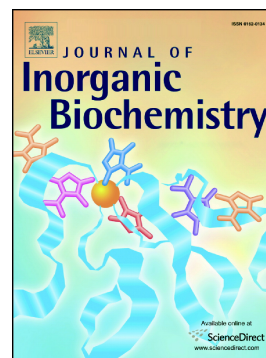


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Coordination Environment Changes of the Vanadium in Vanadium-Dependent Haloperoxidase Enzymes

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Abstract

Vanadium-dependent haloperoxidases are a class of enzymes that catalyze oxidation reactions converting halides to form halogenated organic products and water. These enzymes include chloroperoxidase and bromoperoxidase, which have very different protein sequences and sizes, but regardless the coordination environment of the active sites is surprisingly constant. In this manuscript, data mining of the coordination chemistry of the trigonal bipyramidal geometry for the V-containing-haloperoxidase structures are characterized and compared. The catalytic cycle imposes changes in the coordination geometry of the vanadium to accommodate the peroxido vanadium(V) intermediate in an environment we describe as a distorted square pyramidal geometry. During the catalytic cycle, this intermediate converts to a trigonal bipyramidal intermediate before losing the halogen and forming a tetrahedral vanadium-protein intermediate. Importantly, the catalysis is facilitated by a proton-relay system supplied by the second sphere coordination environment and the changes in the coordination environment of the vanadium(V) making this process unique among protein catalyzed processes. The analysis of the coordination chemistry shows that the active site is very tightly regulated with only minor changes in the coordination geometry. The coordination geometry in the protein structures deviates from that found for both small molecules crystalized in the absence of protein and the reported functional small molecule model compounds. At this time there are no examples

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