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Metallofullerenes are novel forms of fullerene-based materials. “Missing fullerene” C₈₀ is a magic cage in which two, three, even four atoms can be trapped [1-4]. Interestingly, only monometallofullerenes Ca, Sr, Ba@C₈₀ are reported while C₈₀-based monometallofullerenes with I_h symmetry might exhibit novel solid-state properties such as high-T_c superconductivity [5,6].

We report here the first isolation and characterization of Gd@C₈₀. Fig. 1 shows the HPLC chromatogram of the extractives in the toluene solution. The LD-TOF mass spectrometry of the isolated Gd@C₈₀ is inserted in Fig. 2. The high peak at the retention time of 12min, which is assigned to Gd@C₈₀, is due to the optimization of arc-discharge conditions and high-temperature DMF extraction. By using this method, Gd@C₈₀ was isolated in one-step HPLC and the purity was estimated to be more than 98%. The UV-VIS-NIR absorption spectrum of Gd@C₈₀ in toluene solution (as seen in Fig.2) shows different characteristic bands from those of Ca, Sr, Ba@C₈₀, indicating that they have different geometrical or electronic structure. The red-shifted onset of Gd@C₈₀ suggests that the HOMO-LUMO energy gap of Gd@C₈₀ should be smaller than those for Ca, Sr, Ba@C₈₀ [5,6].

Acknowledgment

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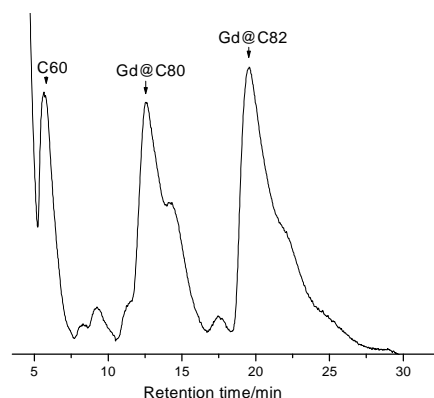


Fig. 1 HPLC chromatogram of the extractives in the toluene solution.

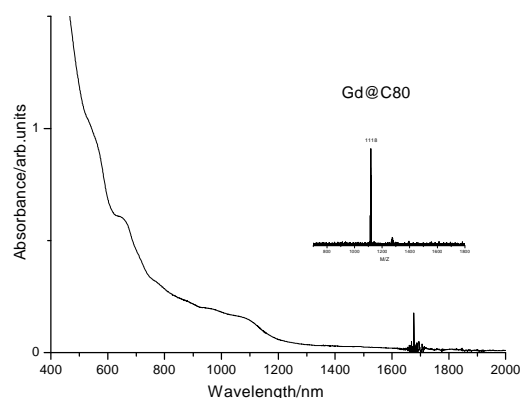


Fig. 2 UV-VIS-NIR absorption spectrum of Gd@C₈₀ in toluene solution, Inset, the LD-TOF mass spectrometry of the isolated Gd@C₈₀