Hydrogenation of Endohedral Metallofullerenes

Jianyuan Zhang, Wujun Fu, Harry C. Dorn

Department of Chemistry, and Carilion Research Institute, Virginia Polytechnic Institute and State University

2 Riverside Circle, Roanoke, VA 24016, USA

Many promising chemical reactions to functionalize empty cage fullerenes, e.g. C_{60} , C_{70} , have been successfully performed on endohedral metallofullerenes (EMFs). One important class of these reactions is the hydrogenation reaction, which change the hybridization state of certain carbon atoms on a fullerene cage from sp² to sp³ and could have both theoretical and practical significance in the understanding of fullerene cages. However, so far little to none work has been done on the hydrogenation reaction on EMFs. In this talk, we present our efforts and results in attempt to accomplish the hydrogenation of trimetallic nitride template EMFs. The reactivity of the M₃N@C₈₀ (M=Sc, Y) towards hydrogenation is directly compared with that of the empty cage fullerenes.