Theoretical calculations of pKa values of biomimetic metal-ligand complexes

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Acireductone dioxygenase (ARD) is a monometallic enzyme involved in the methionine salvage pathway in living organisms. Its distinct chemical properties are determined solely by the identity of the divalent ion bound to it. In this study, we investigate the efficiency of Nickel and Zinc as the metal center of a family of ARD biomimetic models. To explore this, pKa values were determined based on density functional theory (DFT) calculations of eight molecular analogues with a variety of different modifications in order to better assess molecular properties induced by changes in the coordinating environment. Our results show that nickel is the optimal metal center of the complex. As predicted, the pKa values of the complexes with methyl groups were higher than those with a phenyl group.