SPECIATION OF NEPTUNIUM IN WATER

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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 $(NpO_2)^+$ and $(NpO_2)^{2+}$ 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.