Chemical reaction of metal-fullerene in gas phase (2)

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Since the discovery of macroscopic generation and purification procedure of fullerenes and endohedral fullerenes, the geometric structure and the formation mechanism of them has been one of the most intriguing issues. Recently X-ray diffraction study\cite{1} demonstrated that the metal atom(s) are encapsulated with in a fullerene cage. On the other hand, in case of metal-fullerene which were produced by laser-vaporization cluster beam source in gas phase, several question has not yet been fully understood such as the geometric structure, formation mechanism, chemical reactivity, and so on. To examine these question, chemical reaction of pure carbon cluster anions C\textsubscript{n}\textsuperscript{-} and lanthanum-carbon binary cluster anions \textit{LaC}\textsubscript{n}\textsuperscript{-} with NO were performed by using FT-ICR mass spectrometer.\cite{2} Fig.1(a) shows the FT-ICR mass spectrum of the injected and trapped clusters. In order to observe the chemical reaction product on a clean baseline, all clusters except for C\textsubscript{44}\textsuperscript{-}, C\textsubscript{47}\textsuperscript{-}, \textit{LaC}\textsubscript{44}\textsuperscript{-} were excited away from the ICR cell by the selective RF excitation called “SWIFT” technique. Clusters were well thermalized to the room temperature by exposures to argon at a pressure of at 1 \textmu 10\textsuperscript{-5} Torr for 2 seconds after SWIFT. Fig.1(b) shows the mass spectrum measured after this mass selection. Fig.1(c) shows the results of exposure of C\textsubscript{44}\textsuperscript{-}, C\textsubscript{47}\textsuperscript{-}, \textit{LaC}\textsubscript{44}\textsuperscript{-} to NO at 1 \textmu 10\textsuperscript{-5} Torr for 1.0 seconds. C\textsubscript{47}\textsuperscript{-} reacted well and the signal of C\textsubscript{47}(NO)\textsuperscript{-} was observed. On the other hand, C\textsubscript{44}\textsuperscript{-} was not reacted so much, and an only small signal of C\textsubscript{44}(NO)\textsuperscript{-} was observed. Throughout the study odd-numbered C\textsubscript{n}\textsuperscript{-} were more reactive than even-numbered clusters. As shown in the figure, \textit{LaC}\textsubscript{44}\textsuperscript{-} was not reactive with NO. Throughout the study, no chemical reaction of NO molecules and H atom were observed for \textit{LaC}\textsubscript{n}\textsuperscript{-} where \textit{n}=even and \textit{n} \geq 36. This can be explained by the hypothesis that \textit{LaC}\textsubscript{n}\textsuperscript{-} (\textit{n}=even and \textit{n} \geq 36) have no dangling bonds, in other words all carbon atoms of have \textit{SP}\textsuperscript{2} bondings. At this stage we consider that those \textit{LaC}\textsubscript{n}\textsuperscript{-} (\textit{n}=even and \textit{n} \geq 36) are fullerene-like structures with metal atom inside.

References: