Chemical Redox and Exohedral Derivatization: Powerful Tools for Accessing "Insoluble" Endohedral Fullerenes

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New materials based on endohedral metallofullerenes such as $Gd@C_{2n}$ and $Ho@C_{2n}$ have promising medicinal applications, including use as diagnostic imaging and nuclear medicine agents. In order to use the $M@C_{2n}$ species in pharmaceutical formulations, their efficient separation from empty fullerenes and their exohedral derivatization is highly desirable.

Development of $M@C_{2n}$ species has centered on those soluble in "normal" fullerene solvents, particularly several isomers of $M@C_{82}$. However, the majority of $M@C_{2n}$ produced by the standard carbon-arc process are not of the soluble variety. Here, we show how chemical redox manipulation of the charge state of $M@C_{2n}$ is broadly useful for the identification and separation of distinct groupings of previously insoluble lanthanide metallofullerenes. Chemical derivatization of these materials can then be used to confer desirable properties such as water solubility, allowing their in vivo evaluation in applications such as magnetic resonance imaging.