

Mobility of Titanium in F-rich fluids: clues from experiments and thermodynamic calculation

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Mobilities of the high-field-strength element (HFSE) are generally high in fluorine-rich fluids, which has been attributed to the formation of stable HFSE fluoride complexes. However, geochemical properties of these complexes are not clear yet.

Hydrolysis behavior of potassium titanium fluoride (K_2TiF_6) solution has been investigated at temperatures from 200 to 600 °C and pressure of 100 MPa. We gained the cumulative hydrolysis constants (K) at varied temperatures (T), and a nice linear fitting of $\ln K = 9.182 - 10509/T$. Based on the Van't Hoff Equation, the $\Delta_r H_m^\ominus$ and $\Delta_r S_m^\ominus$ of the hydrolysis reaction are supposed to be $+1263 \text{ kJ}\cdot\text{mol}^{-1}$ and $+1104 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$, respectively.

Given that natural fluids usually contain various components or complexes, further thermodynamic calculation used the cumulative hydrolysis constant to give a quantitative evaluation on the mobility of titanium in F-rich fluids with a given conditions of temperature, pH and fluorine content. The results show the mobility of titanium reaches up to thousands of ppm in LT/acidic or HT/alkaline fluids with 2 wt% fluorine, in good agreement with previous rutile solubility experiments. In addition, temperature negatively influences titanium mobility at acidic conditions and positively at alkaline conditions.

Therefore, titanium can migrate effectively under such conditions: a) abundance of fluorine; b) LT/acidic or HT/alkaline fluid circumstances. Among the two requirements above, abundance of fluorine is of crucial importance.