

Synthesis, Isolation and Structural Characterization of Some Metal-Carbides Metallofullerenes

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○Takashi Inoue¹, Yasuhiro Ito¹, Hiroe Moribe¹, Baopeng Cao¹, Tetsuo Tomiyama¹,
Toshiya Okazaki¹, Toshiki Sugai¹, Takako Suematsu², Naoyuki Fujii²
Kazutetsu Nojima² and Hisanori Shinohara^{1,3,4}

(Author's Name: Times, 12pt, Centered)

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¹*Department of Chemistry, Nagoya University, Nagoya 464-8602, Japan*

²*JEOL Ltd., Akishima, Tokyo 196-8558, Japan*

³*Institute for Advanced Research, Nagoya University, Nagoya 464-8602, Japan*

⁴*CREST, Japan Science and Technology Corporation, c/o Department of Chemistry,
Nagoya University, Nagoya 464-8602, Japan*

(Author's Address & Affiliation: Times, 12pt, Italic, Centered)

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Metal-carbide metallofullerene has been known as one of the new class of cluster endohedral fullerenes. (Sc₂C₂)@C₈₄ is the first metal-carbide metallofullerene[1] which has been synthesized and structurally characterized by both ¹³C NMR and powder X-ray diffraction. At the first stage of the investigation, because the molecular formula (stoichiometry) of the fullerene was Sc₂C₈₆, this molecule had simply been considered as normal metallofullerene having a structure Sc₂@C₈₆. However, the (Sc₂C₂)@C₈₄ structure with a Sc₂C₂ carbide cluster inside was clearly determined by ¹³C NMR and powder X-ray diffraction measurements. In this presentation, we report that one of the yttrium metallofullerenes, Y₂C₈₄(III), is a metal-carbide metallofullerene.

A ¹³C NMR spectrum of Y₂C₈₄(III) is shown in Figure 1. The spectrum exhibits in total 17 distinct lines that consist of a series of eleven full-intensity lines, five half-intensity lines and one 1/6-intensity line. Only C_{3v}(8) isomer of IPR C₈₂ can satisfy the number of NMR lines and relative intensity. We interpret that this metallofullerene has a metal-carbide endohedral structure in which two yttrium and two carbon atoms are encapsulated in the C₈₂ fullerene, namely (Y₂C₂)@C₈₂.

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[1] C. R. Wang, T. Kai, T. Tomiyama, T. Yoshida, Y. Kobayashi, E. Nishibori, M. Takata, M. Sakata and H. Shinohara, *Angew. Chem. Int. Ed.*, **40**, 397 (2001).

(References: Times, 12pt, Left)

Corresponding Author: Hisanori Shinohara

TEL: +81-52-789-2482, FAX: +81-52-789-1169, E-mail: noris@cc.nagoya-u.a.jp

(Corresponding Author, TEL, FAX, E-mail: Times, 10pt, Left)