Zinc and Magnesium Low Temperature Solid-State NMR Spectroscopy of Metalloproteins

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ABSTRACT. We will briefly present our most recent results on two protein systems: Alkaline Phosphatase (AP) and the *E. coli.* DNA repair protein N-Ada-17. We will utilize AP to discuss the concept of pH in the context of low temperatures and the consequences of static disorder in solid-state NMR spectroscopy. Given this background, we present the first direct determination of the pK_a for water bound to Zn^{2+} in a *resting* metalloprotein. Further, AP offers the opportunity to investigate the potential pH dependence of the ^{25}Mg NMR spectroscopy of the of a tight binding Mg^{2+} site in metallobiochemistry. Theoretical predictions of the Zn^{2+} and Mg^{2+} electric field gradients will be described and discussed in terms of the potential mechanistic implications of the data. The implications of the Mg^{2+} calculations will be extended to Mg^{2+} dependent DNA repair proteins. Likewise, we will also present the results of low temperature experiments performed on the DNA repair protein Ada. The spectroscopy will be discussed in terms of the potential mechanistic implications.

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