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**ABSTRACT TITLE:** Inorganic Geochemical Controls on Neptunium Transport: Co-Precipitation in Minerals

**ABSTRACT:** Neptunium-237, with a half-life of 2.14 million years, is a contaminant of concern for the U.S. Department of Energy. Multiple oxidation states are accessible, but under subsurface conditions of environmental importance the Np(V) oxidation state is strongly favored. This cation forms a linear dioxo cation, the neptunyl ion, which is soluble in aqueous solutions. Whereas it is tempting to assume that the Np(V) uranyl ion will behave similarly to the U(VI) uranyl ion in the subsurface, there are a variety of reasons to expect otherwise. Specifically, the Np(V)-O bonds within the neptunyl ion are weaker than those in the U(VI) uranyl ion, making the neptunyl ion O atoms more reactive. Also, the charge of the neptunyl ion is lower than that of the uranyl ion, which will impact charge balance mechanisms for co-precipitation reactions.

We hypothesize that the Np(V) neptunyl ion may be co-precipitated into a variety of low temperature mineral structures that form in the subsurface. The analogous situation has been demonstrated in several studies focusing on uranyl ions, but the only studies for neptunyl have examined calcite. In order to derive a predictive understanding of Np(V) incorporation into a variety of minerals, we are experimentally examining incorporation of the neptunyl ion in about a dozen mineral phases that present different cation sites that are incorporation targets. Results to date demonstrate both that incorporation of U(VI) and Np(V) in such structures differ significantly between the two actinyl ions, and also between structure types. We are thus bringing crystal chemical and quantum mechanical models to bear on the study of the local environments of incorporation.