Susceptible Electron Spin Adhering to Yttrium Cluster inside an Azafullerene $C_{79}N$

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Spin-active molecules have broad applications in quantum information processing, nano-electronic devices, and ultrahigh- density memory, among them paramagnetic endofullerenes are specially attracting due to their stable electron spin states and novel geometrical structures. $Y_2@C_{79}N$ is a classical endohedral azafullerene whose ESR spectrum shows three groups of distinct hyperfine signals with 1: 2: 1 intensity ratio due to the coupling between the unpaired spin and two equivalent ^{89}Y nuclei (I = 1/2). As the unpaired spin locates on the internal Y_2 cluster, this molecule is highly stable, and it is expected to find broad applications in information science. Herein, we explored controllable spin and magnetic features of this molecule through changing the temperature or performing chemical modification. It was revealed that the exohedral addend not only conduces to the insufficient spin averaging but also leads to the inhomogeneous spin density distributions. These researches make $Y_2@C_{79}N$ to be candidate for promising information materials and molecular devices.

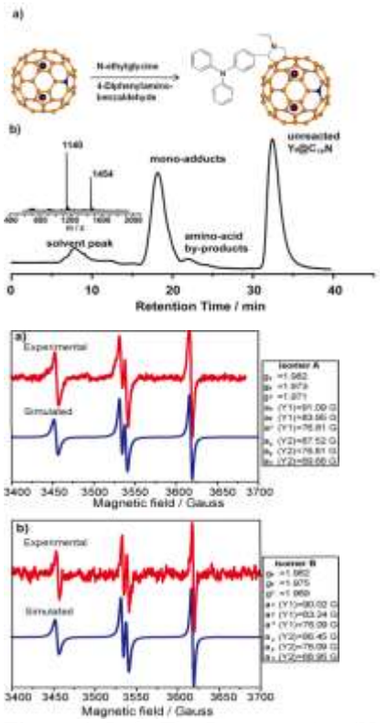

Figure 1. Left: The Prato reaction (N-ethylglycine and 4-Diphenylaminobenzaldehyde treated with $Y_2@C_{79}N$ for 30 mins at 393 K.) b) HPLC profile of reaction products. The inset shows the MALDI-TOF MS for isolated mono-adducts. Right: The experimental (in CS_2 solution at 298 K) and simulated ESR spectra of $Y_2@C_{79}N$ fulleropyrrolidine isomers A (a) and B (b).