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Experimental and computational approaches to investigate high oxidation state redox chemistry of osmium

Three simultaneous reactions that occur on different timescales during the reduction of OsVIII with methanol were investigated. The study combined detailed experimental and quantum mechanical computational work with regard to oxo/hydroxide, high oxidation state osmium (Os) chemistry. The kinetics and thermodynamics of the three reactions were shown to fit a well-defined set of chemical reactions. The comproportionation reaction of OsVIII and OsVI was found to occur via concerted electron-proton transfer whereas the rate-determining step of the reduction of OsVIII with methanol was found to occur via α -C-H (not O-H) hydrogen atom transfer.

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