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Abu Dabbab and Abu Rusheid Rare-Metal Granites and the Thermodynamic Properties of Fluorine in Silicate Melts

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Many post-collisional alkaline granites from the Arabian-Nubian Shield have been identified in the Eastern Desert of Egypt as hosts of rare metals and elements. The mechanism by which these rocks formed is poorly understood, as is the observed correlation between high concentrations of rare metals and fluorine. This relationship may be causative and in order to discover if that is the case, a combination of molecular dynamics, thermodynamics, and geochemical data will be applied to this problem. This study presents bulk rock data from XRF and ICP-MS, as well as mineralogical data from SEM and EPMA for two of these rare-metal granites, Abu Rusheid and Abu Dabbab. They are high in Na, Al, K, Si, and F, and low in Ca, Fe, Mn, P, and Mg. Both localities show enriched concentrations of high field strength elements (HFSE) relative to the primitive mantle, as well as a slight to moderate enrichment of the heavy rare-earth elements relative to light, but Abu Rusheid is generally more enriched than Abu Dabbab. Abu Rusheid has a broader mineral assemblage, including rare-earth phosphates, and higher F content in its minerals, namely in abundant 'zinnwaldite' and fluorite. Molecular dynamics simulations are currently underway to determine the speciation of HFSE compounds in silicate melts. We are describing the force fields of 17 individual compounds, which include both trace (Zr, La) and major (Al, Ca, Na, K, Si) cations as fluoride, oxide, and oxyfluoride species, using small-scale, *ab initio* calculations performed in VASP to calibrate large-scale simulations (LAMMPS). The speciation of these compounds in a simulated silicate melt will be used in thermodynamic models. Such models, when combined with the above data, will allow for the prediction of the behavior of fluorine and high field strength elements in magmatic systems.