

XAFS Analysis of Iodine/Iodide in Povidone Iodine

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Introduction

Povidone iodine (PVP-I) is a complex composed of polyvinylpyrrolidone and iodine. While its sterilization effect due to the included iodine is particularly useful, the toxicity of PVP-I is not completely ignorable. As bed sore ointment, PVP-I which is mixed with refined sugar and buffer reagents is generally used.

As Kubo[1] has pointed out, this has a drawback that the amount of the tri-iodide ions and the iodine molecules in the ointment are influenced by the buffer[1]. In order to prevent the undesirable effect of the buffer, Kubo developed a new PVP-I ointment.

It is common to perform the thiosulfate titration in evaluating the available amount of the iodine in PVP-I. For the new ointment, however, it is difficult to apply this method. In order to circumvent this difficulty, we perform iodine XAFS measurements and evaluate the available iodine in the new type ointment.

Experiments

KI aqueous solution, I₂ ethanol solution and KI-I₂ aqueous solution were prepared for XAFS measurements. Samples containing PVP-I are PVP-I solid, 10%w/w PVP-I aqueous solution, 10%w/w PVP-I aqueous solution with buffer, and newly developed ointment I-III [1]. We also performed measurements on a commercially available ointment. Measurements of iodine XAFS spectra were performed at BL-9A (for L_{1,III}-edge) and NW-10A (for K-edge) in transmission mode at room temperature under atmospheric pressure.

Results and discussion

Figure 1 shows L₁-edge XANES spectra. Significant peak, due to the 2s→5p transition, is found at 5185eV in the spectrum of the I₂ ethanol solution and in almost all the sample containing PVP-I, while no peak is found in the spectra of the KI aqueous solution and the new type ointment III.

The sterilization effect of iodine is due to its oxidation power. In the molecular orbital theory, an iodine molecule has eight molecular orbitals in the valence region. The highest molecular orbital 2σ* is unoccupied because an iodine molecule has fourteen valence electrons. Therefore an iodine molecule, having the unfilled orbital, can behave as an oxidizer which take away electrons from other chemical species. The 2s→5p transition observed in the iodine L₁-edge XANES spectra is the excitation from the 2s core states to the unoccupied orbitals. Because normalized XANES spectra represent the absorption per single atom, the area of the peak which corresponds to the

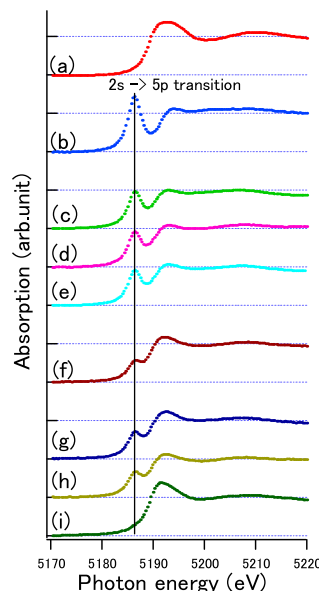


Figure 1: Normalized iodine L₁-edge XANES spectra. (a)KI aq. (b) I₂ EtOH sltn. (c)PVP-I solid (d)10%w/w PVP-I aq. (e)10%w/w PVP-I aq. + buff. (f)commercial ointment (g)-(i)new type ointment I-III

above mentioned 2s→5p transition can be a measure of the average oxidizing power of the iodine atoms in the system. It is found that the new ointment, type I and type II, contain more available iodine than the commercial ointment. Table 1 shows estimated relative values of the amount of the available iodine.

Table 1: Estimated relative values of the amount of the available iodine

The available iodine	
I ₂ EtOH sltn.	100
PVP-I solid	47
10%w/w PVP-I aq.	40
10%w/w PVP-I aq. + buff.	41
commercial	11
new type I	18
new type II	18
new type III	0

References

[1] T. Kubo, 9th Iodine Soc. Symposium, p31-32 (2006).

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