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Metal Ion Dynamics During Metalloenzyme Catalysis

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Elucidation of intermediate structures together with electronic processes occurring at catalytic metal ions and their affect on the enzyme kinetics provide the key to comprehend the catalytic power of metalloenzymes. We combined time-resolved x-ray absorption spectroscopy, pre-steady state kinetic, and computational procedures to study the interaction of catalytic metals with substrates. During turnover of the zinc metalloenzyme *Thermoanaerobacter brockii* alcohol dehydrogenase, we detect a sequence of structural distortions in the coordination number of the catalytic zinc ion followed by concomitant changes in metal-ligand bond distances. We demonstrate that this structural-dynamics is reflected in the perturbation of the metal ion valance via distinct dynamic profile. The present study suggests that catalytic metal ions have a major role in governing the reaction mechanism and kinetics. This provides a novel view on the function of metals in building up the catalytic power within the framework of the active site in metalloenzymes.