

Structural Study of Selective Complexation of Sr(II) in Micellar Solution by XAFS Method

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1 Introduction

Strontium-90 (^{90}Sr) having long radiological half-life is radioactive in nature and it falls under the category of most hazardous of radioactive fallout [1]. Investigation of the effects of ^{90}Sr on environment and human body are one of the most important issues for the management of radioactive elements. Fluorescent probes are sufficiently sensitive to detect a tiny amount of metal ions such as strontium ion (Sr(II)) because of its exquisite sensitivity and selectivity. Therefore, the study of Sr(II) fluorescent probes have been carried out [2, 3].

Recently, we synthesized a Sr(II) selective fluorescent probe, *N*-(2-hydroxy-3-(1*H*-benzimidazol-2-yl)-phenyl methyl)-1-aza-18-crown-6-ether: **BIC**, and studied its fluorescence properties and complexation behavior with Sr(II) . We revealed that the stability constant of Sr(II) -**BIC** complex was 10 times higher than that in aqueous solution. In addition, its detection limit value was also improved up to 300 times by this system. However, the mechanisms of these phenomena have remained obscure. In present study, the local structure of the Sr(II) -**BIC** complex in micelle solutions is determined using EXAFS analyses to reveal the species of Sr(II) complex which formed in the solution.

2 Experiment

BIC was synthesized according to a procedure described previously [4]. An aqueous solution of SrCl_2 (0.001 M), **BIC** (0.001 M), and SDS (100 mM) were prepared. A solution of 0.01 M of SrCl_2 and $\text{Sr(18-crown-6 ether)}$ complex were prepared as reference sample. All of XAFS spectra were measured in fluorescence mode at the BL-27B station in the KEK-PF. The Sr *K*-edge XAFS spectra were recorded within 15.77 – 17.05 keV. Each sample was measured for 1 h. The EXAFS spectra were analyzed using the WinXAS 3.1 program [5]. Theoretical phase shifts and backscattering amplitude functions were generated using the FEFF8.00 code. The amplitude of the reduction factor, S_0^2 , was fixed at 1.0. All of XAFS measurements were performed at room temperature.

3 Results and Discussion

We measured the XAFS spectra of SrCl_2 and $\text{Sr(18-crown-6 ether)}$ complex as reference sample for the XAFS analysis. Fig. 1 shows the k^3 -weighted Sr *K*-edge EXAFS oscillation of Sr(II) complexes in various solutions, and the corresponding magnitude of the Fourier-transformed data. Because O/N and Cl can

behave as ligands for Sr(II) in this system, both Sr-O/N and Sr-Cl models were used to fit the EXAFS data. The Fourier-transformed spectra exhibited two peaks at 2.0 and 3.0 Å in the data of $\text{Sr(18-crown-6 ether)}$ and Sr(BIC) complexes. The larger peak at 2.0 Å can be clearly assigned to a Sr-O/N interaction [6].

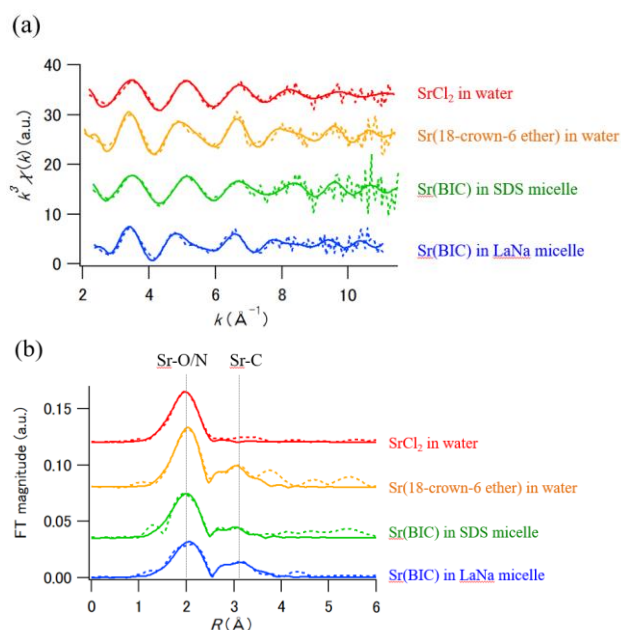


Fig. 1: (a) k^3 -weighted Sr *K*-edge EXAFS oscillation of Sr(II) complexes in solution, and (b) the corresponding magnitude of the Fourier-transformed data. Solid lines and dashed lines indicate the experimental data and theoretical fit, respectively. The phase shift in the Fourier-transformed data was not corrected.

The obtained EXAFS spectra and their fitting results indicated that Sr(II) and **BIC** formed a $\text{Sr(18-crown-6-ether)}$ -like complex in aqueous micellar solution. The EXAFS results also indicated that the hydrophilic head group of surfactant molecule was directly coordinated with Sr(II) . Therefore, we concluded that Sr(II) , **BIC**, and surfactant molecule formed a ternary complexes in aqueous micellar solution, and at least, it is clear that the improvement of the stability constant in micellar solution is attributed to the result of the formation of Sr(BIC) (surfactant) complex.

To understand Sr(II) recognition mechanism in detail, more study is in progress.

Acknowledgement

Sample preparation was conducted at the User Experiment Preparation Lab III that is provided by Comprehensive Research Organization for Science and Society (CROSS). This work was supported by JSPS KAKENHI Grant Number 16K21615.

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