New Endohedral Fullerenes: From Ho3N@C80 to CH2@C70

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Endohedral fullerenes have been shown to offer new types of structures which are quite special for this type of compounds. The included atoms, ion or cluster can stabilize the fullerene cage which is not to be isolated in the empty form like C72 or C74 and even the non-IPR structures C66 and C68 .On the other hand fullerenes can provide an ideal isolated environment with its internal space, which enables the stabilization of highly reactive atoms such as nitrogen (N@C60) and clusters such as Sc2C2 (Sc2C2@C84) or Sc3N (Sc3N@C80). To open the route for new endohedral fullerene structures we report on the influence of the type of the atmosphere in the arc burning process as well as on new nitride cluster fullerenes like Ho3N@C80 and the first isolation and characterization of the smallest included carbene, CH2, in the endohedral fullerene structure CH2@C70. 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 and different mixtures of reactive generation and inert cooling gas was used. The chromatographic separation of the new endohedral structures was carried out by a multi step HPLC including recycling procedures. As preferred structures in this study Ho3N@C80 and CH2@C70 are studied. The isolated endohedral structures were investigated by 13C NMR, UV-Vis, ESR, Raman and IR spectroscopy as well as by cyclic voltammetry. The results of Raman spectroscopic data were compared with the data for other endohedral fullerenes and the interactions of the clusters with cage are analysed. Furthermore ab initio calculations were used to confirm the preferred endohedral structure. In the case of CH2C70 both the exohedral and the endohedral fullerene was prepared and isolated and compared in their spectroscopic properties. As a conclusion of the synthesis of new endohedral fullerenes by vaiation of the atmosphere in the brning chamber a general outlook of the potentialities of this new route in fullerene production is given.