

How Hydrogen Bonds Affect the Growth of Reverse Micelles Around Coordinating Metal Ions

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In comparison to the extensive studies on hydrogen bonds (H-bonds) performed in aqueous solutions to illustrate their critical role in various biological, chemical and physical processes, how H-bonds affect both the structure and function of aggregates in organic phase is poorly understood. In the present work, the role of H-bonds on the hierarchical structure of an aggregating amphiphile-oil solution containing a coordinating metal complex is explored for the first time. Atomistic molecular dynamics simulations are performed in combination with X-ray techniques.

- The presence of the acidic (HNO_3) condition enriches the formation of H-bonds.
- The H-bonds network plays a role in not only stabilizing the metal complexes, but also affecting the growth of reverse micelles.
- The growth of reverse micelle into rod-like shape elevates the extraction efficiency of Eu(III) in the acidic condition.

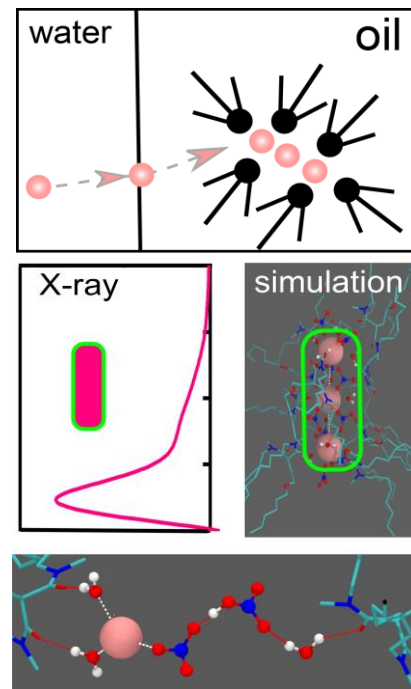


Figure: (top) Schematic representation of the diamide extraction of metal ions. Metal and surfactant are in pink and black, respectively. (middle) Experimental prediction and simulation snapshot of the elongated reverse micelle aggregates in the acidic (HNO_3) system. (bottom) Snapshot from atomistic simulation showing H-bonds bridging Eu^{3+} ions and the DMDOHEMA surfactants.

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