

The Intrinsic Qualities Driving Iron and Nickel Mineral Evolution also Drive their Coordination Sphere Characteristics Across Biological Protein Space.

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Interactions between elements determine the physical properties of minerals and are central in the function of protein active sites. Minerals show an expanding range of mineral electronegativity associations as Earth's surface became progressively more oxidized over the course of its 4.5 billion year history. That is, the differences in electronegativity between the elements within minerals has increased systematically with time, largely in parallel with Earth's increasing near-surface oxidization. To understand if these trends are recapitulated in biology, we examine proteins that have known 3D structures deposited in the Protein Data Bank (PDB) and that incorporate transition metals. By analyzing the amino acid residues that fall within a threshold distance from each metal cluster, we quantify the average hydropathy index (measure of water and amino acid interactions) of metal-binding sites for nickel (Ni), iron (Fe), and their cluster types across the PDB. The data show that Fe, found in a wide range of protein types, both from early and modern metabolisms, is highly flexible in the degree of hydrophobicity of its protein fold space (from -2 to +3 average hydropathy on the Kyte-Doolittle scale). Nickel, found in a far smaller number of protein types used exclusively in earlier metabolisms, displays a smaller and slightly more hydrophilic range of average hydropathy (-3 to +1). Just as average mineral electronegativity differences increase overall with geologic time, so do the differences between the positively charged (soluble, hydrophilic) metal center, and the (increasingly) hydrophobic nature of the metal cluster's coordination sphere at protein binding sites. Ni, more limited than Fe in the electronegativity difference increases of its minerals over geologic time, also has a more limited range than Fe in its biological protein hydropathy space. We will characterize further the coordination spheres of Ni and Fe in available PDB structures to better understand this trend. Insight into how evolution on Earth has been shaped by the electrochemical qualities of specific elements and minerals can help in understanding how different sets of elemental and mineral constituents could enable and affect life's evolution elsewhere in the universe.