Approach to determination of muon stopping sites in proteins

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In order to explore the electron-transfer process in life sciences, we have been carrying out μSR studies using the electron labeling method on cytochrome c, a protein which is a member of the respiratory chain in mitochondria.[1–3] In order to deepen the understanding of the μSR data, we intend to determine the muon stopping sites and the electronic structure. In addition, our LF μSR data showed a level crossing resonance (LCR) signature for cytochrome c indicating that some portion of the muons have a strong energy transfer at a specific LF to the surrounding species at the stopping site (Fig. 1(b)). The observed LCR data around 20 G was similar to that of polyglycine (Fig. 1(c)) (F. L. Pratt, private communication). Proteins are made of amino acids, which are linked by peptide bonds, and polyglycine is the simplest polypeptide made of aliphatic (–CH_2–) parts, peptide bonds (–CONH–), terminal –COOH (or –COO^-), and –NH_2 (or –NH_3^+) groups. The candidates of muon stopping sites are peptide bonds (–CONH–) and terminal –COOH or –NH_2 (Fig. 1(a)).

Under such a background, we carried out μSR measurements of triglycine, tetraglycine, and N-methylacetamide ($CH_3CONHCH_3$), which is the simplest molecule containing a peptide bond, and compared the characteristics of the μSR data with those of glycine, glycylglycine, and polyglycine.

The low LF μSR data of glycine were fitted well using the product of Kubo-Toyabe and Lorentzian functions. LCR was not detected around 20 G, contrary to the cases of cytochrome c and polyglycine. On the other hand, the low LF μSR data of glycylglycine, triglycine and tetraglycine were approximately fitted with the Lorentzian function, and the LCR was observed (Fig. 1(d)). In addition, the missing fraction of the initial asymmetry of oligoglycine under zero magnetic field was approximately 20% of the full asymmetry, and larger than that of glycine (approximately 10%). A similar tendency was observed in the μSR data of N-methylacetamede at 10 K, although the quality of the data was inferior because the sample melted during the treatment (melting point: 300 K), and a cavity appeared in the sample cell. Taking the results of theoretical calculations into account,[4] muon would stop at –COOH (or –COO^-) moiety in glycine, and at CO moiety of peptide bonds in oligoglycine.

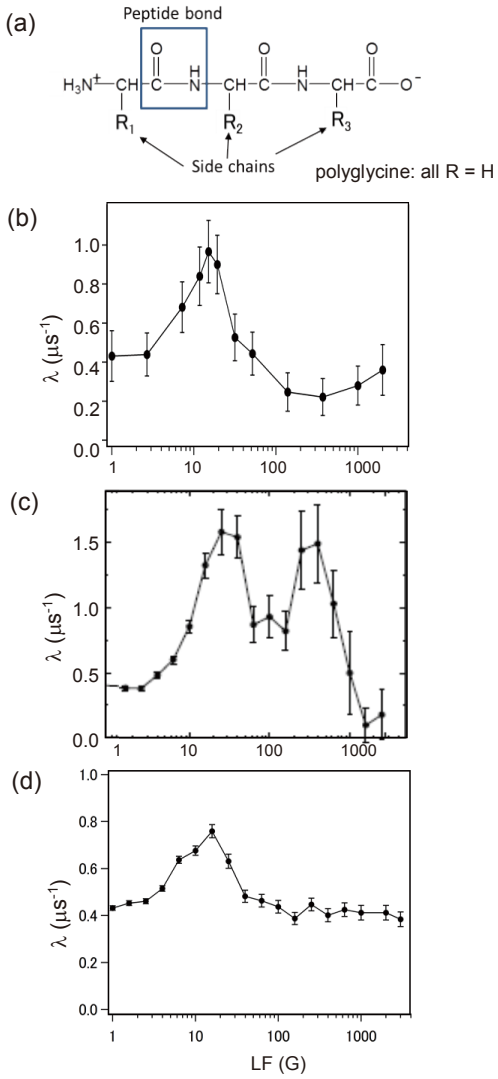

Fig. 1. Schematic structure of protein (a) and longitudinal field dependence of relaxation rates (λ) of cytochrome *c* (18 K) (b), polyglycine (5 K) (c) and tetraglycine (16 K) (d).

The results indicate that the LCR data of cytochrome c originates from the muon stopping at peptide bonds.

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