Bottom-Up Formation of Endohedral Metallofullerenes is Directed by Charge Transfer

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Introduction

An understanding of chemical formation mechanisms is essential to achieve effective yields and targeted products. One of the most challenging endeavors is synthesis of molecular nanocarbon. Endohedral metallofullerenes (EMFs) are of particular interest because of their unique properties that offer promise in a variety of applications. Nevertheless, the mechanism of formation from metal-doped graphite has largely eluded experimental study because harsh synthetic methods are required to obtain EMFs.

Experimental

Here, we report bottom-up formation of mono-metallofullerenes under core synthesis conditions.

Results and Discussion

We find that charge transfer is a principal factor that guides formation, based on characterization of metallofullerenes with virtually all available elements of the periodic table. **Figure 1** shows that the "magic numbers" for the cage sizes for endohedral metallofullerenes can differ substantially from those for empty cages. These results could enable production strategies that overcome long-standing problems that hinder current and future applications of metallofullerenes.

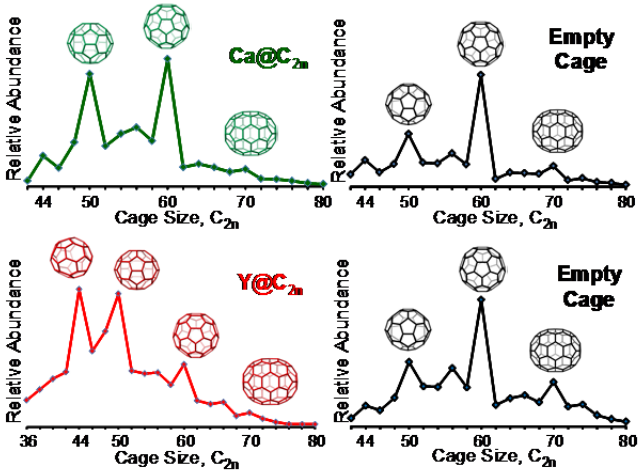

Fig. 1. Cluster cations formed by laser evaporation of metal-doped graphite for selected elements of Group II (top) and Group III (bottom) metals with corresponding $M@C_{2n}$ and C_{2n} distributions, Positive ions are representative of neutral distributions. $M@C_{44}$ (M = metal) contains four sets of triple sequentially fused pentagons, $M@C_{50}$ exhibits five sets of double fused pentagons, and all pentagons are isolated for $M@C_{60}$.

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