Theoretical understanding on chlorine isotope fractionation between apatite-group minerals and fluid

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The chlorine isotope compositions (δ^{37}Cl) show a variation from ca. -14‰ to +16‰ on the earth, and up to +24‰ in the Apollo basalts and glasses [1]. Due to insufficient understanding of chlorine isotope fractionation behaviors, it still remains great challenges to trace genesis of ore-deposits and migration of metals in magmatic-hydrothermal processes using this novel isotope system. In an attempt to explore the main driving mechanisms of volatile isotope fractionation, the chlorine isotope fractionation behaviors between minerals and melt/fluid containing volatiles have been investigated by using the quantum mechanics (density functional theory, DFT) and *ab initio* molecular dynamics simulation (AIMD).

The differences in ion-chlorine coordination and hydration effect in fluid, together with the bonding strengths in minerals, induce obvious chlorine isotope fractionations at low temperature. The equilibrium chlorine isotope fractionation follows the sequence of low salinity fluid < basic high salinity fluid < acidic high salinity fluid. The largest chlorine isotope fractionation of -1.5‰ was estimated between hydroxy-chlorapatite and fluid at 400 K. It is well consistent with the δ^{37}Cl signatures of mantle reservoir in the Earth, but much smaller than the spreading of δ^{37}Cl in the Moon, reflecting the different controls govern the chlorine isotope fractionation in terrestrial (equilibrium dominates) and extra-terrestrial magma degassing and crystallization evolution (kinetic controls).

[1]Barnes J D and Sharp Z D. (2017). Reviews in Mineralogy and Geochemistry, 82(1): 345-378.