

Abstract Submitted
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Cage-Core Interactions in Fullerenes Enclosing Metal Clusters with Multiple Scandium and Yttrium Atoms. LIU DAN, FRANK HAGELBERG, Jackson State University — Pronounced stability has been reported for metallofullerenes of the form $N\text{Sc}_3@C_N$ ($N = 68, 78$) /1/. In response of these and related findings, Density Functional Theory studies have been performed on the relation between cage-core interactions and the geometry as well as stability of endofullerenes with metal impurities containing Sc and Y. Substantial electron transfer from the metal core to the fullerene cage combines with electron backdonation, involving the interaction between the occupied orbitals of the negatively charged cage and the unoccupied d orbitals of the positively charged core. The Hückel $4n+2$ rule, well established in organic chemistry, is shown to provide a valuable heuristic tool for understanding the intramolecular electron transfer and the related stability gain /1/. The usefulness of the aromaticity concept for explaining and predicting the architecture of metallofullerenes is further exemplified by the units $\text{Sc}_2@C_{84}$ and $\text{Y}_2@C_{84}$ which were analyzed in spin triplet and singlet conditions. The Sc_2 core turns out to be realized by two separated ions, while Y_2 forms a bound subunit. These findings are in agreement with conclusions based on the $4n + 2$ rule, assisted by Nucleus Independent Chemical Shift (NICS) calculations. /1/ Stevenson, S.; Fowler, P.W.; Heine, T.; Duchamp, J.C.; Rice, G.; Glass, T.; Harich, K.; Hadju, F.; Bible, R.; Dorn, H.C. *Nature*, 2000, 408, 427, /2/ S. S. Park, D. Liu, F. Hagelberg, *J. Phys. Chem. A* 109, 8865 (2005).

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