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Behavior of Bifunctional Phosphonium-Based Ionic Liquids in Solvent Extraction of Rare Earth Elements - Quantum Chemical Study

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ABSTRACT The complex-forming ability of thirty different bifunctional phosphonium-based ionic liquids (IL) in solvent extraction of rare earth elements (REE) has been investigated through density functional theory (DFT) simulations. The study enabled ranking various organic-solvent-borne ionic liquids for the extraction ability of their anionic or cationic moieties towards heavy and light rare earth element aqua-complexes from the pregnant solutions. The complexation energy estimated under interfacial or bulk organic phase conditions was used as quantitative index to discriminate the best complex-forming combinations between bifunctional phosphonium-based ionic liquids and rare earth elements. Anionic moieties with P=O and P-O functional groups proved superior in terms of complex-forming ability with rare earth elements as compared with P=S and P-S containing anions. Ammonium-based cationic moieties with short alkyl chain as well as imidazolium and pyrrolidinium cationic moieties led to stronger IL-REE complexes. This strength of complexation can be promoted further with phosphonium-based ionic liquids provided pulp digestion towards pregnant solutions is carried out with nitric and hydrochloride acids instead of sulfuric acid. DFT simulations revealed that while anionic moieties of phosphonium based ionic liquids are covalently bound with rare earth elements, the IL cationic moieties are involved only through outer-sphere interactions in the IL-REE complexes. Nevertheless, these cationic moieties are shown to influence the anion electron-donor properties resulting in changes in the ionic liquid complex-forming ability.

KEYWORDS Ionic liquids; Rare earth elements; Solvent extraction; DFT simulation

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