Li *K*-Edge XANES Spectra of Lithium-Doped Fullerenes and Lithium Borate Glasses

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Li *K*-edge XANES spectra for lithium doped fullerenes, Li_xC_{60} and Li_xC_{70} (x = 14±2), and for lithium borate glasses, xLi_2O-$(100-x)B_2O_3$, were measured using a beamline BL-2 of the SR Center at Ritsumeikan University [1]. All samples were powdered to collect their XANES spectra in the total electron yield mode. The vacuum level in the sample chamber was higher than 1.0 x 10^{-5} Pa during measurements. The lithium-doped fullerenes were synthesized at the laboratory of one of the authors (M. K.).For preparing lithium borate glasses, chemicals were melted at 1100-1200 ℃ and then quenched.

Figure 1 shows Li *K*-edge XANES spectra of Li_xC_{60} and Li_xC_{70} (x = 14±2) and reference samples. Spectra of **Li_xC_{60} C 1** and **Li_xC_{60} C 2** show the first and second runs of the measurements of a sample **Li_xC_{60} C** under Ar atmosphere, respectively. Similar measurement was done for a different sample, **Li_xC_{60} U 1**. A spectrum of **Li_xC_{60} U 2** is for the sample partially exposed to the air. A spectrum of **Li_xC_{70} E 1** is for a sample of Li_xC_{70} measured under Ar atmosphere, and that of **Li_xC_{70} E air** is for the sample exposed to the air.

Broad and somewhat split absorptions appear around 57-69 eV in the spectra of **Li_xC_{60} C 1**, **Li_xC_{60} C 2**, and **Li_xC_{60} U 1**, the whole features of which are similar to those of the reference samples such as Li_3N, but quite different from those of lithium halides like LiF, where the lithium atoms are in the isolated ionic states and show sharp absorption peaks due to the core exciton [2,3]. This indicates that lithium atoms in lithium-doped fullerenes do interact with C_{60}, like interacting Li and N atoms in Li_3N.

Compared to these absorptions, the corresponding broad absorption in **Li_xC_{70} E 1** is somewhat shifted to higher energies, meaning that the Li-C_{70} interaction is different from the Li-C_{60} one.

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When exposed to the air, the spectral features (**Li_xC_{60} U 2** and **Li_xC_{70} E air**) become similar, though the positions are a little in low energy, to those of the reference samples of Li_2CO_3 and Li_2O.

Figure 2 shows Li *K*-edge XANES spectra of lithium borate glasses xLi_2O-$(100-x)B_2O_3$ together with the reference samples. The whole spectral features of xLi_2O-$(100-x)B_2O_3$ (x = 20-45) resemble those of Li_2CO_3 and Li_2O. However, the spectra are rather broad with a relatively strong rising up at the low-energy side of the absorption. This may be indeed characteristic of the lithium atoms in amorphous glassy materials unlike crystalline ones.

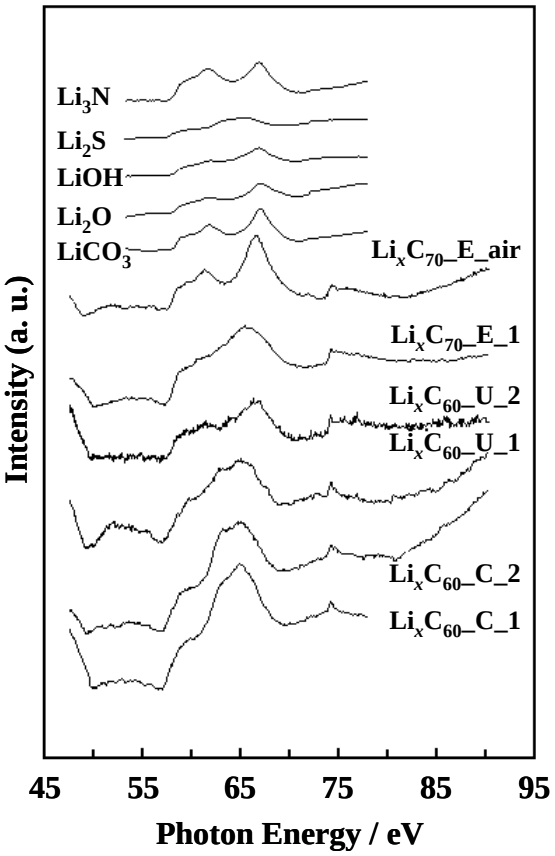

Figure 1. Li *K*-edge XANES spectra of Li_xC_{60} and Li_xC_{70} (x = 14 ± 2) and reference samples.

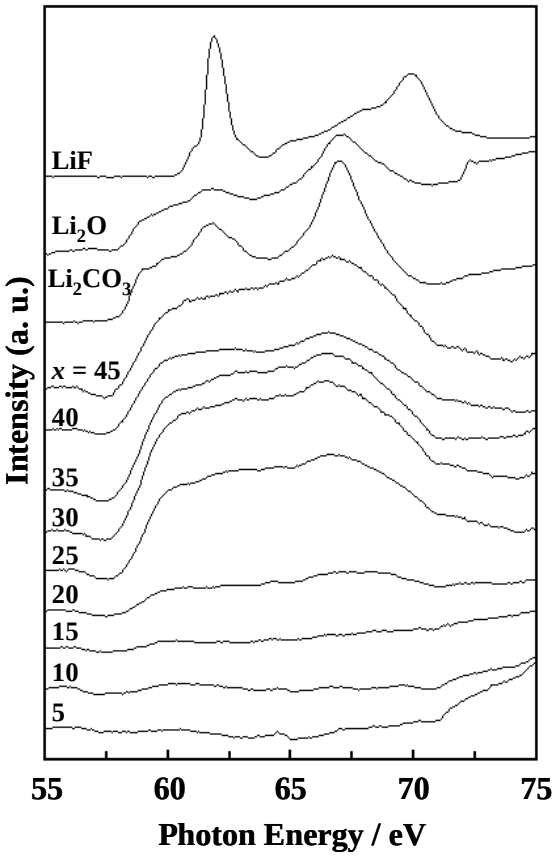

Figure 2. Li *K*-edge XANES spectra of lithium borate glasses xLi$_2$O-$(100-x)$B$_2$O$_3$ and reference samples.

References

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