

W0152

Metal Ions in Biological Systems: Information from Crystallographic and Theoretical Studies. Jenny P. Glusker, Amy K. Katz, Charles W. Bock, The Institute for Cancer Research, Fox Chase Cancer Center, Philadelphia, PA 19111, Philadelphia Univ., Philadelphia, PA 19144.

Approximately one third of all enzymes utilize metal ions. Our aim is to improve our understanding of the functions and characteristics of metal ions in biological systems. The Cambridge Structural Database (CSD), in conjunction with theoretical calculations, was used to study the stereochemistry of ligand binding. Descriptions will be given of energy calculations assessing the tendency of individual metal ions to ionize water (thereby liberating hydrogen ions). We have also examined the geometry of water structure around metal ions and the energetic consequences of replacing one of the water molecules with a different ligand. The relative tendency of metal ions to bind O, N, or S (the most likely choice in proteins) and the local effects of two metal ions in close proximity, will also be discussed. Our conclusions are checked by examining metalloproteins in the Protein Databank (PDB). The overall aim is to develop a database of results from our analyses indicating why an enzyme may or may not choose a specific metal ion.

This work was supported by grants CA-10925 and CA-06927 from the National Institutes of Health and by an appropriation from the Commonwealth of Pennsylvania.