

Electronic Supplemental Information (ESI) for:

**One-pot Synthesis of New Thio-Derivatives of C₆₀ with the
Unexpected Formation of a Thiazolidine-Fulleropyrrolidine**

Chuanbao Chen,^a Xiaofang Li,^b and Shangfeng Yang*^a

^a *Hefei National Laboratory for Physical Sciences at Microscale, CAS Key Laboratory of Materials for Energy Conversion & Department of Materials Science and Engineering, University of Science and Technology of China (USTC), Hefei 230026, China*

^b *School of Chemistry and Chemical Engineering, Hunan University of Science and Technology, Xiangtan, Hunan 411201, China*

Contents

S1. Mass, ¹H NMR, ¹³C NMR, FTIR, and UV-Vis spectra of compound **3**

S2. The spectroscopic data of compounds **6** and **8**

S3. The spectroscopic data of compounds **10** and **12**

S1. Mass, ^1H NMR, ^{13}C NMR, FTIR, and UV-Vis spectra of compound **3**

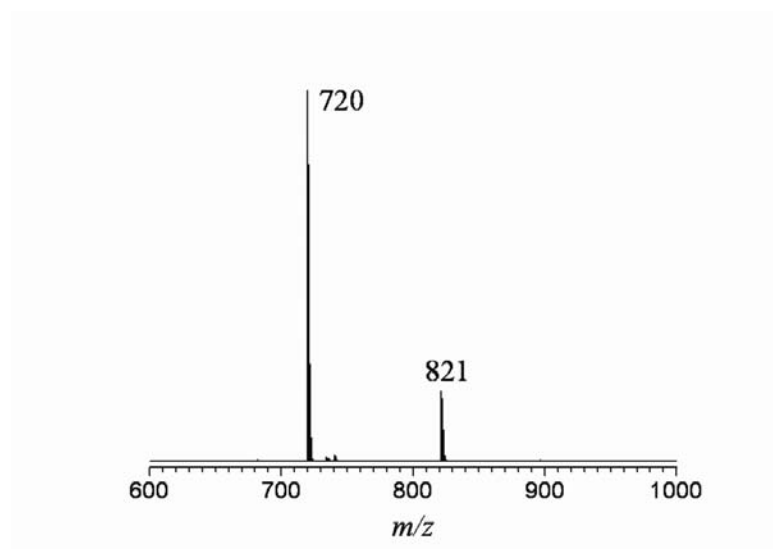


Fig. S1 Positive ion laser desorption time-of-flight (LD-TOF) mass spectrum of compound **3**.

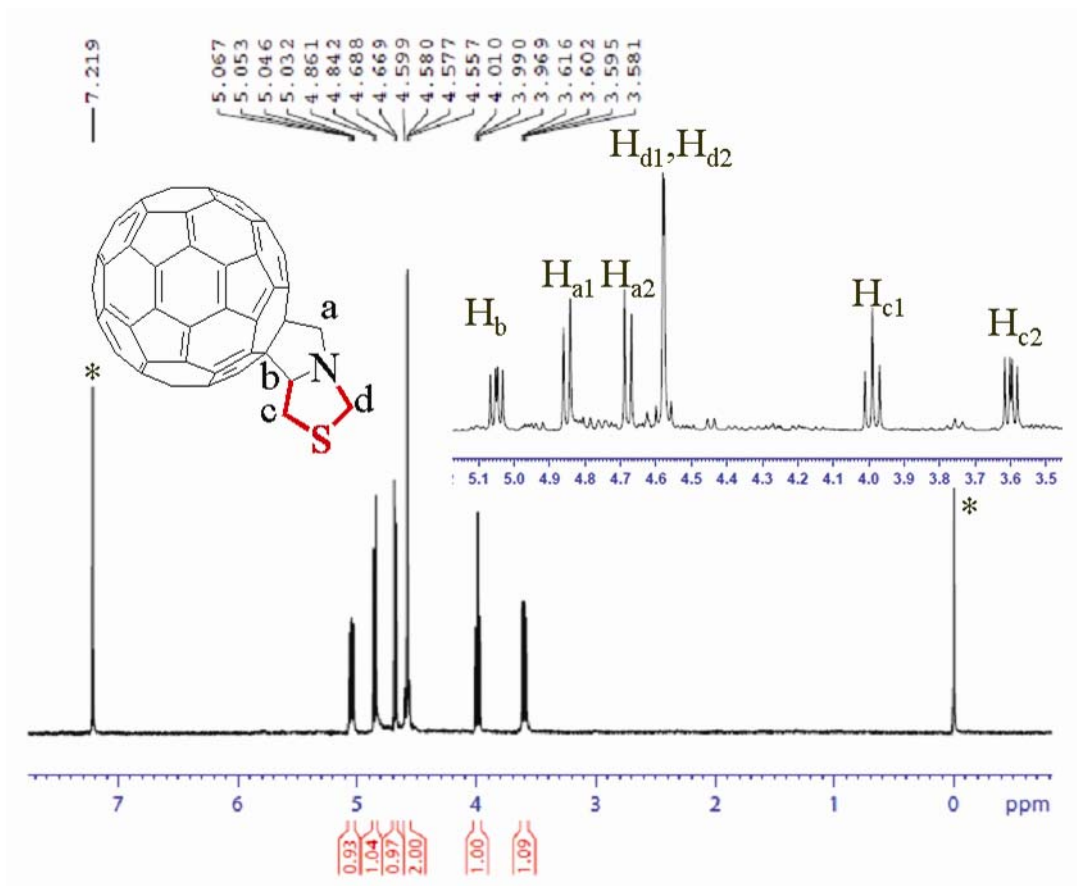


Fig. S2 The ^1H NMR spectrum of compound **3** in $\text{CS}_2/\text{CDCl}_3$. The asterisks represent solvent lines.

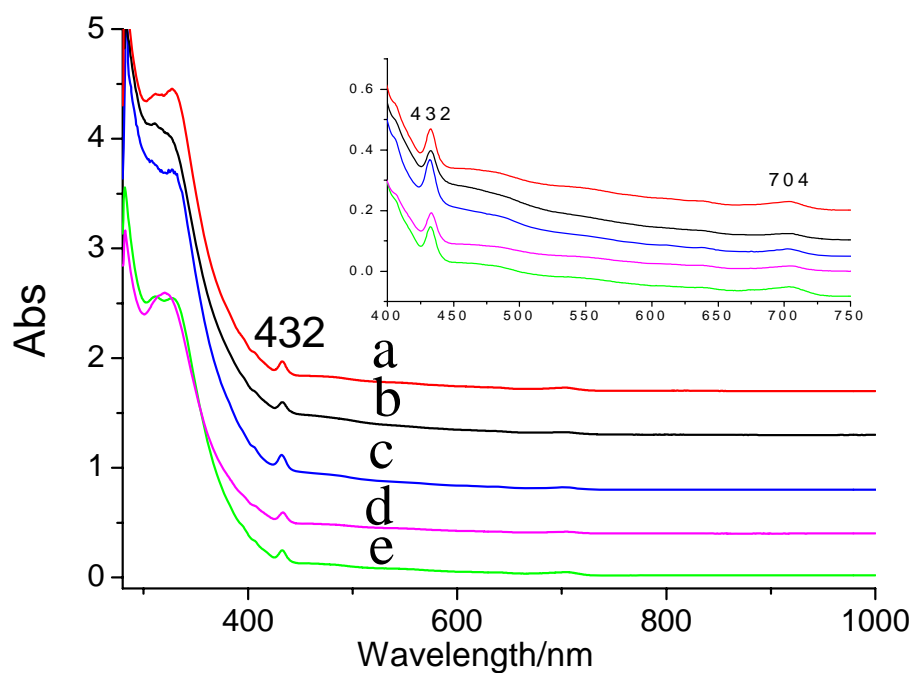


Fig. S3 UV-vis spectra of compounds **3** (a), **6** (b), **8** (c), **10** (d), **12** (e). Inset: enlarged spectral range of 400-750 nm.

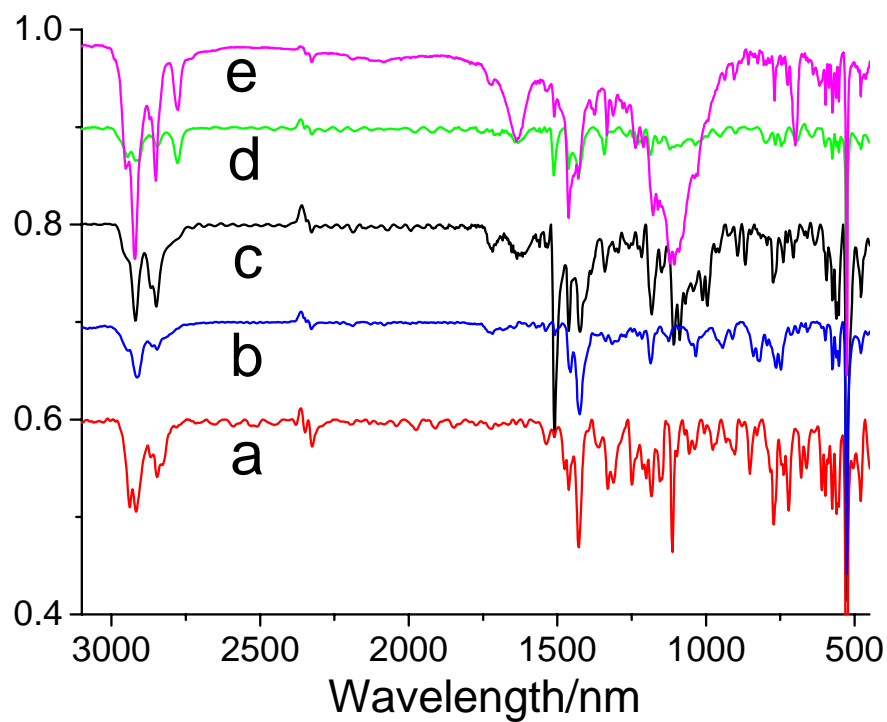


Fig. S4 FTIR spectra of compounds **3** (a), **6** (b), **8** (c), **10** (d), **12** (e).

S2. The spectroscopic data of compounds 6 and 8.

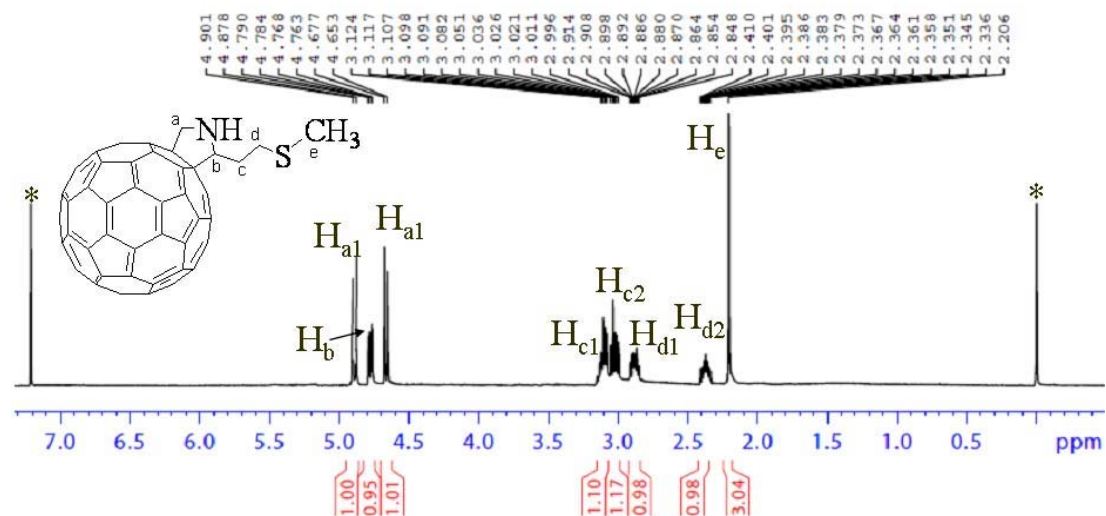


Fig. S5 The ¹H NMR spectrum of compound 6 in CS₂/CDCl₃. The asterisks represent solvent lines.

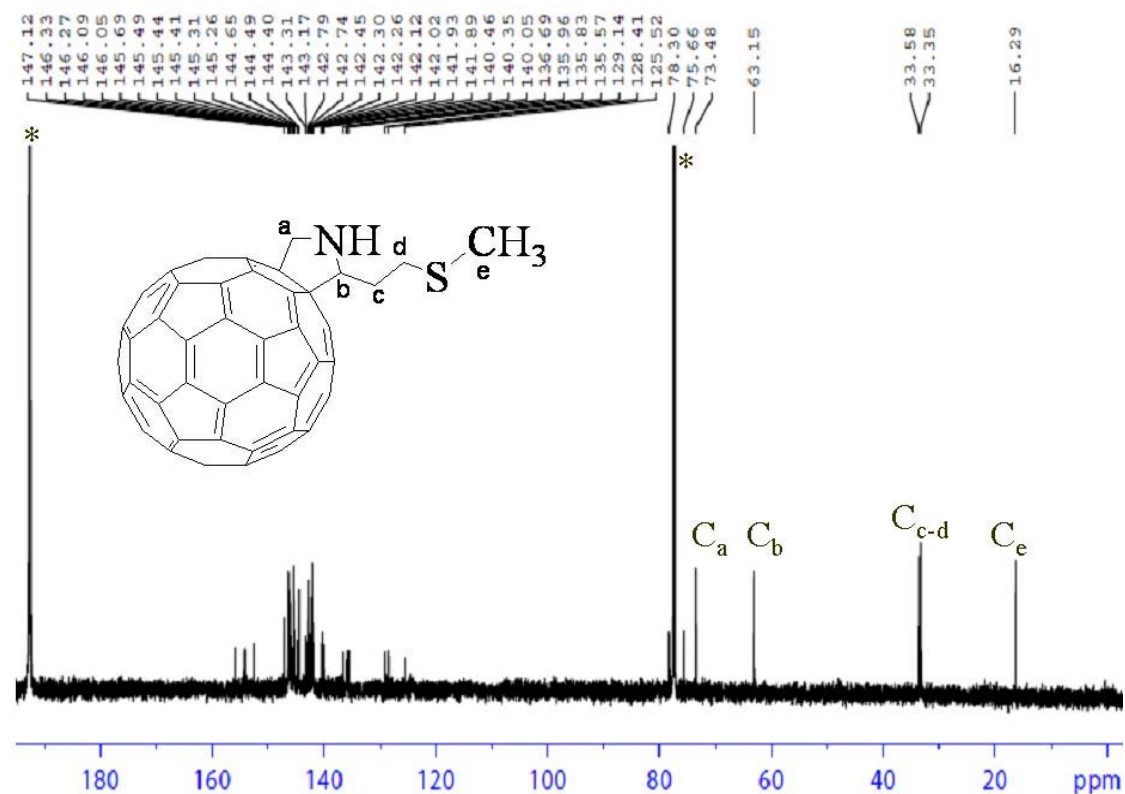


Fig. S6 The ¹³C NMR spectrum of compound 6 in CS₂/CDCl₃. The asterisks represent solvent lines.

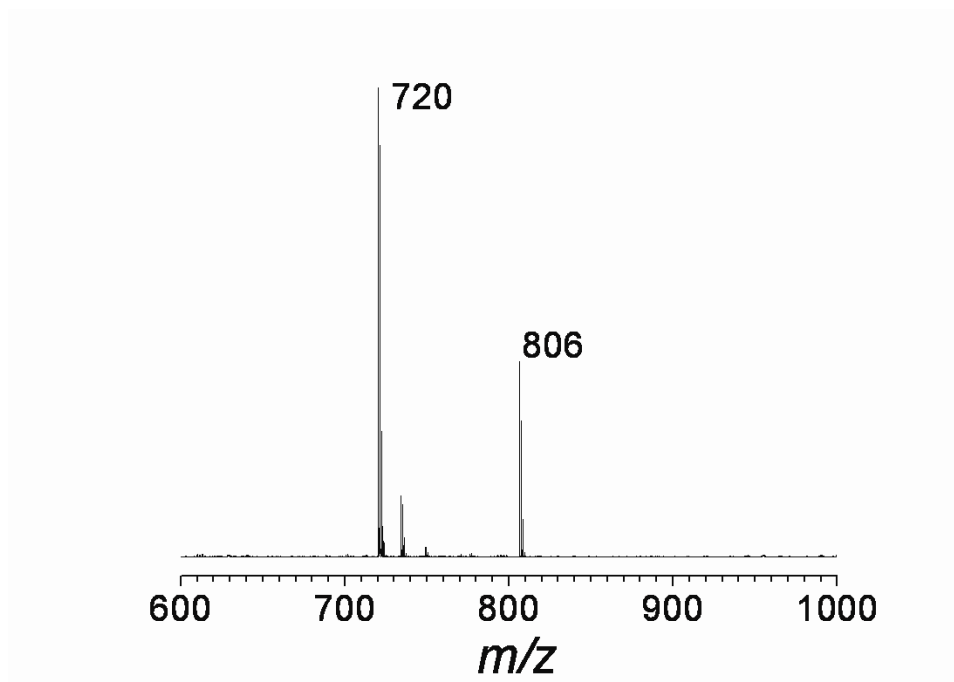


Fig. S7 Positive ion laser desorption time-of-flight (LD-TOF) mass spectrum of compound **8**.

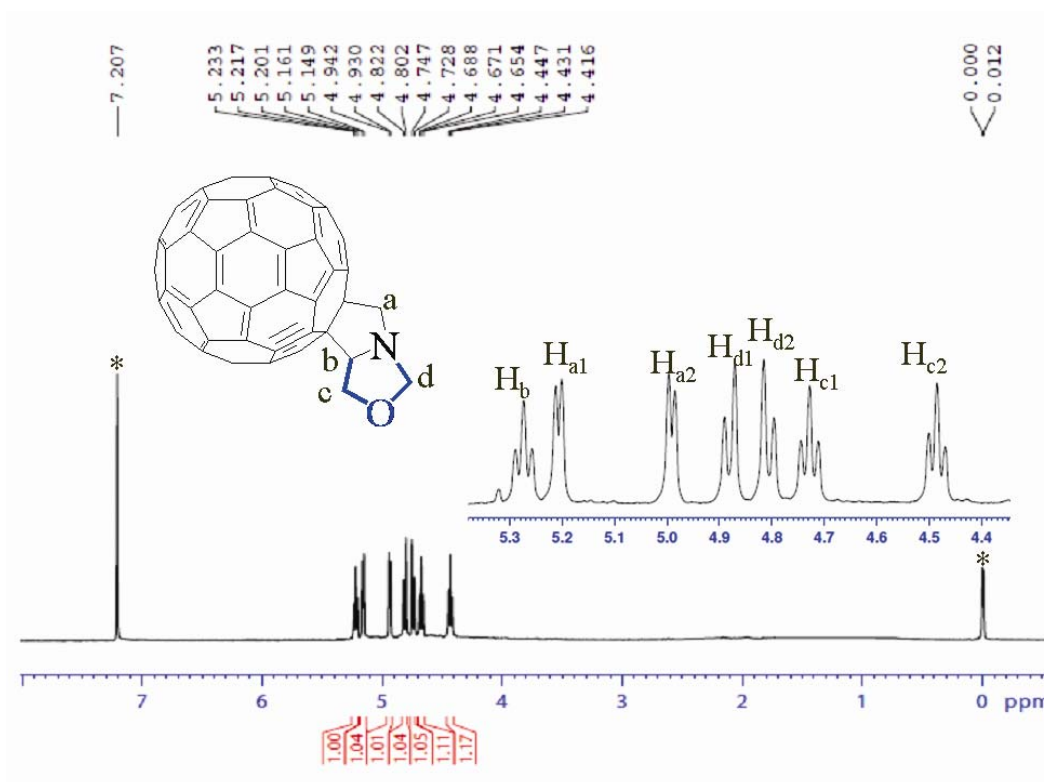


Fig. S8 The ¹H NMR spectrum of compound **8** in CS₂/CDCl₃. The asterisks represent solvent lines.

S3. The spectroscopic data of compounds 10 and 12

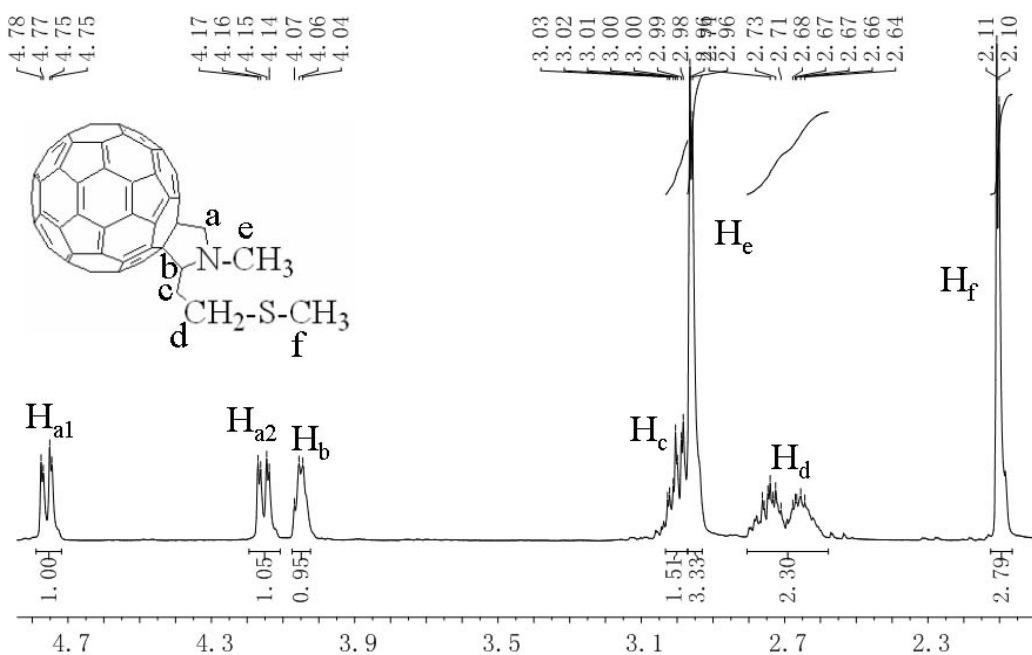


Fig. S11 The ¹H NMR spectrum of compound 10 in CS₂/CDCl₃.

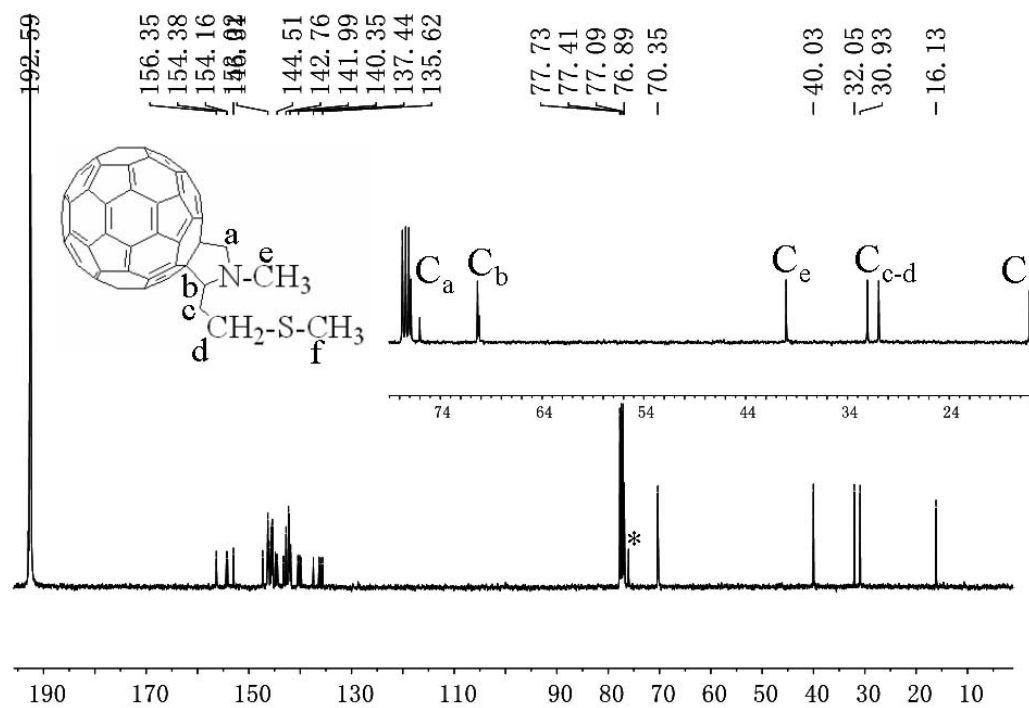


Fig. S12 The ¹³C NMR spectrum of compound 10 in CS₂/CDCl₃. The asterisk represents the impurity from the solvent.

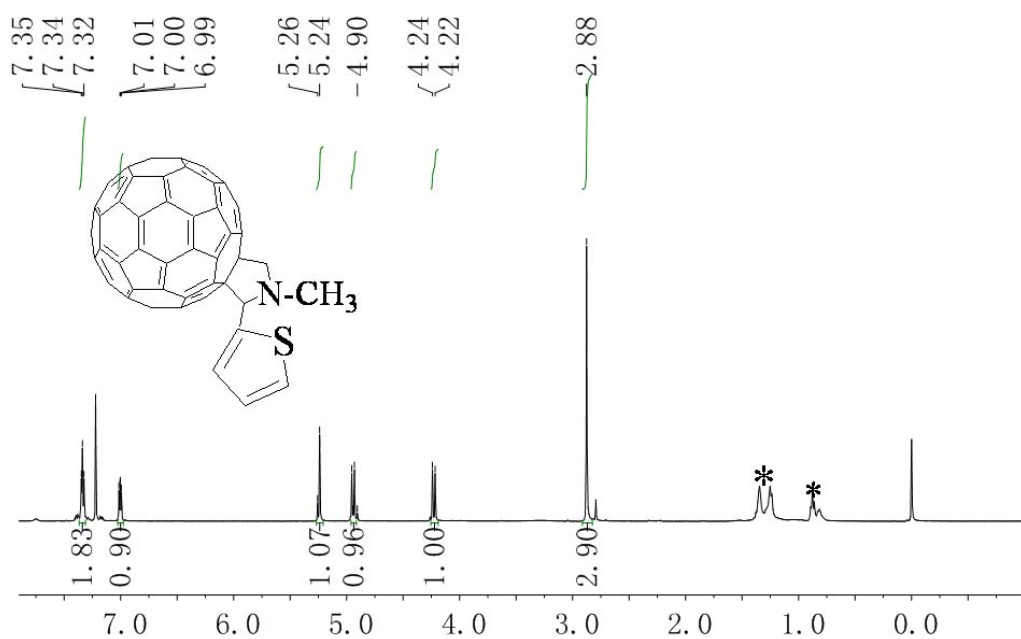


Fig. S13 The ¹H NMR spectrum of compound **12** in CS₂/CDCl₃. The asterisks represent the impurities from the solvent.

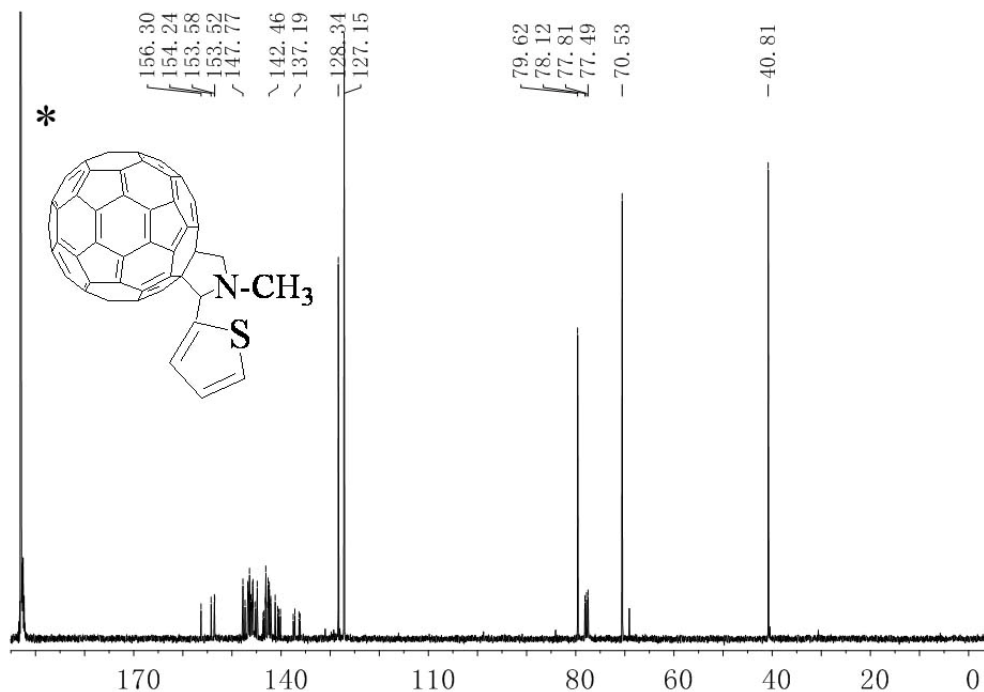


Fig. S14 The ¹³C NMR spectrum of compound **12** in CS₂/CDCl₃. The asterisks represent solvent lines.