mono}]^+$	200	201	200	42.7 x 42.7 x 42.7	300	2
$[UO_2(NO_3)(CMPO)_{mono}]^+$ (NO_3^- cst)[a)]	200	201	200	42.7 x 42.7 x 42.7	300	2
$[UO_2(NO_3)(CMPO)_{mono}]^+ + NO_3^- + CMPO$	200	200	200	42.9 x 42.9 x 42.9	300	2
$[UO_2(NO_3)_2(CMPO)_2]$	200	200	200	42.8 x 42.8 x 42.8	300	2
$[UO_2(NO_3)_2(CMPO)_2]$ (NO_3^- cst)[a)]	200	200	200	42.8 x 42.8 x 42.8	300	2

Table S1: Characteristics of the simulated systems.

[a)] NO_3^- constrained to be bidentate

Solute	Temp (K)	BMI^+	PF_6^-	E_{solv}
***Cis* – CMPO**	300	-51 (4)	-48 (3)	-99 (5)
***Cis* – CMPO**	400	-50 (5)	-49 (4)	-99 (6)
***Trans* – CMPO**	300	-57 (4)	-34 (3)	-92 (4)
***Trans* – CMPO**	400	-55 (4)	-37 (4)	-93 (6)
$[UO_2(NO_3)(CMPO)_{bi}]^+$	300	340 (7)	-547 (12)	-207 (12)
$[UO_2(NO_3)(CMPO)_{bi}]^+$	400	342 (8)	-529 (10)	-186 (9)
$[UO_2(NO_3)(CMPO)_{mono}]^+$	300	331 (7)	-583 (9)	-252 (9)
$[UO_2(NO_3)(CMPO)_{mono}]^+$	400	359 (8)	-579 (11)	-221 (9)
$[UO_2(NO_3)_2(CMPO)_2]$	300	-101 (5)	-42 (5)	-148 (8)
$[UO_2(NO_3)_2(CMPO)_2]$	400	-114 (7)	-52 (7)	-166 (8)
$[UO_2(NO_3)_2(CMPO)_2]$ (NO_3^- cst)[a)]	300	-101 (5)	-62 (5)	-163 (6)
$[UO_2(NO_3)_2(CMPO)_2]$ (NO_3^- cst) [a)]	400	-115 (7)	-69 (6)	-184 (8)

Table S2: Interaction energies (kcal/mol) and fluctuations (between brackets) of the different solutes with the [BMI][PF_6] "dry" ionic liquid and its ionic components.

[a)] NO_3^- constrained to be bidentate

Solute	BMI^+	PF_6^-	H_2O	E_{solv}
***Cis* – CMPO**	-40 (4)	-44 (3)	-32 (6)	-115 (7)
***Trans* – CMPO**	-33 (3)	-36 (3)	-39 (4)	-108 (5)
$[UO_2(NO_3)(CMPO)_{bi}]^+$	312 (8)	-488 (10)	-82 (9)	-260 (11)
$[UO_2(NO_3)(CMPO)_{bi}]^+$ (NO_3^- cst) [a)]	279 (8)	-437 (11)	-53 (8)	-211 (10)
$[UO_2(NO_3)(CMPO)_{mono}]^+$	263 (12)	-402 (21)	-180 (23)	-320 (13)
$[UO_2(NO_3)(CMPO)_{mono}]^+$ (NO_3^- cst) [a)]	304 (6)	-475 (10)	-92 (7)	-264 (9)
$[UO_2(NO_3)_2(CMPO)_2$	-108 (8)	-55 (8)	-65 (7)	-228 (9)
$UO_2(NO_3)_2(CMPO)_2$ (NO_3^- cst) [a)]	-96 (7)	-58 (8)	-40(8)	-195 (10)

Table S3: Interaction energies (kcal/mol) and fluctuations (between brackets) of the different solutes with the [BMI][PF_6][H_2O] "humid" ionic liquid and its different components.

[a)] NO_3^- constrained to be bidentate

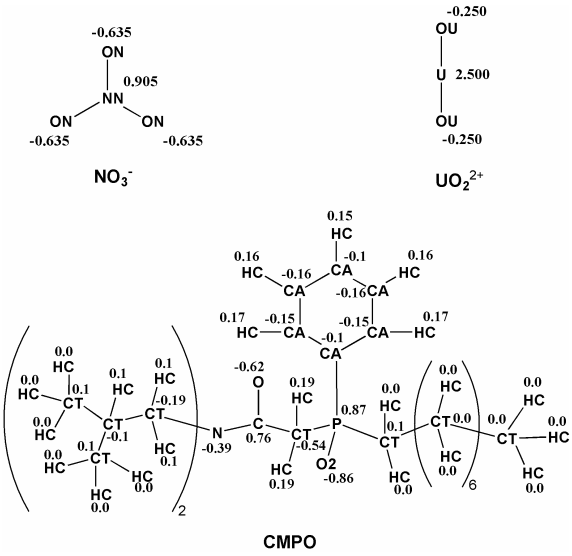


Figure S1: Charges and AMBER atom types of the different solutes.

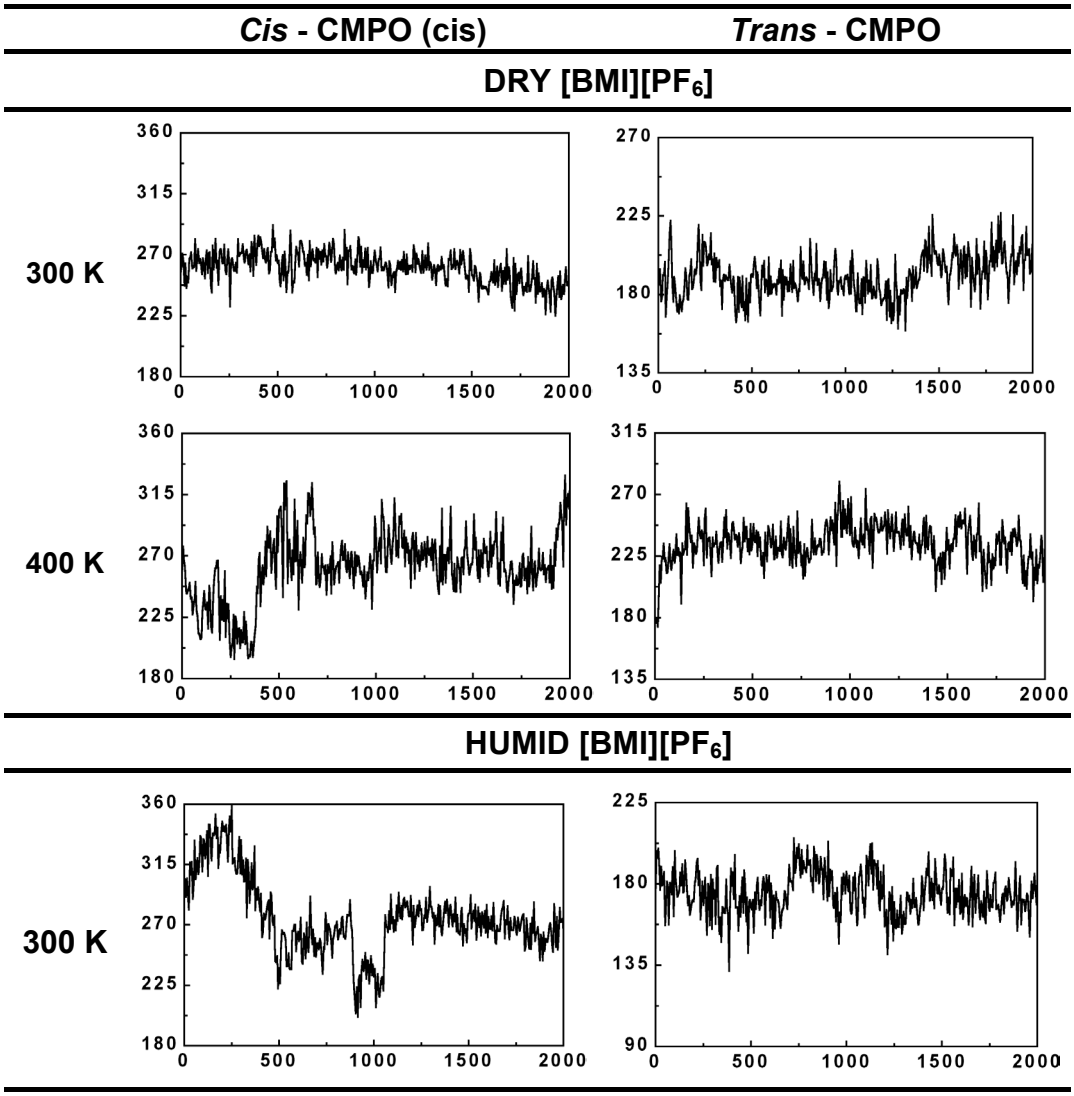


Figure S2: CMPO in "dry" and "humid" [BMI][PF_6]: Variation of the OC-PO dihedral as a function of time (ps). Starting in a *cis* form (left) and a *trans* form (right)

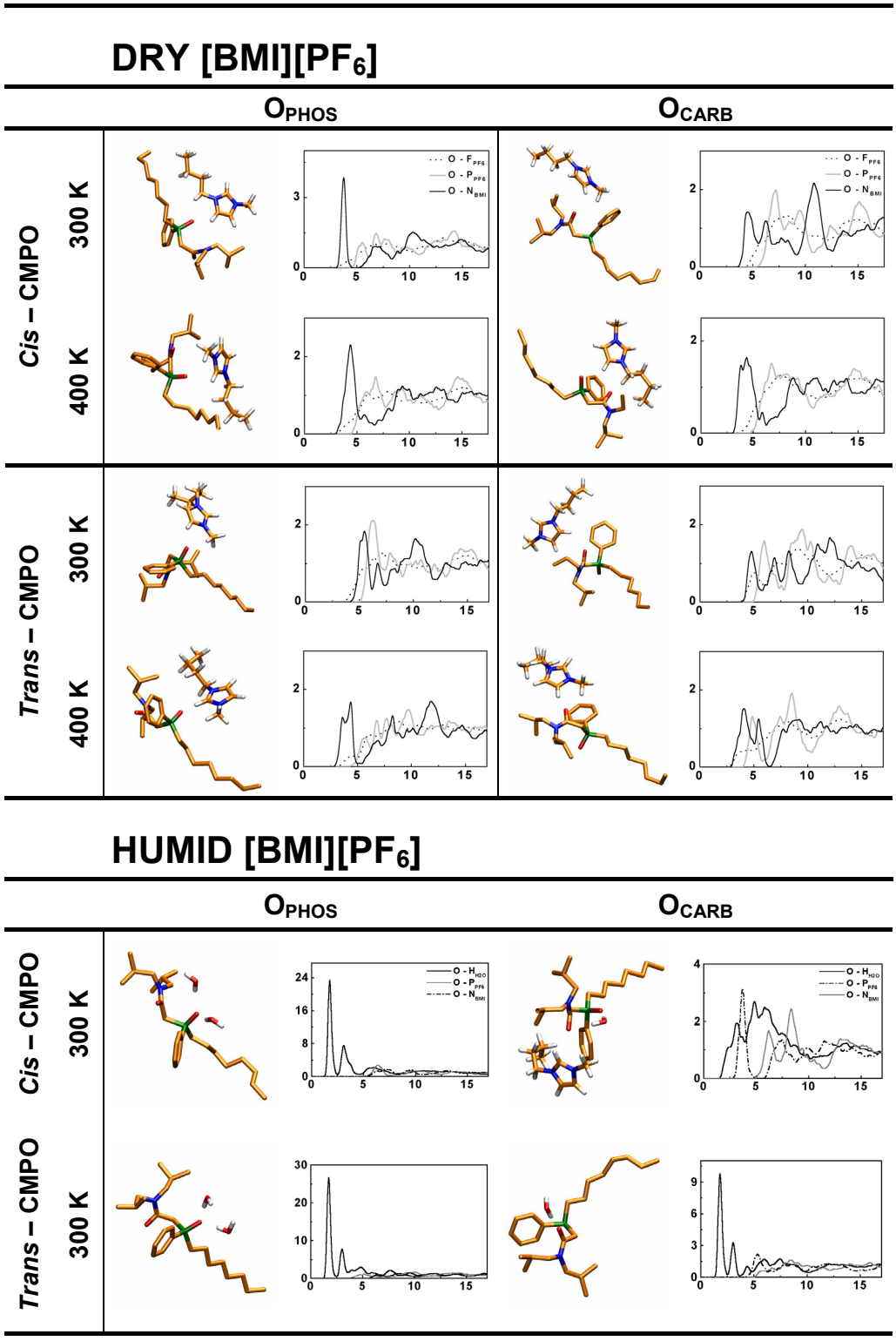


Figure S3: Free CMPO ligands in "dry" and "humid" [BMI][PF_6]: Final snapshot of the first solvation shell around the O_{PHOS} and O_{CARB} and corresponding radial distribution functions.

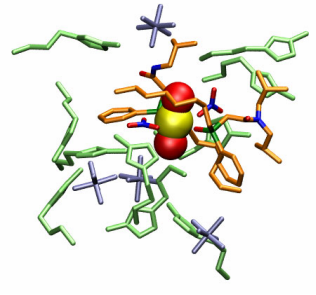
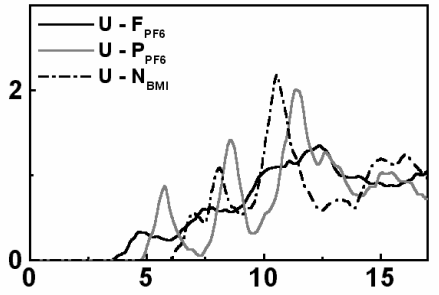
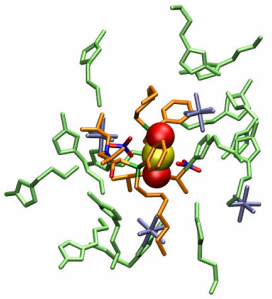
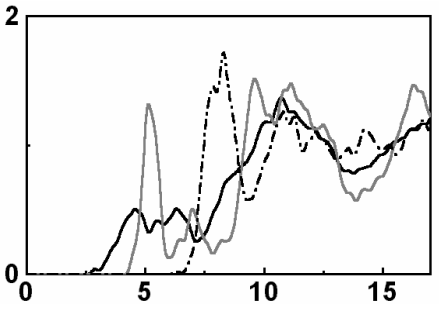
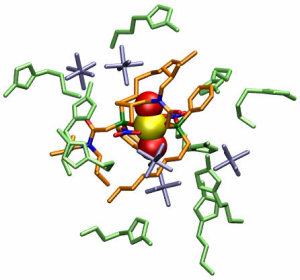
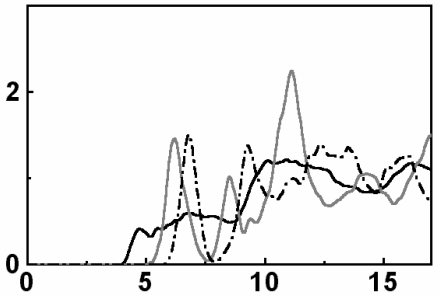
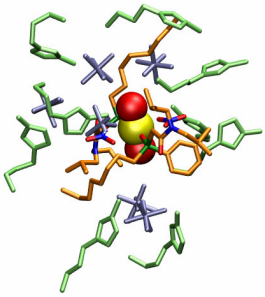
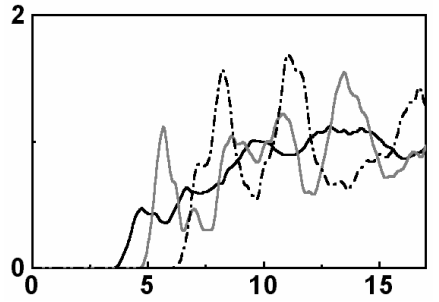
Temp (K)	Snapshot	RDF
NO_3^- Unconstrained		
300 K		
400 K		
NO_3^- Constrained bidentate		
300 K		
400 K		

Figure S4: $[UO_2(NO_3)_2(CMPO)_2]$ complexes in "dry" [BMI][PF_6]: Final snapshot of the first solvation shell (up to 8 Å) around the UO_2^{2+} cation and radial distribution function around the U atom.