

Cu^{II} ion coordination to an unprotected pentadecapeptide containing two his residues: competition between the terminal amino and the side-chain imidazole nitrogen donors.

Autorzy

Chiara Conato
Wojciech Kamysz
Henryk Kozłowski
Marek Łuczowski
Z. Maćkiewicz
F. Mancini
Piotr Młynarz
Maurizio Remelli
Daniela Valensin
Gianni Valensin

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The complex-formation equilibria of the pentadecapeptide TLEGTKKGHKLHLDY, the 114–128 protein fragment of SPARC, with the Cu^{II} ion have been investigated, at $I = 0.1 \text{ mol} \cdot \text{dm}^{-3}$ (KNO₃) and $T = 298.2 \text{ K}$. Protonation and complex-formation constants have been determined potentiometrically, and formation enthalpies measured by direct solution calorimetry; the complex-formation model and species stoichiometry have been carefully checked by means of UV/Vis absorption, CD and EPR spectroscopy. The structure hypotheses of the complex species are also based on detailed study of the ¹H and ¹³C NMR spectra of the ligand in both the absence and presence of copper ions. The involvement in complex-formation of both the terminal amino and imidazole groups has been suggested and their specific behaviour at different pH values elucidated.

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