

Multiple scattering XAS calculations for the characterization of the binuclear (type 3) copper sites of hemocyanins and related model compounds.

E. Borghi¹ and P.L. Solari²

¹ Dipartimento di Chimica, Università La Sapienza, P.le A. Moro 5, 00185 Roma, Italy

² European Synchrotron Radiation Facility, B. P. 220, 38043 Grenoble, France

Our study [1] on the met- and met-azido-Hcs forms from *Octopus vulgaris* (mollusc) and *Carcinus aestuarii* (arthropod) at pH 7.5 and on some related binuclear models without XRD [2] has considered and resolved some fundamental aspects of their binuclear type 3 copper site (*i.e.* correct values of the Cu-Cu distances, apical distortion when present, at the copper site, presence and type of bridging groups).

In this contribution, we will show how, only by advanced multiple scattering (MS) calculations it has been possible to refine the EXAFS modulation of the absorption spectra and to overcome some severe problems that mainly derive from the presence of two absorbing atoms and from the fact that the metal-metal contribution in the absorption spectra overlaps with the Cu-His signals. We will also present some results indicating the role of the MS calculations in the XANES edge region, which show how it is possible to extract quantitative structural information from the absorption data also in a binuclear core in order to refine the fine structure of the site.

1. Borghi E., Solari P. L., Beltramini M., Bubacco L., Di Muro P., Salvato B., *Biophys. J.* 82, 3254-3268 (2002).

2. Casella L., Carugo O., Gullotti M., Garofani S., Zanella P., *Inorg. Chem.* 32, 2056-2067 (1993).