New routes to stable endohedral nitride cluster fullerenes

Lothar Dunsch,[1] Petra Georgi,[1] Jens Naock[1] and Matthias Krause[1]

[1] IFW Dresden
Helmholtzstr. 20
Dresden D-01069
Germany

Recently nitride cluster fullerenes have been shown to offer new types of endohedral structures. The included cluster can stabilizes generally the fullerene cage like icosahedral C80 which is not to be isolated in the empty form. Even non-IPR cage structures like C68 can be stabilized by nitride clusters. On the other hand these fullerenes provide an ideal environment with its internal space, stabilizing of such nitrogen containing clusters which have not been isolated as such.

To open a new route for endohedral nitride cluster fullerene structures we report on the application of a reactive atmosphere in the arc burning process to get a efficient production of these new cluster fullerenes. The situation in the gas atmosphere and the reaction products are described in detail.

The second main point of this study was the influence of the metal in the nitride cluster on the stability of the fullerene. Thus a large variety of nitride cluster fullerenes has been prepared. Among them are structures like Sc3N@C80, Y3N@C80, Ho3N@C80, Er3N@C80, Tb3N@C80, Sc2ErN@C80 and ScEr2N@C80.

The fullerene structures under study were produced by the Krtschmer- Huffman method using metal filled and empty graphite rods. The influence of the preparation conditions was studied with respect to the atmosphere in the arc burning chamber. Different mixtures of reactive gas NH3 and the inert cooling gas were used.

As the endohedral fullerene Me3N@C80 is the main product in the fullerene soot the chromatographic separation of these new endohedral structures turns out to be very simple as the fullerene can be isolated in a high purity by a one step procedures.

The isolated endohedral structures were investigated by UV-Vis IR spectroscopy as well as by cyclic voltammetry. The results demonstrate a large band gap of all materials and were compared with the data for empty fullerenes. The influence of the metal on the band gap is discussed in detail.

As a conclusion of the synthesis of new endohedral fullerenes by reactive atmospheres in the burning chamber a general outlook of the potentialities of this new route in fullerene production is given.