Chemical Functionalization of $Sc_3N@C_{80}$

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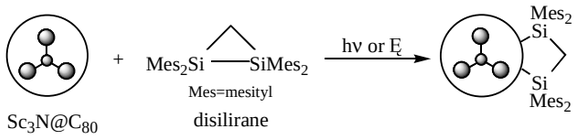
Endohedral metallofullerenes have attracted special interest, because of the unique properties that are unexpected for empty fullerenes. Recently, the novel endohedral $Sc_3N@C_{80}$ has been prepared in remarkably high yield [1]. $Sc_3N@C_{80}$ contains a planar Sc_3N cluster confined within a C_{80} cage with I_h symmetry. $Sc_3N@C_{80}$ can be formally described as a positively charged planer cluster of atoms inside a negatively charged icosahedral carbon cage, $(Sc_3N)^{6+}C_{80}^{6-}$ [1].

In our series of studies on the chemical functionalization of fullerenes with organosilicon compounds, we have reported the bis-silylation of fullerenes with disilirane [2]. In this context, it is worthy to note that disilirane can act as a mechanistic probe to clarify the electronic and chemical characteristics of fullerenes. Although $Sc_3N@C_{80}$ and $La_2@C_{80}$ have the same carbon cage with the same oxidation state ($C_{80}(I_h)^{6-}$), LUMO level of $Sc_3N@C_{80}$ [3] is much higher that of $La_2@C_{80}$ [4]. In this study, we report the redox property and the reactivity of $Sc_3N@C_{80}$ vs. $La_2@C_{80}$.

Thermal and photochemical reaction of $Sc_3N@C_{80}$ with 1,1,2,2-tetrakis(2,4,6-trimethylphenyl)-1,2-disilirane were performed (Scheme). Interestingly, photochemical reaction afforded mono-adducts, which structure determination was carried out by means of NMR measurement (Figure).

[1] Stevenson, S., *et al*., *Nature* **1999**, *401*, 55.
[2] For a review, see: Akasaka, T., *et al*., *J. Synth. Org. Chem. Jpn*. **2000**, *58*, 1066.
[3] Kobayashi, K., *et al*., *J. Comput. Chem.* **2001**, *22*, 1353.
[4] Kobayashi, K., *et al*., *Chem. Phys. Lett*. **1995**, *245*, 230.

Scheme



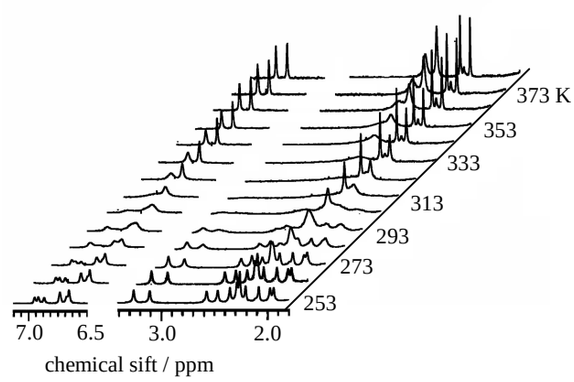


Figure. VT-^{1}H NMR spectra of mono-adducts