

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

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Metal-carbide metallofullerene has been known as one of the new class of cluster endohedral fullerenes. $(Sc_2C_2)@C_{84}$ 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 Sc_2C_{86} , this molecule had simply been considered as normal metallofullerene having a structure $Sc_2@C_{86}$. However, the $(Sc_2C_2)@C_{84}$ structure with a Sc_2C_2 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, $Y_2C_{84}(III)$, is a metal-carbide metallofullerene.

A ¹³C NMR spectrum of $Y_2C_{84}(III)$ 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 C_{82} 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 C_{82} fullerene, namely $(Y_2C_2)@C_{82}$.

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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, 10pt, Left)

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