# Niobium and tantalum in hydrothermal systems: Thermodynamic description of Nb and Ta hydroxo- and fluoride complexes over a wide range of temperatures and pressures

N. N. AKINFIEV[1*], E. V. LUKYANOVA[1], V. S. KORZHINSKYA[2], N. P. KOTOVA[2] AND A. V. ZOTOV[1]

[1]IGEM RAS, Staromonetny per., 35, 119017, Moscow, Russia (*correspondence: akinfiev@igem.ru)

[2]IEM RAS, 142432, Chernogolovka, Russia

Despite tantalum (Ta) and niobium (Nb) are essential metals in modern society their geochemical behaviour, especially in hydrothermal fluids is still poorly known. The goal of this study is to identify stoichiometry of Nb and Ta aqueous species and to estimate stability of their complexes' formation in a wide range of temperatures (0 – 600 °C) and pressures (0.1 – 300 MPa).

The whole set of the available experimental data on $Nb_2O_5$ [1] [2] and $Ta_2O_5$ [3] solubility in hydrothermal HF-NaF-KF-NaOH fluids were processed by the OptimA program [4] to estimate Gibbs free energies, *g(T,P)*, of aqueous species at given *T, P* point. It was assumed that solubility of metal oxides in the near neutral fluids is characterized by the hydroxocomplex $MeO_2(OH)(aq)$, while under acid conditions of HF bearing fluids the dissolution reactions are defined by two species, namely $MeO_2F(aq)$ and $MeO(OH)F_2(aq)$, where Me stands for Nb or Ta. The fluoride negatively charged complex, $MeO_2F_2^-$ is significant in alkaline fluoride-bearing solutions.

The estimated *g(T,P)* values for hydroxide and fluoride complexes were then used to generate the HKF model (Tanger and Helgeson, 1998) parameters of these species by use of the OptimB [4]. As a result thermodynamic description of Nb and Ta aqueous species is available to perform various thermodynamic models of hydrothermal transport and accumulation of these metals in a wide range of temperatures (0 – 600 ºC), pressures (0.1 – 300 MPa) and fluid compositions.

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