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Probing the structure of proteins in physiological conditions by X-ray absorption and UV/Visible spectroscopies

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Myoglobin (Mb) is one of the best-characterized metalloproteins found in mammalian muscle cells, which facilitates oxygen diffusion in muscle cells. It has the ability to bind small ligand molecules to the Fe atom at the center of its heme plane. Despite extensive studies, a microscopic description of ligand detachment and rebinding in Mb remains unclear. X-ray absorption spectroscopy (XAS) is an ideal probe to retrieve the local geometric and electronic structure in disordered systems. In order to draw meaningful conclusions about the XAS it is important to know the form of the protein during the course of the measurements. UV-Visible spectroscopy is particularly sensitive to the form of the protein, including the oxidation state of the Fe and the bound ligand, so by combining it simultaneously with XAS we can ensure measurements on undamaged and uncontaminated protein. Using these two techniques we have measured six different forms of Mb under physiological conditions (in solution, pH 7). EXAFS features were investigated using MXAN code, and the TDDFT analysis scrutinizes details of pre-edge features show their remarkable sensitivity to the local protein geometry and the chemical nature of the ligand. We will report on the structures obtained for Mb and on some recent time-resolved XAS measurements where we investigate the binding of CO and NO to Mb. Our results are in good agreement with the structures determined by x-ray crystallography.

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