Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

The passage of TBP-Uranyl complexes from aqueous-organic interface to the organic phase: insights from molecular dynamics simulation

Pooja Sahu, Sk. Musharaf Ali and Kalasanka Trivikram Shenoy*

Chemical Engineering Division, Bhabha Atomic Research Center, Mumbai, India- 400085

*musharaf@barc.gov.in

Table S1: Bonded Forcefield Parameters

Molecules/Ions	bonds	K (kcal/mol)	r_{eq}
UO_2^{2+}	U-OU	500	1.80
NO_3^-	N-ON	300	1.26
H_3O^+	H-O	553	0.96
HNO_3	O-H	553	1.03
	N-O	300	1.26
Dodecane	C-C	300	1.54
TBP	O2-P	525	1.48
	P-Os	230	1.61
	Os-C	320	1.41
	C-C	310	1.53
	C-H	340	1.09
	Angles	K (kcal/mol)	θ_{eq}
UO_2^{2+}	OU-U-OU	150	180.0
NO_3^-	O-N-O	150	120.0
H_3O^+	H-O-H	100	104.5
HNO_3	H-O-N	45	105.3
	O-N-O	150	120.0
Dodecane	C-C-C	125	114.0
TBP	O2-P-Os	100	108.2
	P-Os-C	100	120.5
	Os-C-C	50	109.5
	Os-C-H	50	109.5
	Os-P-Os	45	102.6
	C-C-C	40	109.5
	C-C-H	50	109.5
	H-C-H	35	109.5

Table S2: Non bonded forcefield parameters

molecules/ions	site	σ (Å)	ε (kcal/mol)
UO_2^{2+}	U	2.81	0.400
	OU	3.12	0.200
NO_3^-	N	3.15	0.170
	O	2.86	0.211
H_3O^+	H	1.00	0.000
	O	2.96	0.211
HNO_3	H	1.00	0.000
	N	3.25	0.170
	O	2.96	0.211
Dodecane	CH2	3.95	0.092
	CH3	3.75	0.195
TBP	O2	2.96	0.210
	P	3.74	0.200
	Os	3.0	0.170
	C	3.4	0.110
	H	2.65	0.016

Figure S1. Final snapshots and corresponding density profiles for all simulated biphasic systems