

μ SR Investigations of the Spin Dynamics of Central Metal Ions of Proteins

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The structural genomics, which is aiming at understanding of structure-functions relationships of proteins, is now a worldwide initiative in the field of biology. Studies on metalloproteins are one of the central issues in this field, because the occurrence of metal centers in proteins is high, as about 1/3 of proteins coded by genomes are metalloproteins. Metalloproteins utilize the chemistry of metals to their advantage to perform varied biological functions with specificity and control. Therefore, functions of metalloproteins are known to be varied by not only their 3D-structures but also electronic state around central metal ions.

In order to study the dynamic properties of central metal ions, we have prepared some models of the heme-proteins as shown in the figure and applied μ SR measurements on them at the RIKEN-RAL Muon Facility in the UK and at PSI in Switzerland. All measurements have been done at the room temperature. We have investigated Fe-porphyrins and its derivatives with Cl, imidazole and peptides as axial ligand. The Fe-porphyrin has the same molecular structure of the basic part of the central metal ions of heme-proteins which are the one of most important class of metalloproteins. Since the heme is commonly contained in a lot of proteins as prosthetic group, understandings of the electronic state of this Fe-porphyrin is very important as the first step to study functions of the metalloproteins.

In the case of Fe(TPP)Cl (sample No. 2), for instance, a fast depolarization behavior has been measured even in the 4 kG, although no such strong depolarization rate has been observed in TPP (Sample No.1) which has no Fe ions. We have repeated longitudinal-field μ SR measurements on all samples and have tried to obtain qualitative parameters of dynamically fluctuating internal fields at the muon site. In our presentation, we will discuss a relationship between the dynamics of central metal ion and molecular structures around the central metal ion.

