Chemical reaction of metal-fullerene in gas phase メタルフラーレンの気相反応

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[ABSTRACT] Since the discovery of metal-fullerenes, the geometric structure had been the most exciting issue. Especially, the question "whether metal atom(s) are encapsulated or not" has been examined by several experimental methods and theoretical calculations. Recent X-ray diffraction study has proven ⁽¹⁾ that some metal-fullerenes such as $Sc@C_{82}$ and $Sc_2@C_{84}$ that were prepared in macroscopic amount encapsulate metal atom(s). On the other hand, the assignment of geometric structure of metal-fullerenes that were produced by the supersonic cluster beam source has been very difficult. To understand the geometric structure of these metal-fullerenes we produced metal-fullerenes by two different ways, one is the laser vaporization of a metal-carbon composite disk and the other is gas phase association of C_{60} with metal atoms. Then we tried to determine the location of the metal in these spices by comparison of their reactivity with NO by FT-ICR (Fourier Transform Ion Cyclotron Resonance) mass spectrometer.

Fig. 1 shows a example of FT-ICR mass spectra of the reaction process for LaC_{44} with NO. The top panel Fig. 1(a) shows the FT-ICR mass spectrum of carbon cluster anions (C_n) and lanthanum-carbon cluster anions (LaC_n) as injected from a laser vaporization of lanthanum-carbon composite disk by using supersonic cluster beam source. In order to observe the chemisorption reaction product on a clean baseline, all clusters except for LaC_{44} were excited away from the ICR cell by the selective RF excitation called "SWIFT" (Stored Waveform Inverse Fourier Transform) technique. Clusters were well thermalized to the room temperature by exposures to argon at a pressure of at 1×10^{-5} Torr for 10 seconds after SWIFT. Fig. 1(b) shows the mass spectrum measured after this mass selection. Fig.1(c) shows the results of exposure of LaC_{44}^{-1} to NO at 1×10^{-5} Torr for 20 seconds. As shown in the figure, the LaC_{44}^{-1} were clearly unreactive with NO. Compared with the results of oxidation of YC_n⁺ done



Fig.1 FT-ICR mass spectra of the reaction process for LaC_{44} with NO.

by McElvany and co-workers ⁽²⁾ (the comparison is indirectly, because they used N₂O for reaction), this result suggests that the lanthanum atom is encapsulated in the C₄₄ fullerene cage. The chemical reaction experiments for positive and negative clusters of LaC₄₄ LaC₅₀ LaC₆₀ from the composite disk are compared with the reaction of LaC₆₀ generated from the gas-phase associating.

References (1) M.Takata et al., Nature, **377**, 46 (1995). (2) S.W.Mclvany, J.Phys.Chem., **96**, 4935, (1992).

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