FT-ICR studies of metal-carbon binary clusters for formation mechanism of endohedral fullerene

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A FT-ICR (Fourier Transform Ion Cyclotron Resonance) mass spectrometer directly connected to the laser vaporization cluster beam source was implemented in order to study the clustering process of endohedral metallo-fullerene (Figure 1). Cluster beams were generated by laser-vaporizations of various sample materials used for arc-discharge generation of metal-containing fullerene and SWNT (single-wall carbon nanotube), i.e. La, Y, Sc, Gd, Ce, Ca, and Ni-Y.

An example of FT-ICR mass spectra is shown in Figure 2 for La-C binary clusters. It is remarkable that almost no pure carbon clusters are observed, except for the small signal of C_{60}. Positive La-C, Y-C, Sc-C, Gd-C, Ce-C binary clusters commonly showed strong MC_{2n}^{+} signal in the range of $36 < 2n$ with intense magic numbers at MC_{44}^{+}, MC_{50}^{+} and MC_{60}^{+}. It was speculated that the even-numbered clusters corresponded to the annealed random caged clusters observed in our molecular dynamics simulations.

The apparent minimum sizes of metallo- and di-metallo- clusters strongly suggest that all of these carbon clusters have the caged form with one or two metal atoms inside.

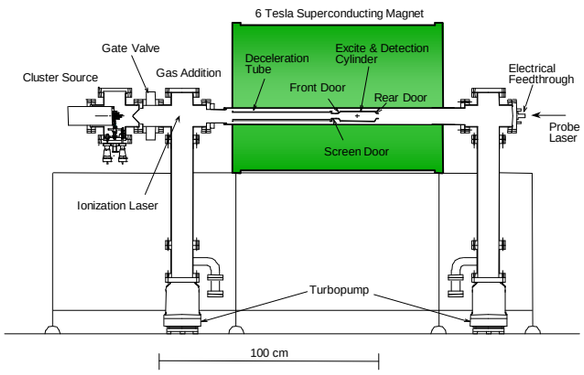

Figure 1. FT-ICR apparatus with direct injection cluster beam source

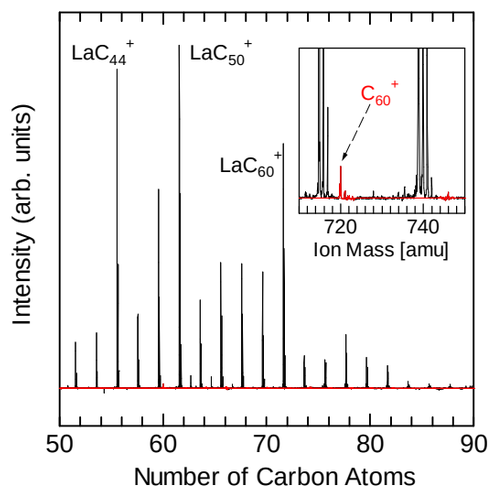

Figure 2 Lanthanum-carbon binary clusters