

SPECIATION OF NEPTUNIUM IN WATER

JEAN-PHILIPPE BLAUDEAU, *Department of Chemistry, The Ohio State University, Columbus, OH 43210 and Department of Chemistry, Ohio Wesleyan University, Delaware, Ohio, 43015*; KEN V. ADAIR, *Department of Chemistry, Ohio Wesleyan University, Delaware, Ohio, 43015*; BRUCE E. BURSTEN, *Department of Chemistry, The Ohio State University, Columbus, OH 43210*.

The speciation of neptunium in water was modeled using density functional theory (DFT) methods. Aqueous neptunium exists in four oxidation states: +3, +4, +5, and +6. The first two forms exist as the bare ions, but the +5 and +6 states exist as $(\text{NpO}_2)^+$ and $(\text{NpO}_2)^{2+}$ species, respectively. The coordination number for the number of water molecules around each of these species is determined and compared to experiment - which uses XANES (X-ray Absorption Near-Edge Spectroscopy) and eXAFS (extended X-ray Absorption Fine Structure) spectroscopy. The DFT calculations include generalized gradient corrections.