

Buckyball Maracas: New Endohedral Fullerene Structures, Reactivity and Mechanistic Aspects

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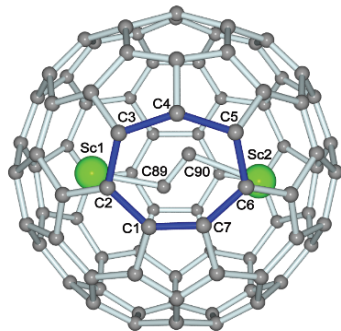
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Endohedral clusterfullerenes were serendipitously discovered in 1999 with the isolation of $\text{Sc}_3\text{N}@\text{C}_{80}$, the first member of what has become an extensive family of interesting compounds. Most of these compounds have been shown to be fairly unreactive due to their unique electronic structure, which formally contains a highly positive cluster encapsulated inside a carbon cage that is highly negatively charged (the accepted model for $\text{Sc}_3\text{N}@\text{C}_{80}$ involves the transfer of six electrons to form $[\text{Sc}_3\text{N}]^{6+}[\text{C}_{80}]^{6-}$).

We recently isolated and characterized two new scandium carbide endohedral structures, $\text{Sc}_2\text{C}_2@C_{2v}(9)\text{-C}_{86}$ and $\text{Sc}_2\text{C}_2@C_s(\text{hept})\text{-C}_{88}$. The former compound represented the first observation of the $C_{2v}(9)$ C_{86} cage and exhibited a distorted but ordered scandium cluster inside. The second compound is much more unique in that it possesses a heptagonal ring on its carbon surface, making it the only C_{88} endohedral cage with such a heptagon, see structure below. Extensive theoretical calculations suggest that the C_{88} compound is formed directly by the insertion of a C_2 unit into a specific location of the C_{86} compound, to yield a kinetically trapped compound which is not the thermodynamically favored one.

Finally, we have also been involved in the synthesis and characterization of new Uranium-based endohedral fullerenes and have obtained X-Ray crystal structures for several of these compounds, which reveal interesting metal-cage interactions and totally unprecedented compounds with formula: $\text{U}_2\text{X}@\text{C}_{78}$, where $\text{X} = \text{C}, \text{O}, \text{or N}$. The C-based compounds have been crystallized and the encapsulated U_2C cluster exhibits unprecedented bonding with totally unanticipated properties.



The synthesis, purification and characterization of these interesting endohedral fullerenes will be presented and discussed, along with very recent results about uranium-based endohedrals.