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Molecular insights into rare earth element complexation in late-stage carbonatitic brine melt systems

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Carbonatites are one of the major global sources of light rare earth elements (REEs). In the late stage of their formation, primary carbonatitic melts are modified by hydrothermal processes forming highly complex brine-melt systems. Despite their importance, the structure of and REE speciation in these high temperature melts remain poorly understood at the molecular scale. As these melts do not persist in natural systems, their investigation requires *in situ* experimental or computational approaches. Here, we investigate the REE speciation in a model H_2O–Na_2CO_3–NaCl-REE brine-melt with 4.55 wt% H_2O by ab initio molecular dynamics (AIMD) simulations. As the coordination dynamics and ligand exchange processes at relevant temperatures of about 1000 K is much slower than the timescale of AIMD, we use enhanced sampling methods and combine AIMD with well-tempered metadynamics to access the underlying free energy landscape. Our simulations show that REE complexes are dominantly stabilized by carbonate ligands (CO_3^{2-}), while chloride plays a secondary role in the first coordination shell. The results suggest a strong stabilization of REE-carbonate complexes under magmatic brine-melt conditions and provide molecular-scale insight into processes that may control REE mobility and fractionation during the evolution of carbonatitic systems.