It appears that only in the last two cases $I_R(h)$ could have been determined directly from the dispersion function $f'(\lambda) + f''(\lambda)$.

The influence of statistical and systematic errors on the results will be discussed.

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L4

Local Coordination Geometry in Fe and Ca Metalloproteins by XANES using Synchrotron Radiation

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X-ray absorption spectroscopy using synchrotron radiation is opening new perspectives in the study of fundamental biological problems of structure and function of metalloproteins because of its unique capability to give direct structural information on the metal active sites of proteins in solution. The direct structural information in X-ray absorption spectra arise because of their interpretation in terms of electron scattering by neighbour atoms of the electrons photoemitted at the metal site. EXAFS oscillations arising from single scattering processes can give distances, coordination numbers and the type of neighbour atoms!

A recent development on the X-ray absorption near edge structure: XANES [1] extending over about 50 eV energy range demonstrates that this part of the X-ray absorption spectrum also can be interpreted in terms of electron scattering by neighbour atoms. The spectra show strong multiple scattering resonances, like low energy electron spectroscopy, determined by atomic geometrical distribution of the neighbour atoms. The actual 'state of art' is such that after distance determination by EXAFS, XANES is able to distinguish between different possible geometrical structures [2].

We report XANES spectra of hemoglobin and related heme-proteins where we have found evidence of:

(1) Fe displacement relative to the porphyrin plane which cannot be determined by other methods in solution.

(2) Variation of the ligand bonding angle Fe–C–O and Fe–C–N in hemoglobin in solution where CO is tilted and CN is vertical relative to the porphyrin plane.

(3) Time resolved XANES can provide information on the dynamics of atoms in the active sites during protein function.

In calcium proteins [4, 5] troponin-C and calmodulin [6] different orientations of COO^- groups of aspartic and glutamic residues bound to Ca^{2+} in the EF-hand loop can be distinguished and different sites are identified.

The presence of the allosteric role of Mg^{2+}, and the effects of drugs on calmodulin have been found.

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L5

Iron EXAFS Studies of the Iron–Molybdenum Cofactor of Nitrogenase and the 3Fe Ferredoxin II of *Desulfovibrio Gigas*

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Chemical and physical analyses indicate that the iron–molybdenum cofactor (FeMo(co)) of nitrogenase contains 6–8 mol of iron and 4–6 mol of sulfur per mol of molybdenum. The physical properties of this cofactor suggest that it contains a novel Mo–Fe–S cluster. Extended X-ray absorption fine structure (EXAFS) data taken at the Mo edge indicate that the molybdenum has two or three iron atoms and four or five sulfur atoms as nearest neighbors. Several models are consistent with these data. More information concerning the iron environment is needed to better define the structure of the FeMo(co). In this talk, we will present our recent results [1] on the iron edge EXAFS of the FeMo(co) from *Azotobacter vinelandii*