

## Supporting Information

### The V-shaped Polar Molecules Encapsulated into $C_s(10528)$ - $C_{72}$ : Stability and Nonlinear Optical Response

Li-Jie Wang, Rong-Lin Zhong, Shi-Ling Sun, Hong-Liang Xu,\* Xiu-Mei Pan\* and

Zhong-Min Su\*

*Institute of Functional Materials Chemistry, Faculty of Chemistry Northeast Normal University,*

*Changchun 130024, Jilin (P. R. China)*

*E-mail: [hlxu@nenu.edu.cn](mailto:hlxu@nenu.edu.cn), [zmsu@nenu.edu.cn](mailto:zmsu@nenu.edu.cn)*

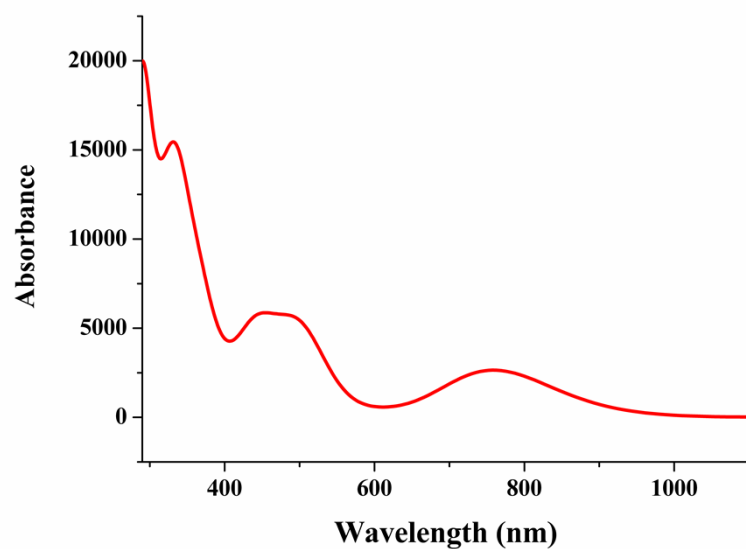


Figure S1. UV-vis-NIR absorption spectra of  $Sc_2S@C_{72}$  obtained by BHandHLYP functional