Synthesis and Isolation of the Titanium-Scandium Endohedral Fullerenes-Sc2TiC@Ih-C80, Sc2TiC@D5h-C80 and Sc2TiC2@Ih-C80 - DTU Orbit (02/03/2019)

Synthesis and Isolation of the Titanium-Scandium Endohedral Fullerenes-Sc2TiC@Ih-C80, Sc2TiC@D5h-C80 and Sc2TiC2@Ih-C80: Metal Size Tuning of the TiIV/TiIII Redox Potentials

The formation of endohedral metallofullerenes (EMFs) in an electric arc is reported for the mixed-metal Sc-Ti system utilizing methane as a reactive gas. Comparison of these results with those from the Sc/CH4 and Ti/CH4 systems as well as syntheses without methane revealed a strong mutual influence of all key components on the product distribution. Whereas a methane atmosphere alone suppresses the formation of empty cage fullerenes, the Ti/CH4 system forms mainly empty cage fullerenes. In contrast, the main fullerene products in the Sc/CH4 system are Sc2Cn@C80 (the most abundant EMF from this synthesis), Sc2Cn@C80 isomers of Sc2C2@C82, and the family Sc2C2n (2n=74, 76, 82, 86, 90, etc.), as well as Sc4CH@C80. The Sc-Ti/CH4 system produces the mixed-metal Sc2TiC@C2n (2n=68, 78, 80) and Sc2TiC2@C2n (2n=80) clusterfullerene families. The molecular structures of the new, transition-metal-containing endohedral fullerenes, Sc2TiC@Ih-C80, Sc2TiC@D5h-C80, and Sc2TiC2@Ih-C80, were characterized by NMR spectroscopy. The structure of Sc2TiC@Ih-C80 was also determined by single-crystal X-ray diffraction, which demonstrated the presence of a short Ti=C double bond. Both Sc2TiC- and Sc2TiC2-containing cluster-fullerenes have Ti-localized LUMOs. Encapsulation of the redox-active Ti ion inside the fullerene cage enables analysis of the cluster-cage strain in the endohedral fullerenes through electrochemical measurements.

General information
State: Published
Organisations: University of California at Davis, Leibniz Institute for Solid State and Materials Research Dresden (IFW)
Number of pages: 10
Pages: 13098-13107
Publication date: 2016
Peer-reviewed: Yes

Publication information
Journal: Chemistry-a European Journal
Volume: 22
Issue number: 37
ISSN (Print): 0947-6539
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.9 SJR 2.265 SNIP 1.02
Web of Science (2017): Impact factor 5.16
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.03 SJR 2.352 SNIP 1.068
Web of Science (2016): Impact factor 5.317
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.99 SJR 2.461 SNIP 1.195
Web of Science (2015): Impact factor 5.771
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.51 SJR 2.526 SNIP 1.222
Web of Science (2014): Impact factor 5.731
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 5.68 SJR 2.643 SNIP 1.239
Web of Science (2013): Impact factor 5.696
ISI indexed (2013): ISI indexed yes