

Supporting Information

Half-sandwich scandium dibenzyl complexes bearing penta- or tetra-arylcyclopentadienyl ligands: Synthesis, structure and syndiospecific styrene polymerization activity

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1. Selected NMR spectra

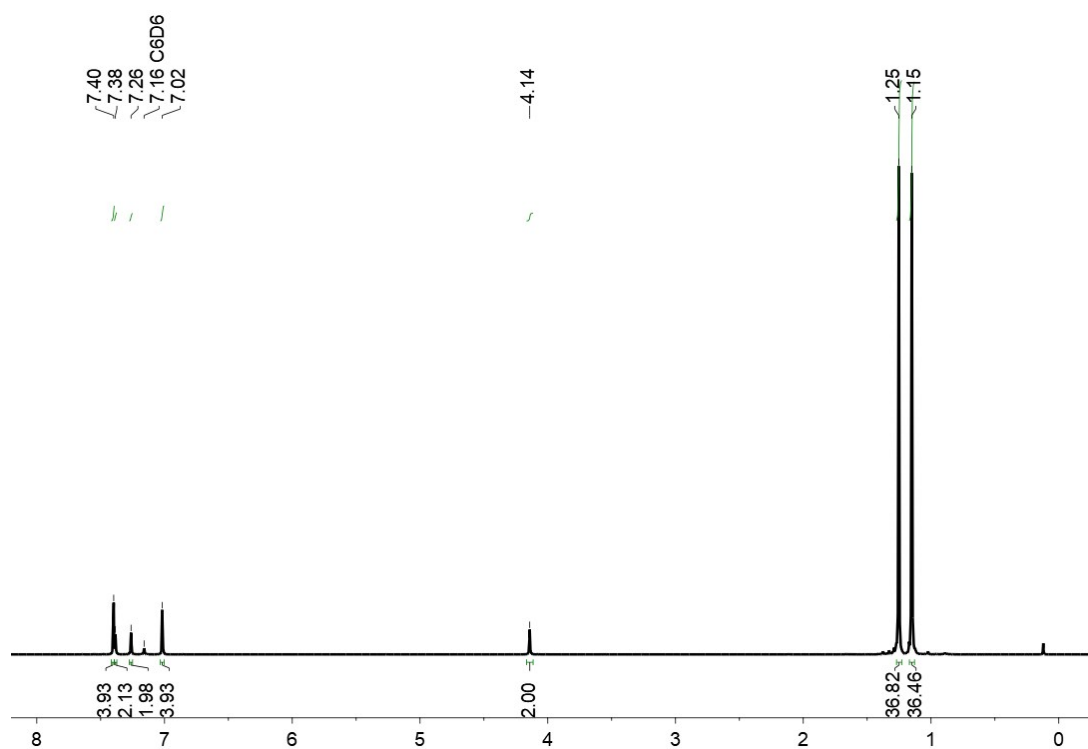


Figure S1. ¹H NMR spectrum (500 MHz) of **L**₃ in C₆D₆ at 25 °C.

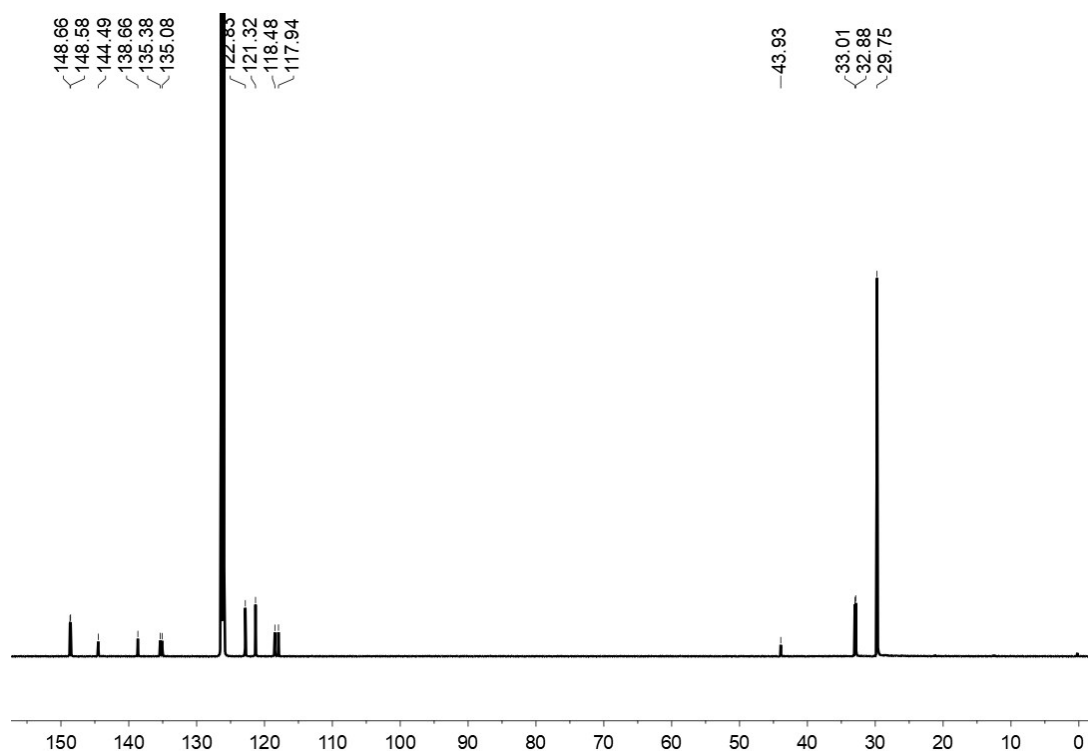


Figure S2. ¹³C {¹H} NMR spectrum (126 MHz) of **L**₃ in C₆D₆ at 25 °C.

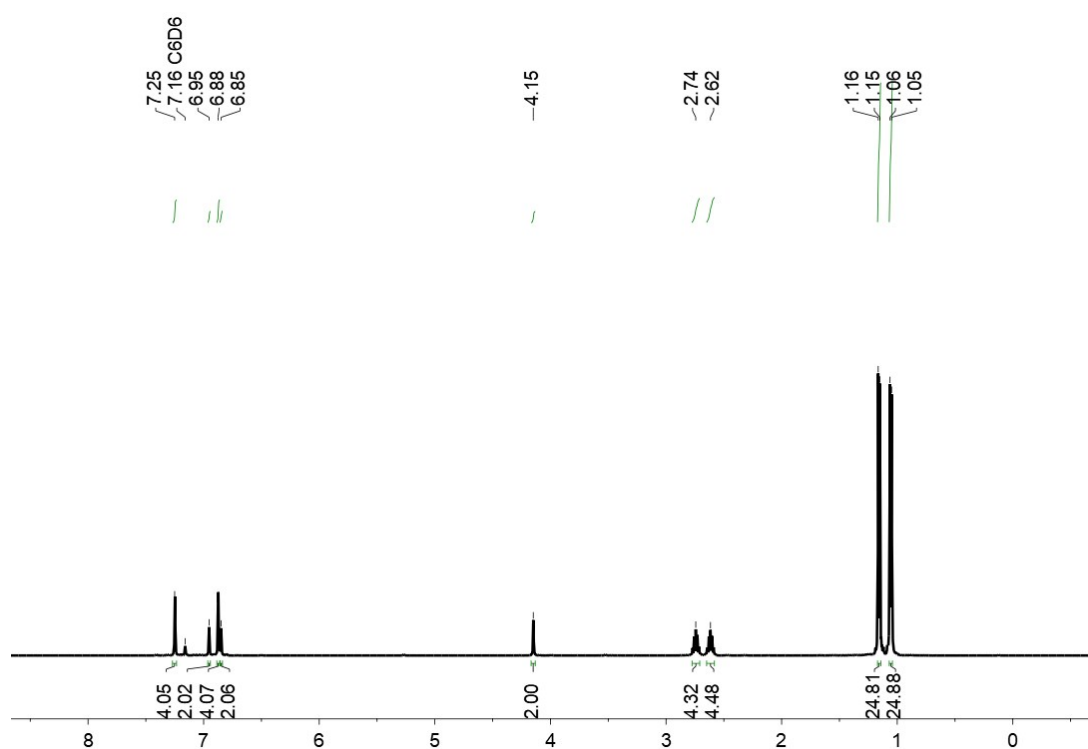


Figure S3. ¹H NMR spectrum (500 MHz) of **L**₄ in C₆D₆ at 25 °C.

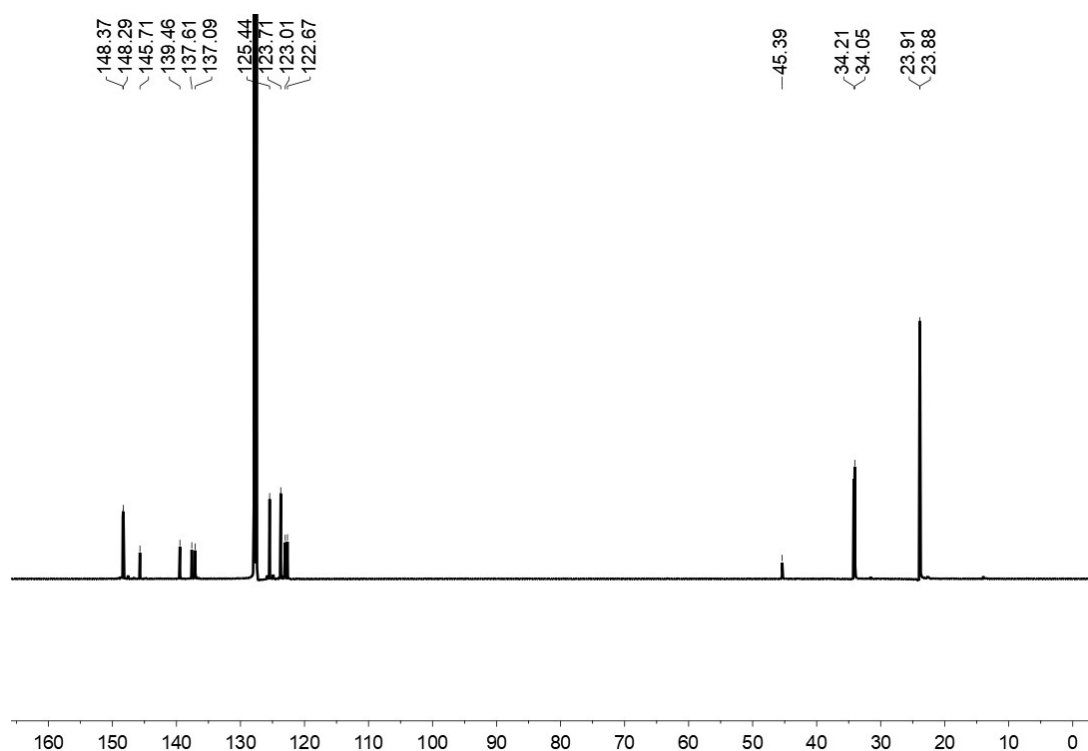


Figure S4. ¹³C {¹H} NMR spectrum (126 MHz) of **L**₄ in C₆D₆ at 25 °C.

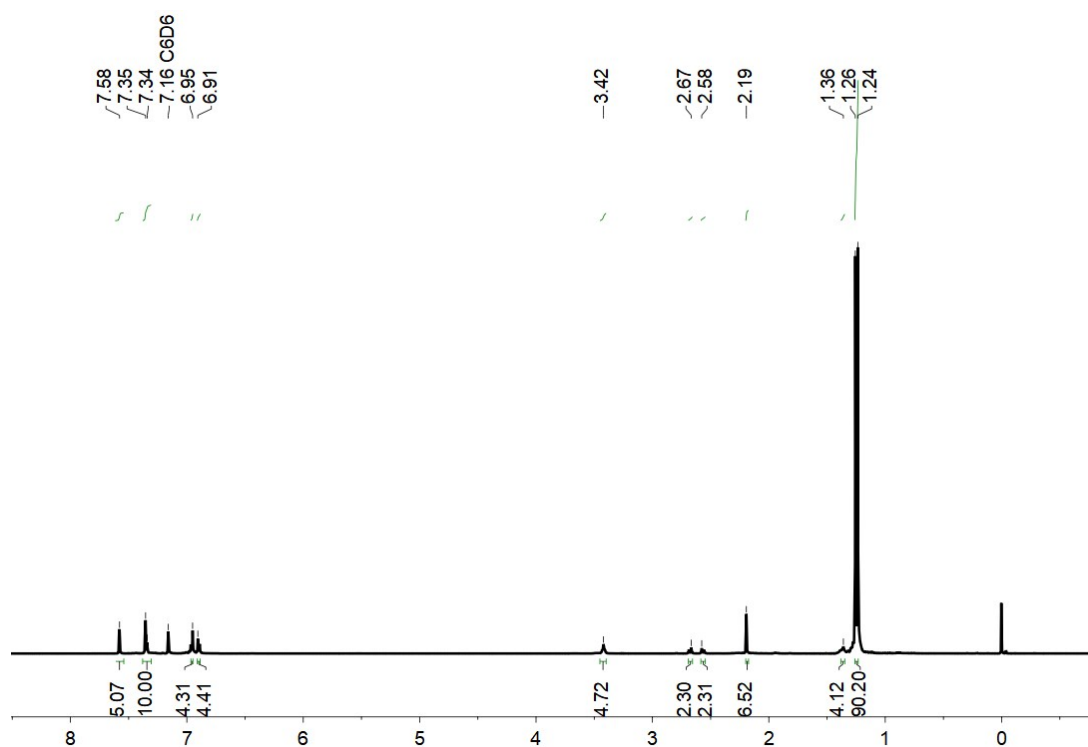


Figure S5. ¹H NMR spectrum (500 MHz) of complex **1** in C₆D₆ at 25 °C.

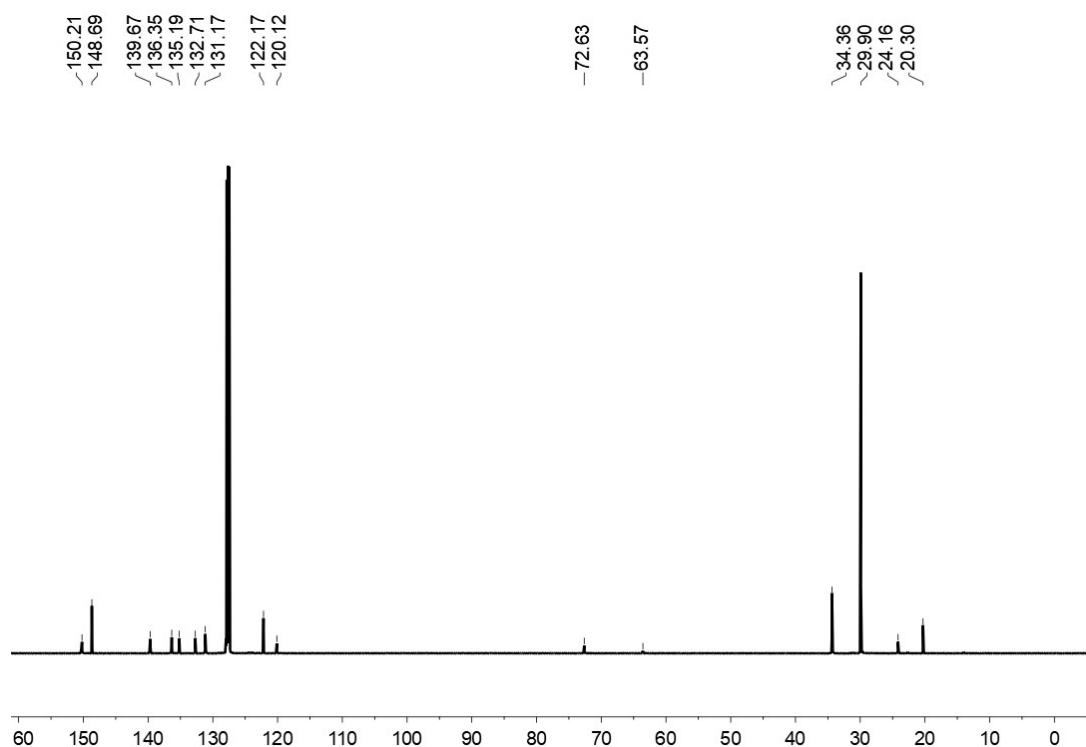


Figure S6. ¹³C {¹H} NMR spectrum (126 MHz) of complex **1** in C₆D₆ at 25 °C.

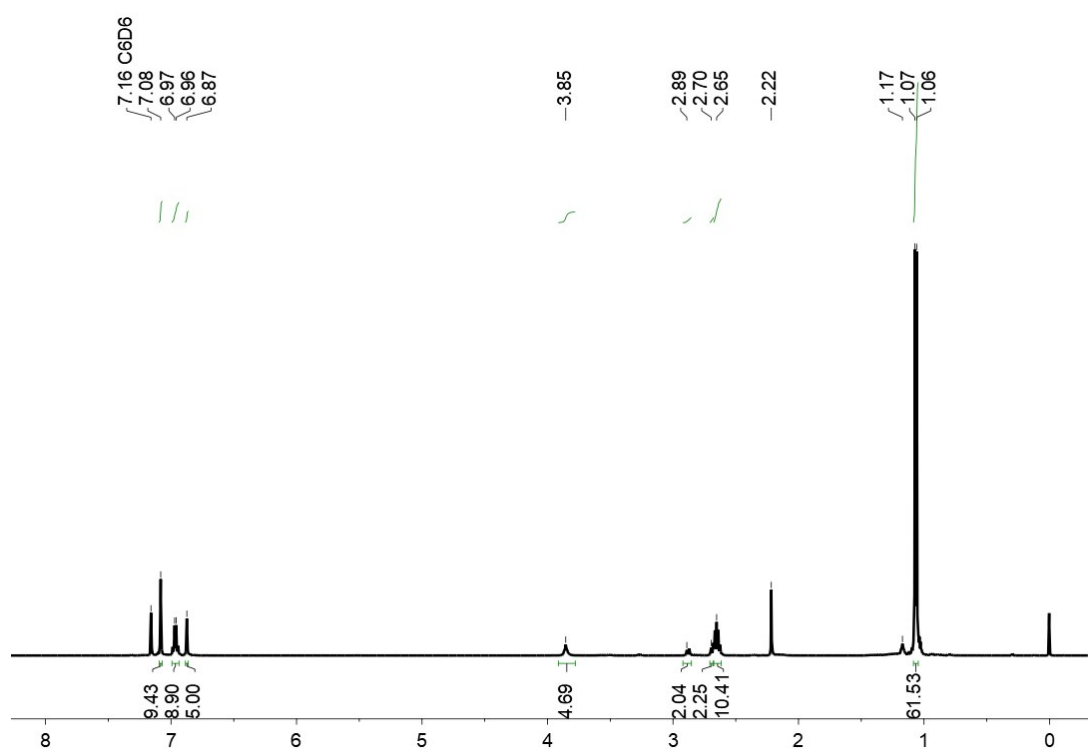


Figure S7. ¹H NMR spectrum (500 MHz) of complex **2** in C₆D₆ at 25 °C.

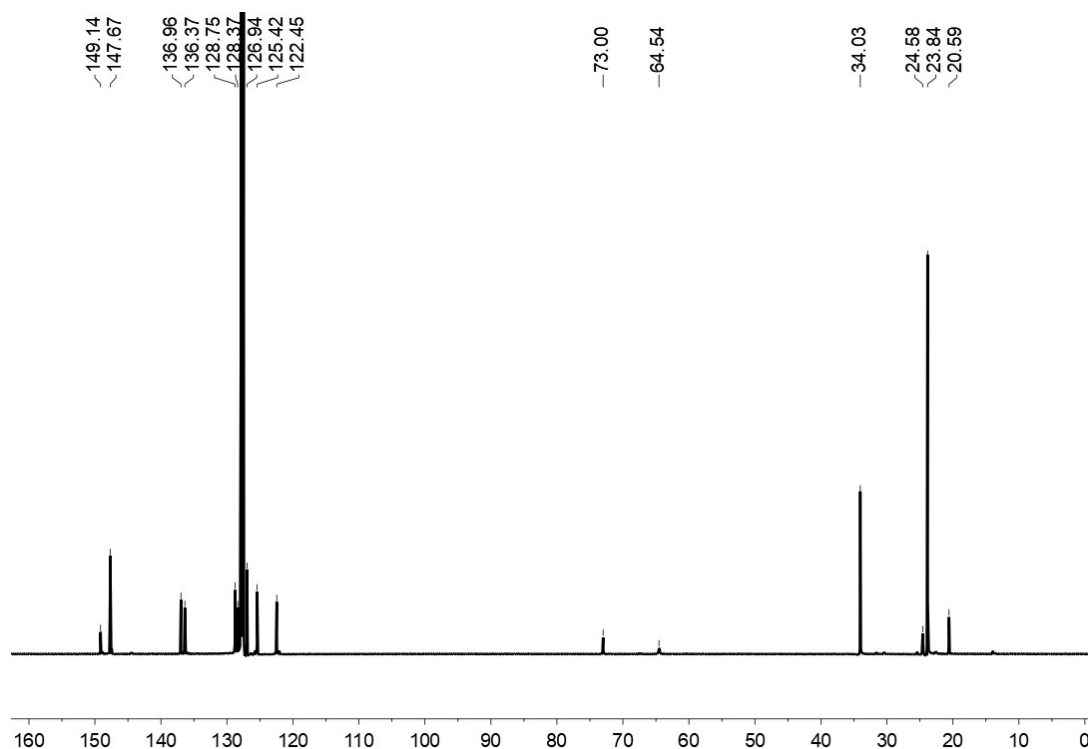


Figure S8. ¹³C {¹H} NMR spectrum (126 MHz) of complex **2** in C₆D₆ at 25 °C.

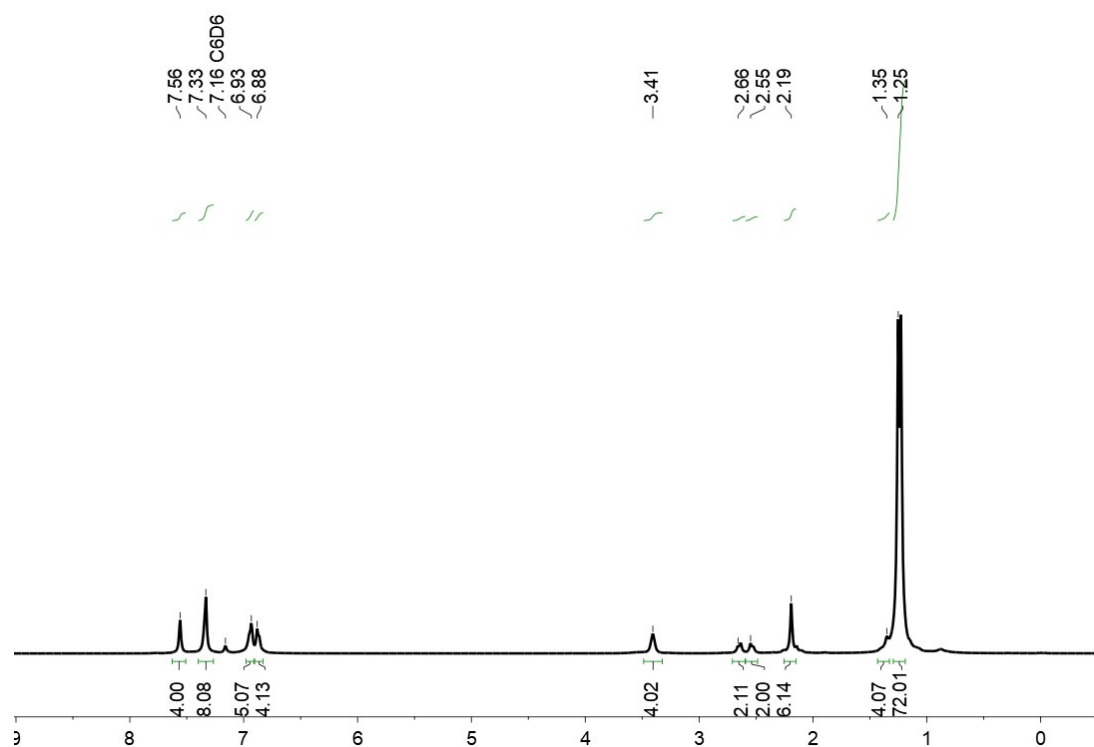


Figure S9. ¹H NMR spectrum (500 MHz) of complex **3** in C₆D₆ at 25 °C.

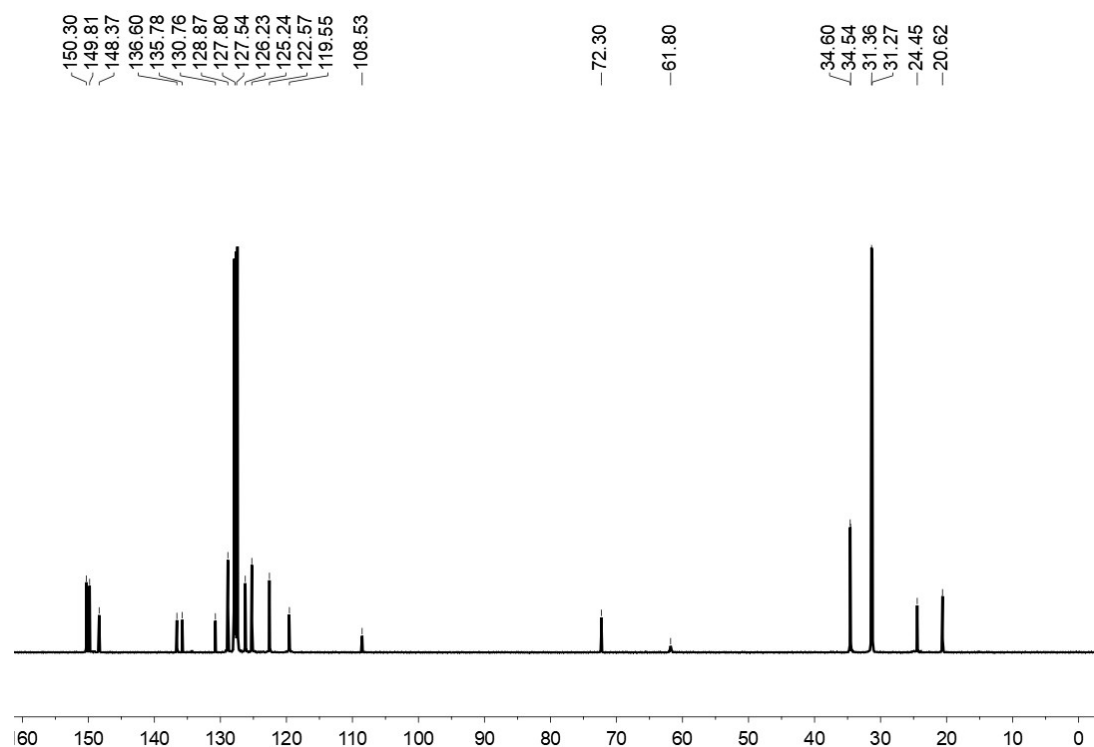


Figure S10. ¹³C {¹H} NMR spectrum (126 MHz) of complex **3** in C₆D₆ at 25 °C.

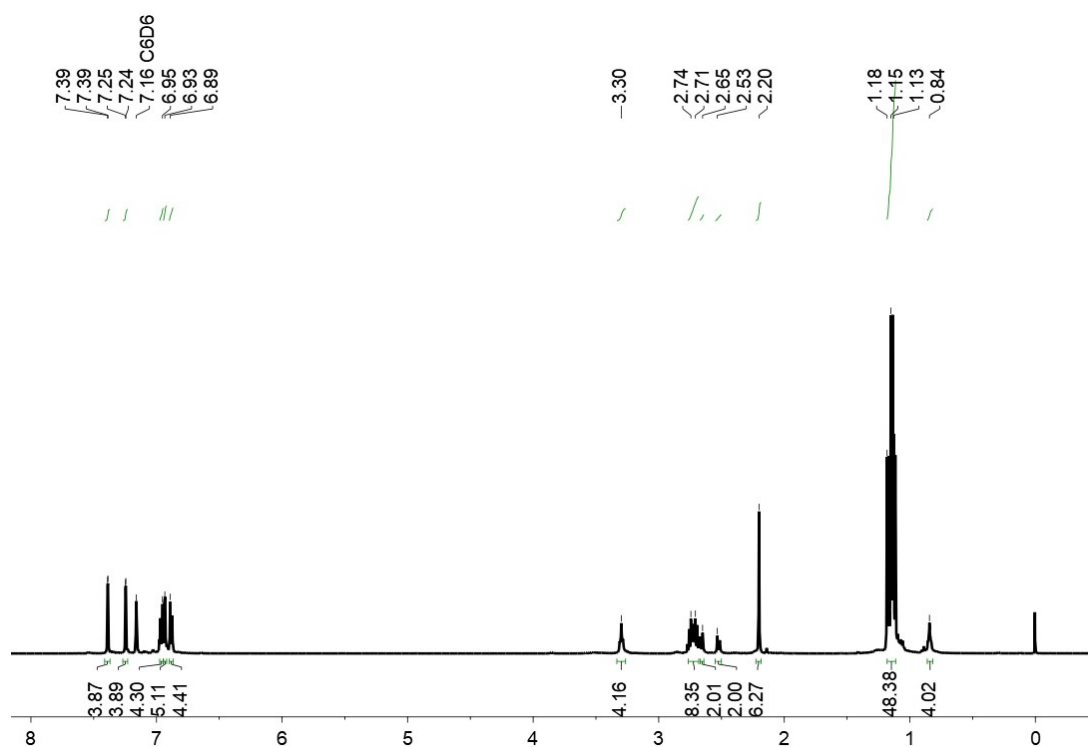


Figure S11. ¹H NMR spectrum (500 MHz) of complex **4** in C₆D₆ at 25 °C.

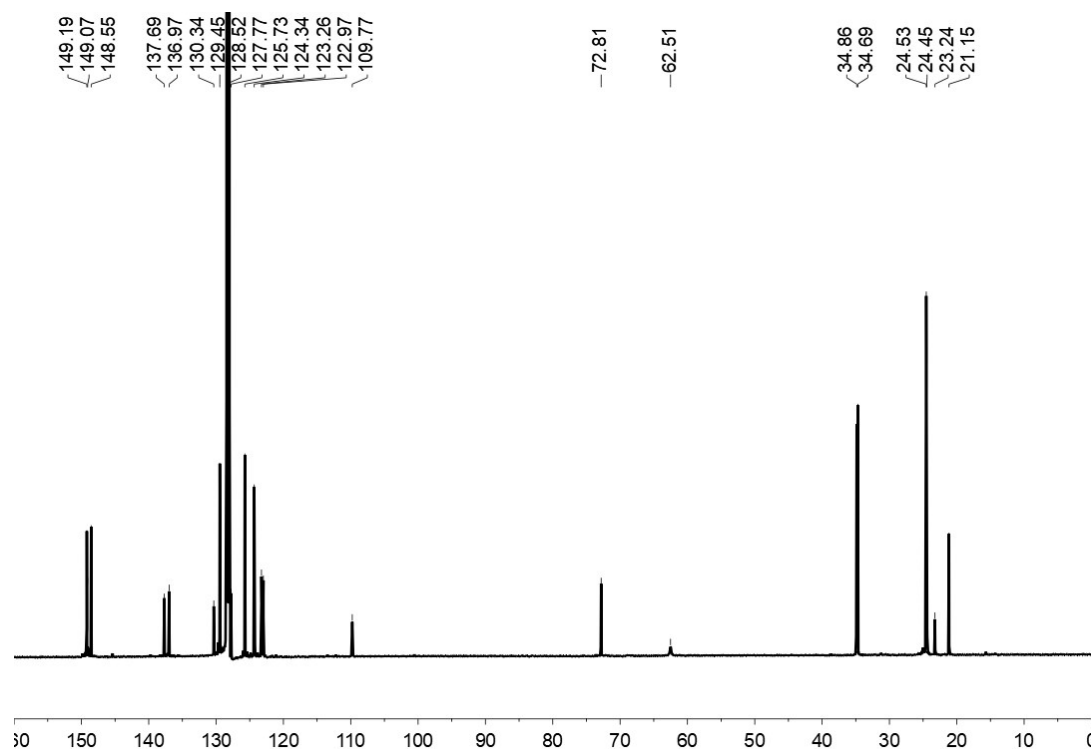


Figure S12. ¹³C {¹H} NMR spectrum (126 MHz) of complex **4** in C₆D₆ at 25 °C.

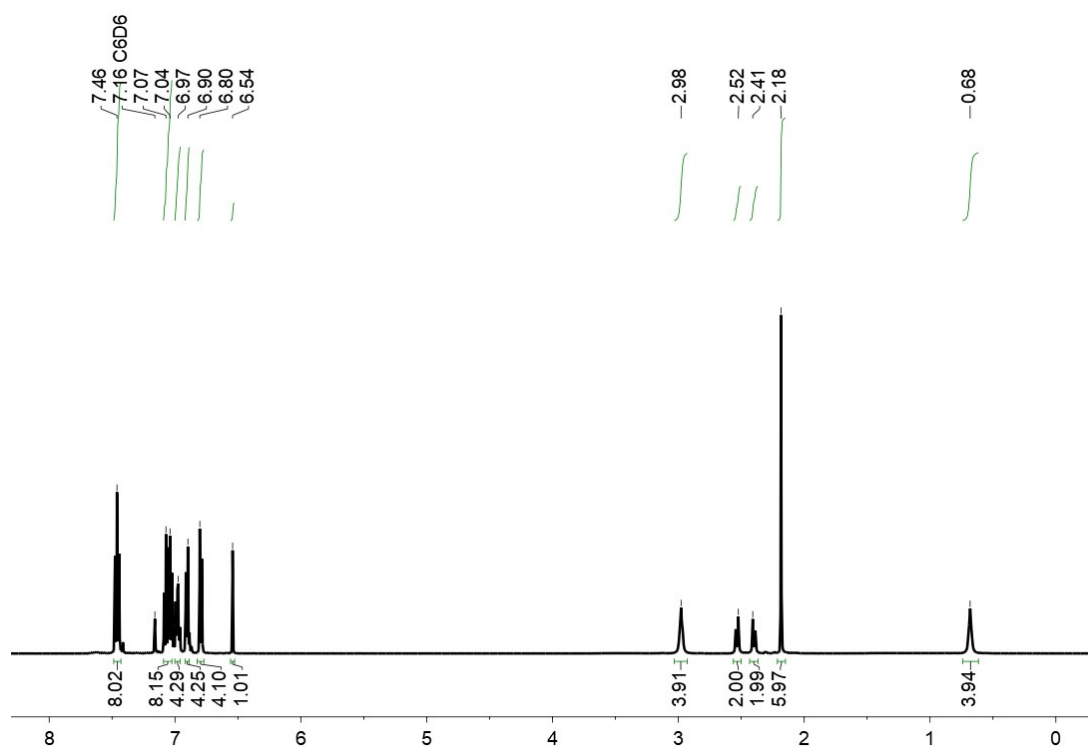


Figure S13. ¹H NMR spectrum (500 MHz) of complex **5** in C₆D₆ at 25 °C.

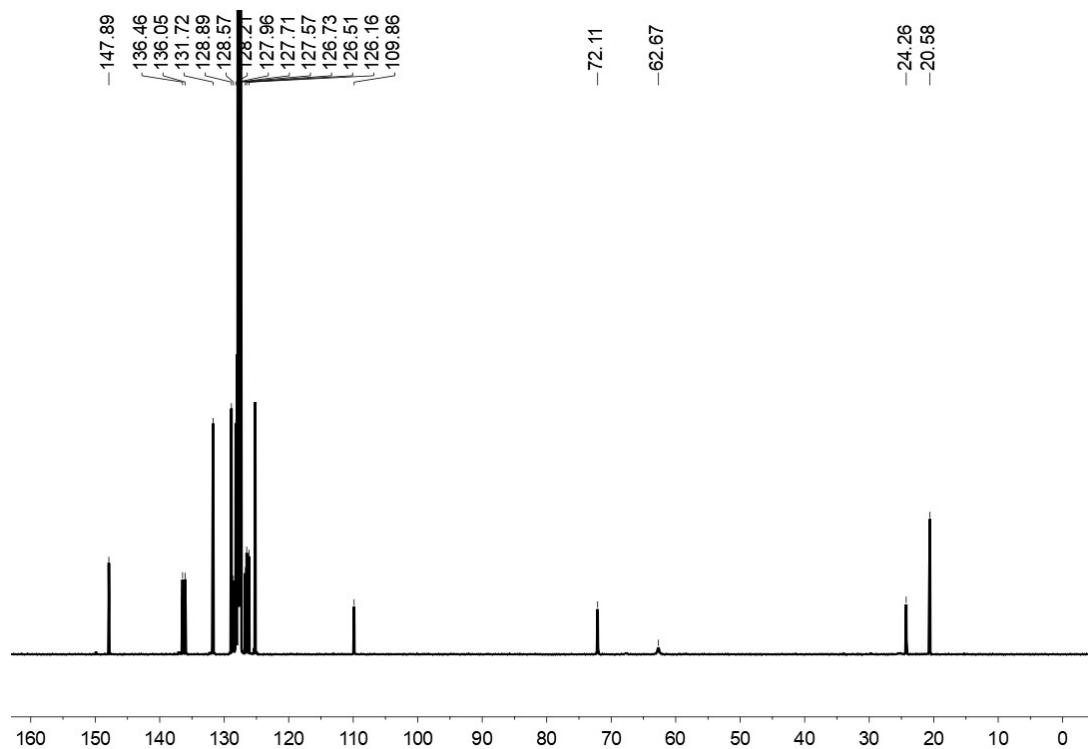


Figure S14. ¹³C {¹H} NMR spectrum (126 MHz) of complex **5** in C₆D₆ at 25 °C.

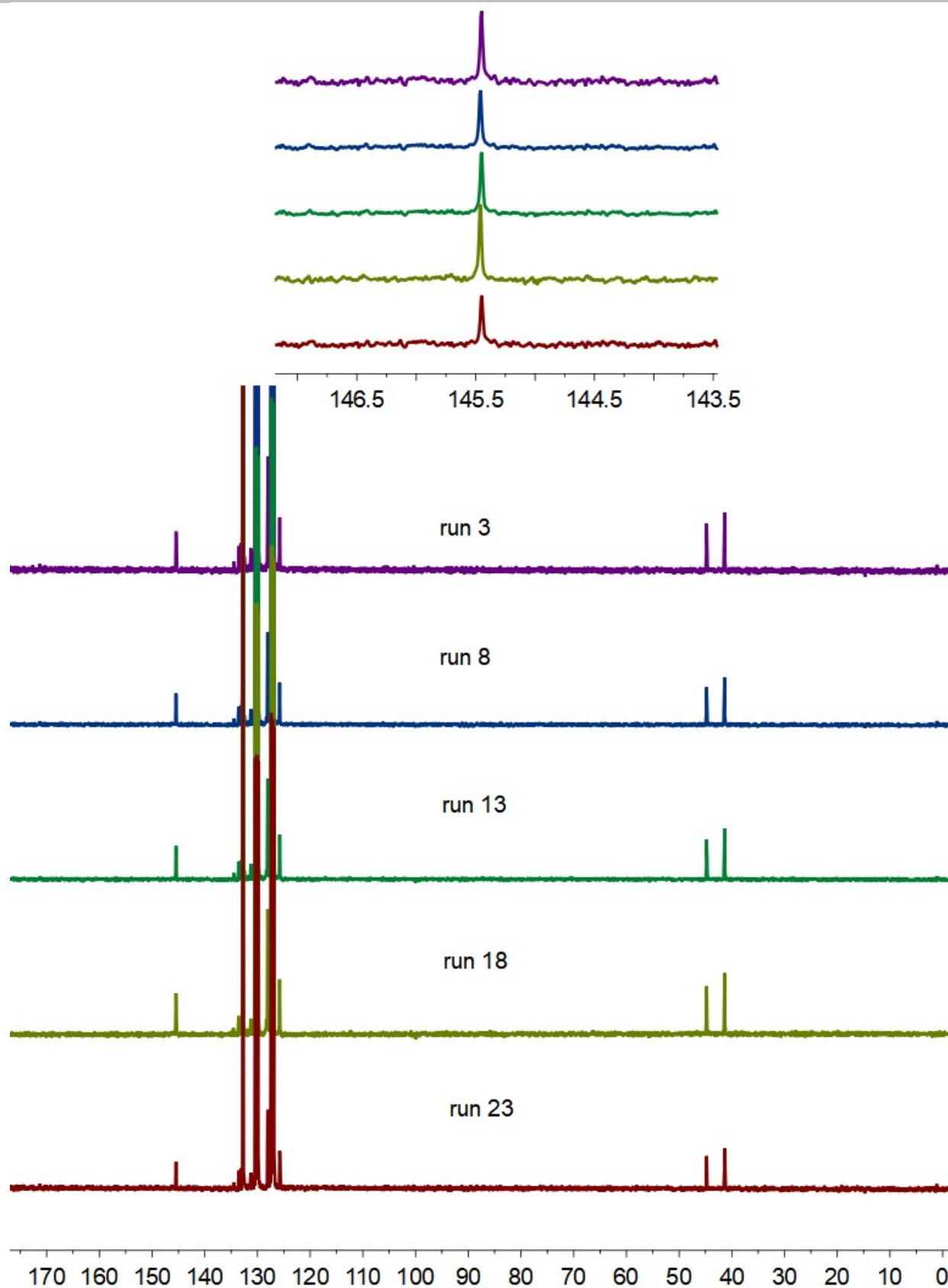


Figure S15. ^{13}C $\{^1\text{H}\}$ NMR spectrum of sPs in $\text{C}_6\text{D}_4\text{Cl}_2$ (rrr >99%) at 100°C , obtained with complexes **1-5** (run 3, 8, 13, 18, 23 in Table 1).

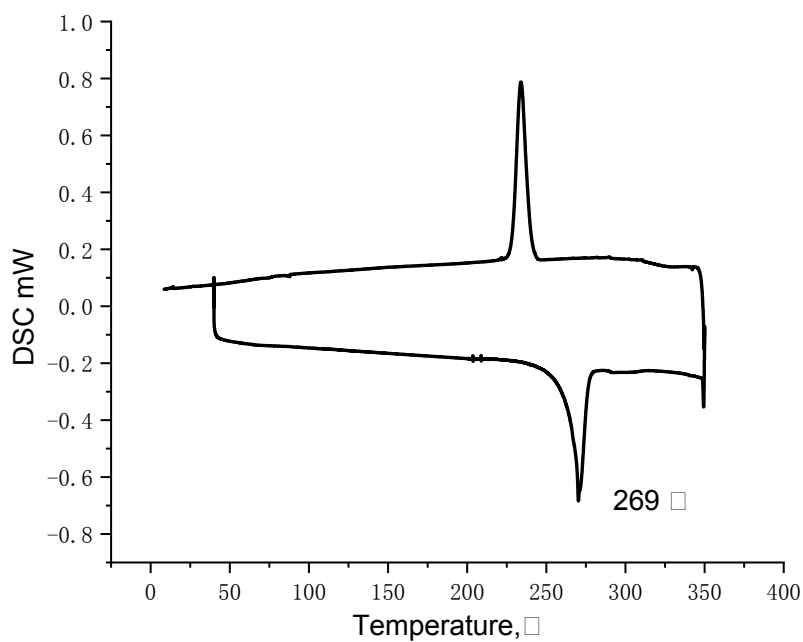


Figure S16. DSC curve of sPS (run 3 in Table 2).

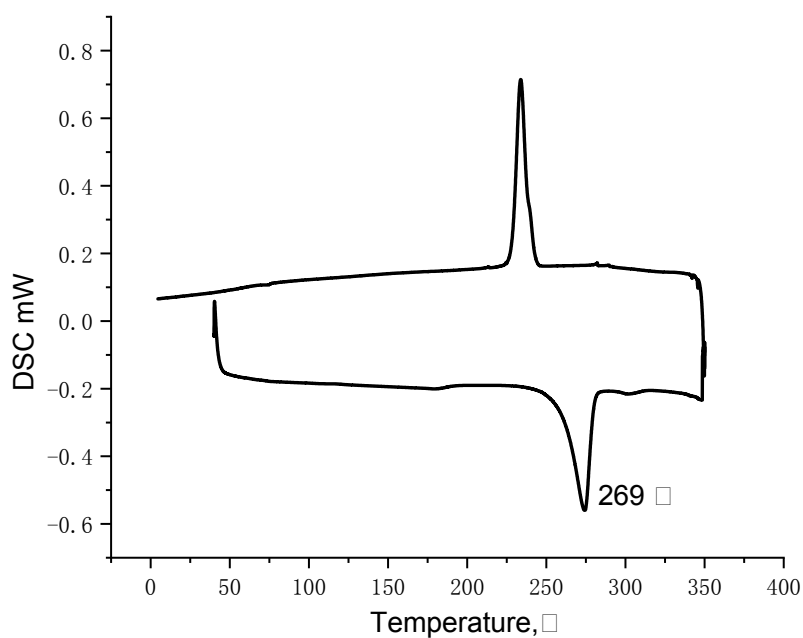


Figure S17. DSC curve of sPS (run 8 in Table 2).

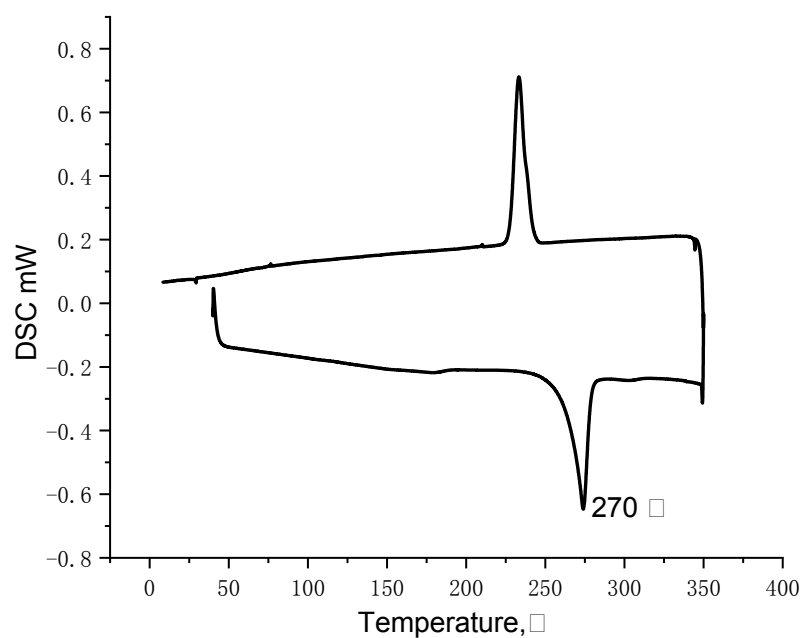


Figure S18. DSC curve of sPS (run 13 in Table 2).

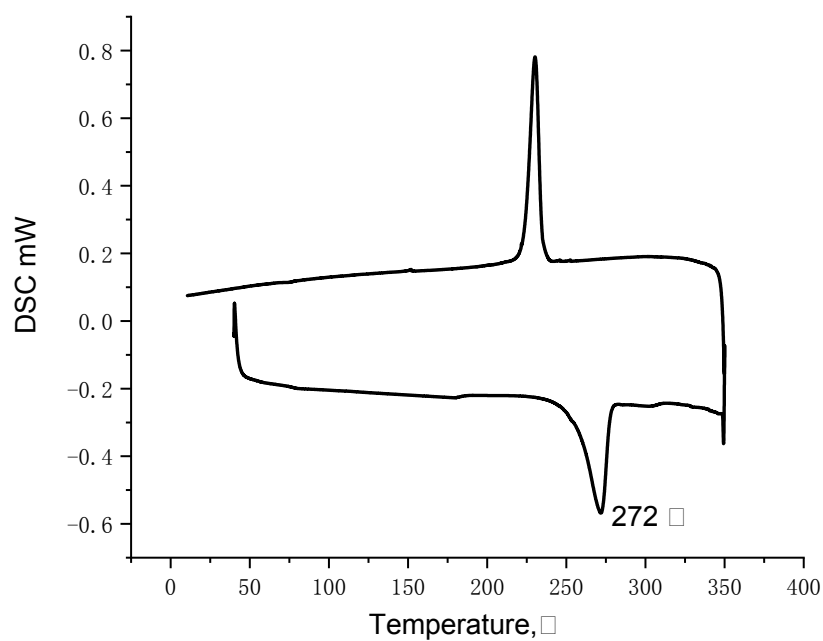


Figure S19. DSC curve of sPS (run 18 in Table 2).

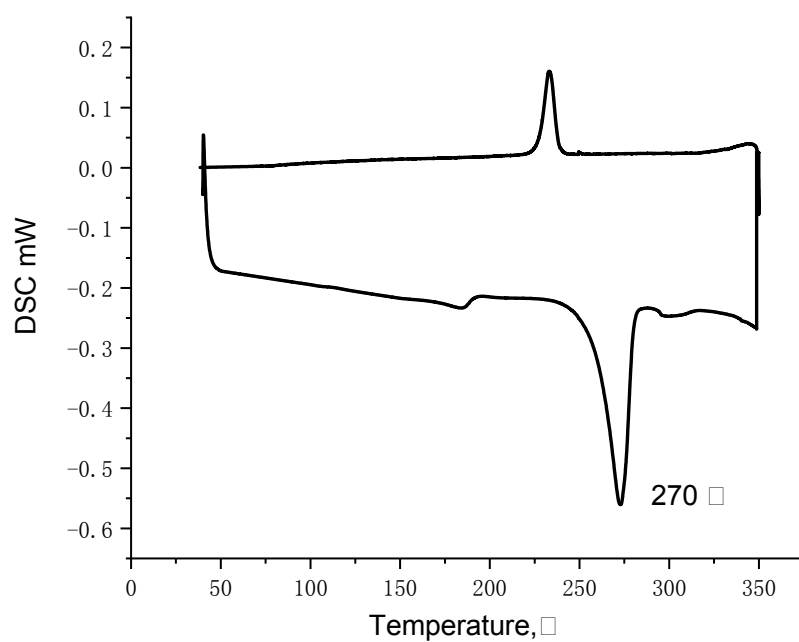


Figure S20. DSC curve of sPS (run 23 in Table 2).