

^1H NMR Spectra of SC4A, STC4A, MVAd $^{2+}$, and MVNp $^{2+}$ in D $_2$ O:

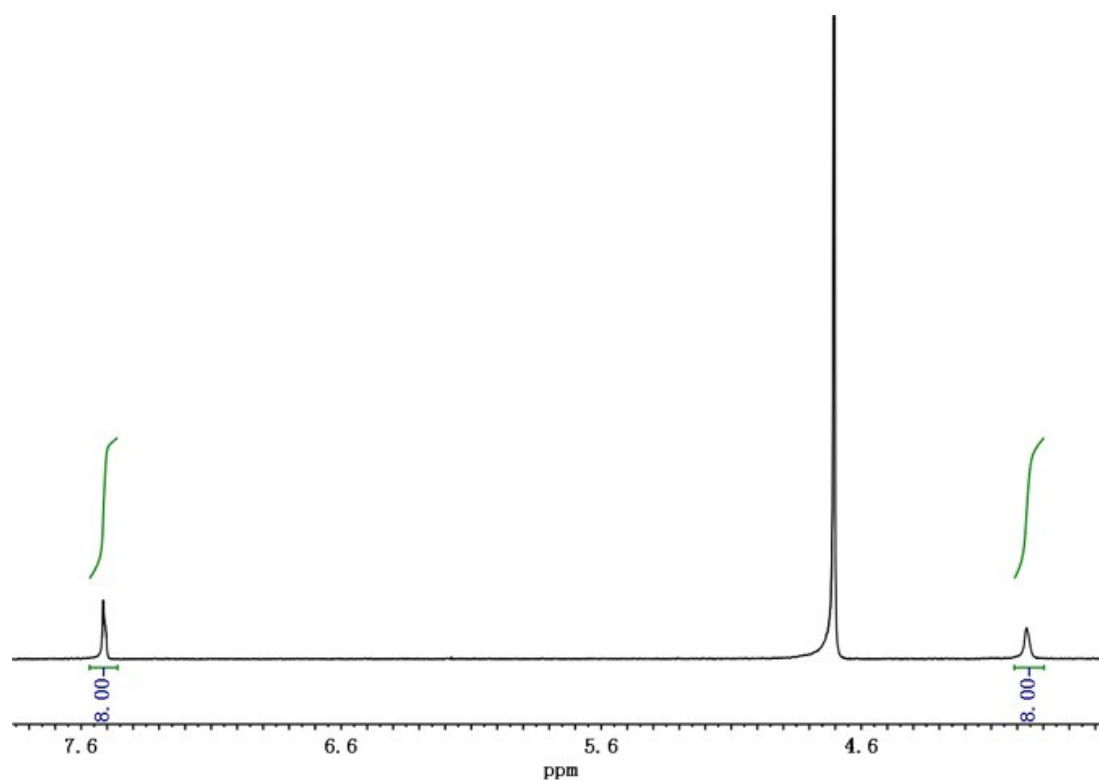


Figure S1. ^1H NMR spectrum of SC4A in D $_2$ O.

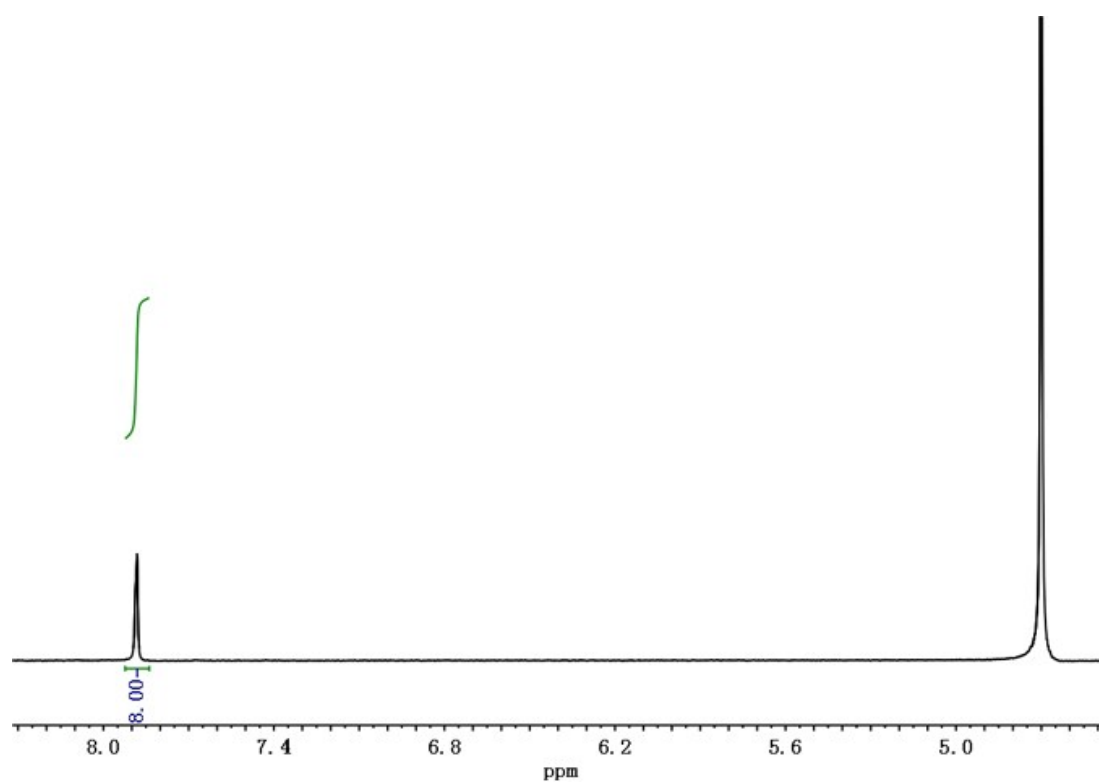


Figure S2. ^1H NMR spectrum of STC4A in D $_2$ O.

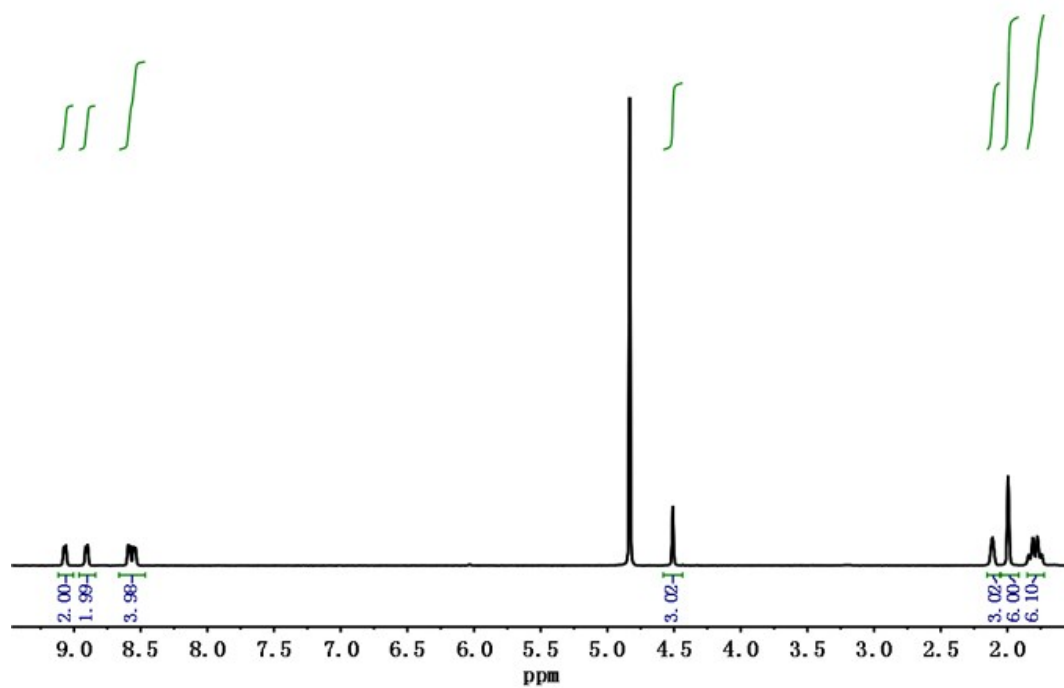


Figure S3. ¹H NMR spectrum of MVAd²⁺ in D₂O.

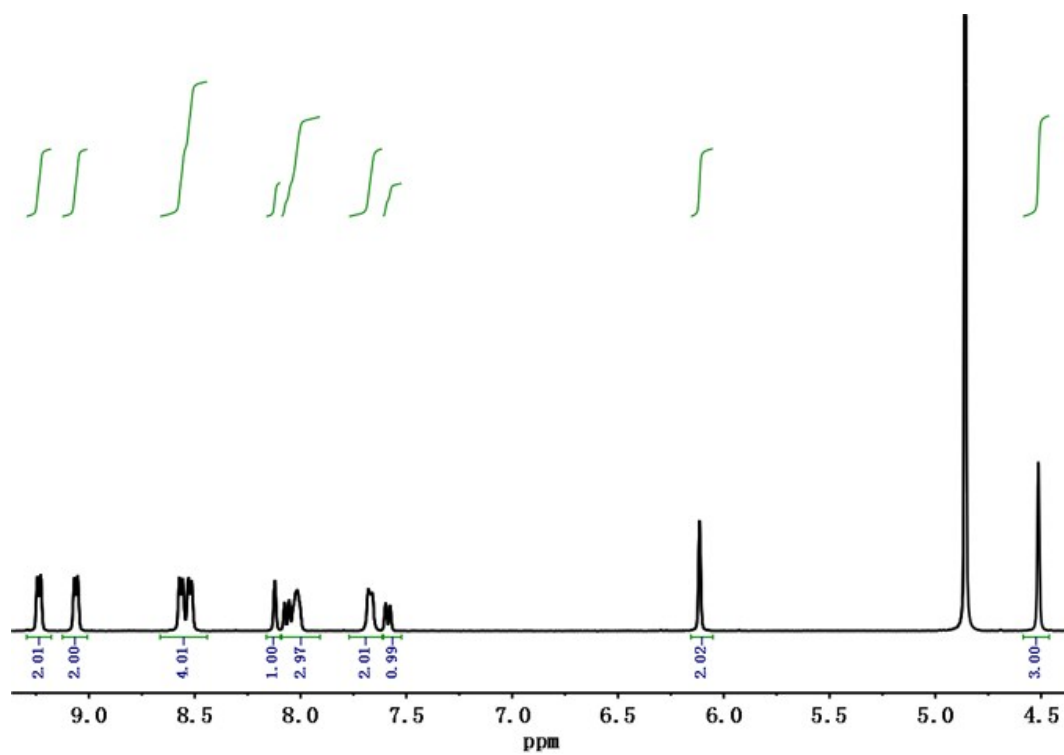


Figure S4. ¹H NMR spectrum of MVNp²⁺ in D₂O.

^{13}C NMR Spectra of SC4A, STC4A, MVAd $^{2+}$, and MVNp $^{2+}$ in D $_2$ O:

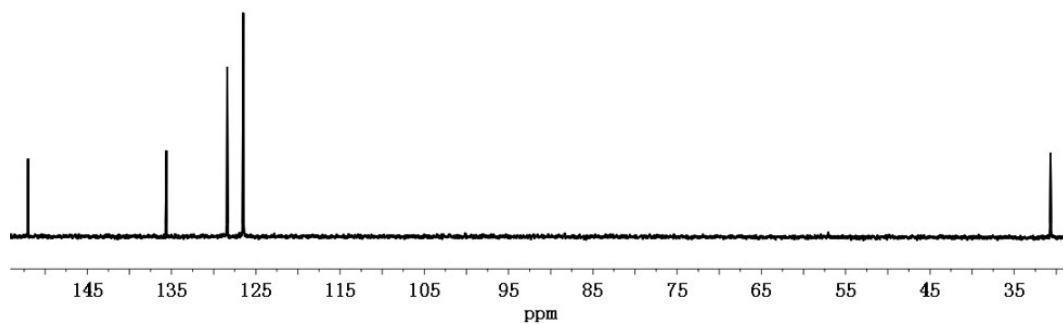


Figure S5. ^{13}C NMR spectrum of SC4A in D $_2$ O.

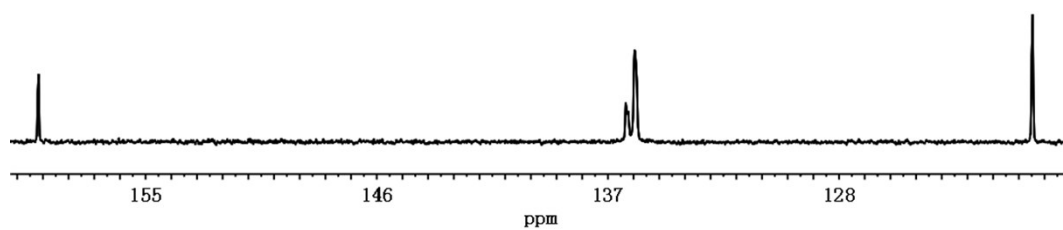


Figure S6. ^{13}C NMR spectrum of STC4A in D $_2$ O.

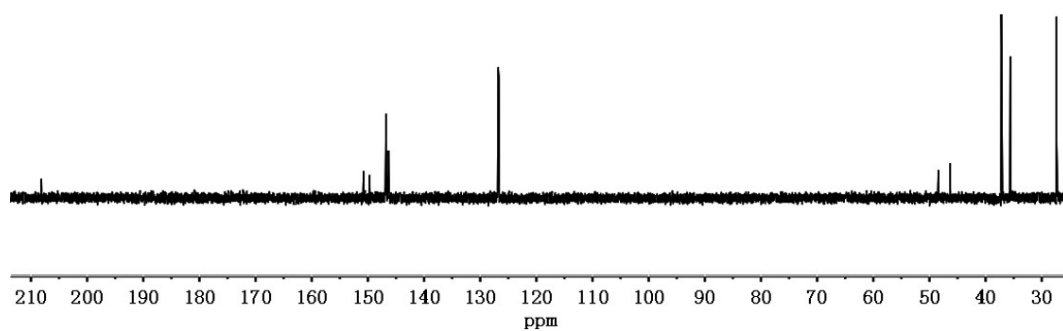


Figure S7. ^{13}C NMR spectrum of MVAd $^{2+}$ in D $_2$ O.

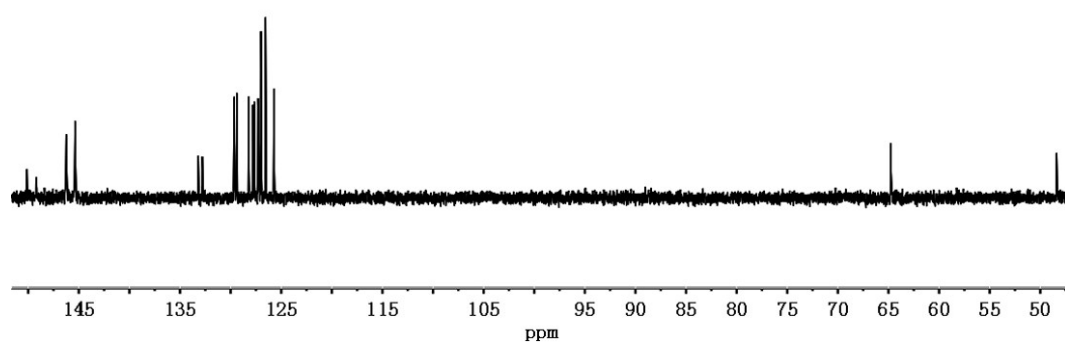


Figure S8. ^{13}C NMR spectrum of MVNp^{2+} in D_2O .

Elemental Analysis Data of SC4A, STC4A, MVAd²⁺, and MVNp²⁺:

Anal. Calcd (%) for C₂₈H₂₀O₁₆S₄Na₄•8H₂O (SC4A•8H₂O): C, 34.43; H, 3.71. Found (%): C, 34.21; H, 4.01.

Anal. Calcd (%) for C₂₄H₁₂O₁₆S₈Na₄•6H₂O (STC4A•6H₂O): C, 28.46; H, 2.39. Found (%): C, 28.23; H, 2.68.

Anal. Calcd (%) for C₂₃H₂₈ON₂²⁺•2Br⁻•3H₂O (MVAd²⁺•2Br⁻•3H₂O): C, 49.12; H, 6.09. Found (%): C, 49.33; H, 6.38.

Anal. Calcd (%) for C₂₂H₂₀N₂²⁺•Br⁻•I⁻•2H₂O (MVNp²⁺•Br⁻•I⁻•2H₂O): C, 47.59; H, 4.36. Found (%): C, 47.73; H, 4.52.