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Free energy study of uranyl complexes across water-oil and water-oil+tri-butyl phosphate (TBP) interfaces[1] MANORI JAYASINGHE, THOMAS L. BECK, University of Cincinnati — Free energy profiles of heavy metal ion complexes, UO_2 $(NO_3)_2$, UO_2 $(NO_3)_2TBP_2$, and TBP, across the water-hexane and water hexane+TBP (50%/50%) interfaces, were calculated from molecular dynamics simulations. These complexes and interfaces are relevant to recently developed heavy-ion separation techniques. The solute complex with TBP, UO_2 $(NO_3)_2TBP_2$, shows strong interfacial activity in contrast to the free energy barrier for UO_2 $(NO_3)_2$ at the water-hexane interface. Increased TBP concentration in the oil phase reduces the interfacial activity and better solvates the ion complexes and their ligands. The solute complex with TBP oriented parallel to the water-hexane+TBP interface binds more strongly to the hexane+TBP phase than to the pure hexane phase. The (un-complexed) TBP orientational probability distribution shows the polar head buried in water, while the nonpolar tails are buried in the oil phase, and hence TBP exhibits interfacial activity. The calculated density profiles at the interface show that TBP acts not only as a carrier for uranyl transport across the interface, but also as an "interface modifier". Our simulation results are in agreement with the recent study of uranyl transport across chemically modified membranes with TBP based metal ion carriers.

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