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Interaction Modes and Absolute Affinities of α-Amino Acids for Mn^{2+}: A Comprehensive Picture

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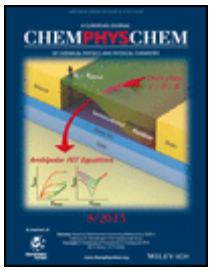

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Abstract

Manganese is involved as a cofactor in the activation of numerous enzymes as well as the oxygen-evolving complex of photosystem II. Full understanding of the role played by the Mn^{2+} ion requires detailed knowledge of the interaction modes and energies of manganese with its various environments, a knowledge that is far from complete. To bring detailed insight into the local interactions of Mn in metallopeptides and proteins, theoretical studies employing first-principles quantum mechanical calculations are carried out on [Mn-amino acid]$^{2+}$ complexes involving all 20 natural α-amino acids (AAs). Detailed investigation of [Mn-serine]$^{2+}$, [Mn-cysteine]$^{2+}$, [Mn-phenylalanine]$^{2+}$, [Mn-tyrosine]$^{2+}$, and [Mn-tryptophan]$^{2+}$ indicates that with an electron-rich side chain, the most stable species involves interaction of Mn^{2+} with carbonyl oxygen, amino nitrogen, and an electron-rich section of the side chain of the AA in its canonical form. This is in sharp contrast with aliphatic side chains for which a salt bridge is formed. For aromatic AAs, complexation to manganese leads to partial oxidation as well as aromaticity reduction. Despite multisite binding, AAs do not generate strong enough ligand fields to switch the metal to a low- or even intermediate-spin ground state. The affinities of Mn^{2+} for all AAs are reported at the B3LYP and CCSD(T) levels of theory, thereby providing the first complete series of affinities for a divalent metal ion. The trends are compared with those of other cations for which affinities of all AAs have been previously obtained.