

Supporting Information for:

Cobaltocenium-containing polybenzimidazole polymers for alkaline anion exchange membrane applications

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Fig. S1: H-D exchange experiment of $\text{DMCp}_2\text{Co}^+\text{PF}_6^-$ cations in $\text{H}_2\text{O}/\text{D}_2\text{O}$ and $\text{D}_2\text{O}/\text{KOH}$.

Fig. S2: H-D exchange experiment of $\text{DCCp}_2\text{Co}^+\text{PF}_6^-$ cations in $\text{H}_2\text{O}/\text{KOH}$ and $\text{D}_2\text{O}/\text{KOH}$.

Fig. S3: ^{13}C NMR spectra for (a) Cp_2Co^+ (b) $\text{DMCp}_2\text{Co}^+\text{PF}_6^-$ (c) $\text{DCCp}_2\text{Co}^+\text{PF}_6^-$ in 1M $\text{KOH}/\text{D}_2\text{O}$ at 80°C at various times.

Fig. S4: Mass spectra for (a) Cp_2Co^+ , (b) $\text{DMCp}_2\text{Co}^+\text{PF}_6^-$, and (c) $\text{DCCp}_2\text{Co}^+\text{PF}_6^-$

Fig.S5: Arrhenius plots of hydroxide conductivity of cobaltocenium-containing polybenzimidazole membranes.

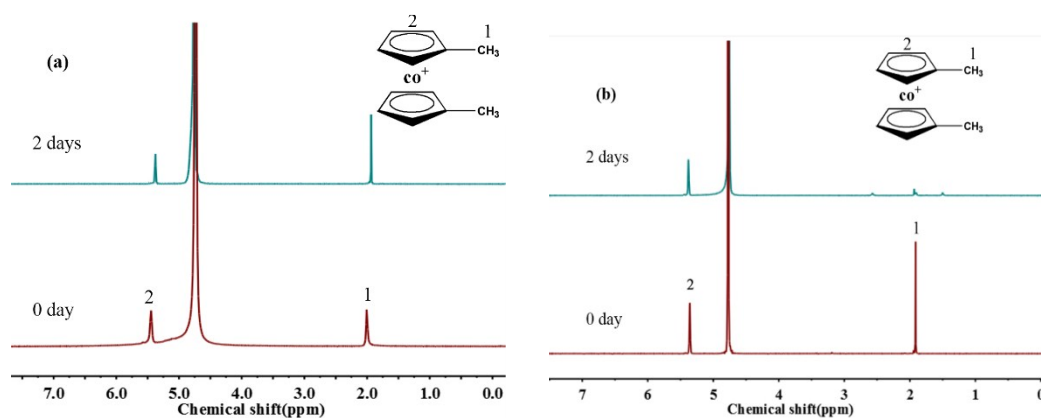


Fig. S1: ^1H NMR spectra evidence for H-D exchange of $\text{DMCp}_2\text{Co}^+\text{PF}_6^-$ in 1mol/L (a) $\text{H}_2\text{O}/\text{KOH}$ and (b) $\text{D}_2\text{O}/\text{KOH}$ at 80°C after 2 days: It can be seen that the ^1H signal belongs to $-\text{CH}_3$ (2.02 ppm) in $\text{D}_2\text{O}/\text{KOH}$ decreases. But the ^1H signals for $\text{H}_2\text{O}/\text{KOH}$ show no change, indicating that the H-D exchange occurs mainly on $-\text{CH}_3$.

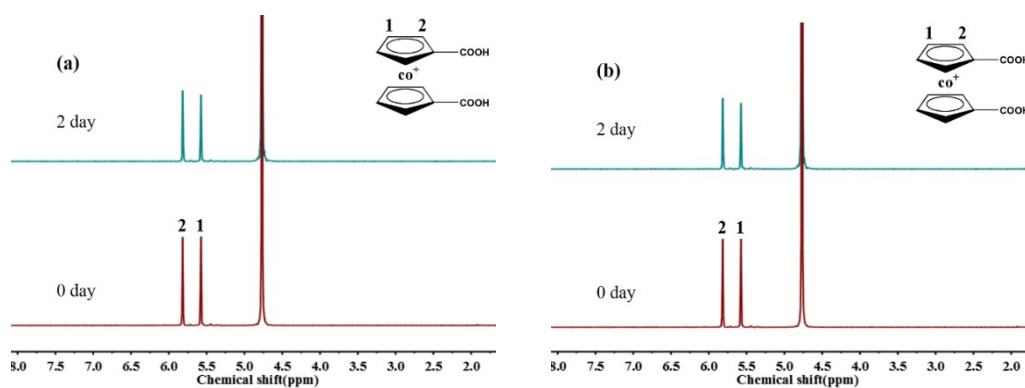
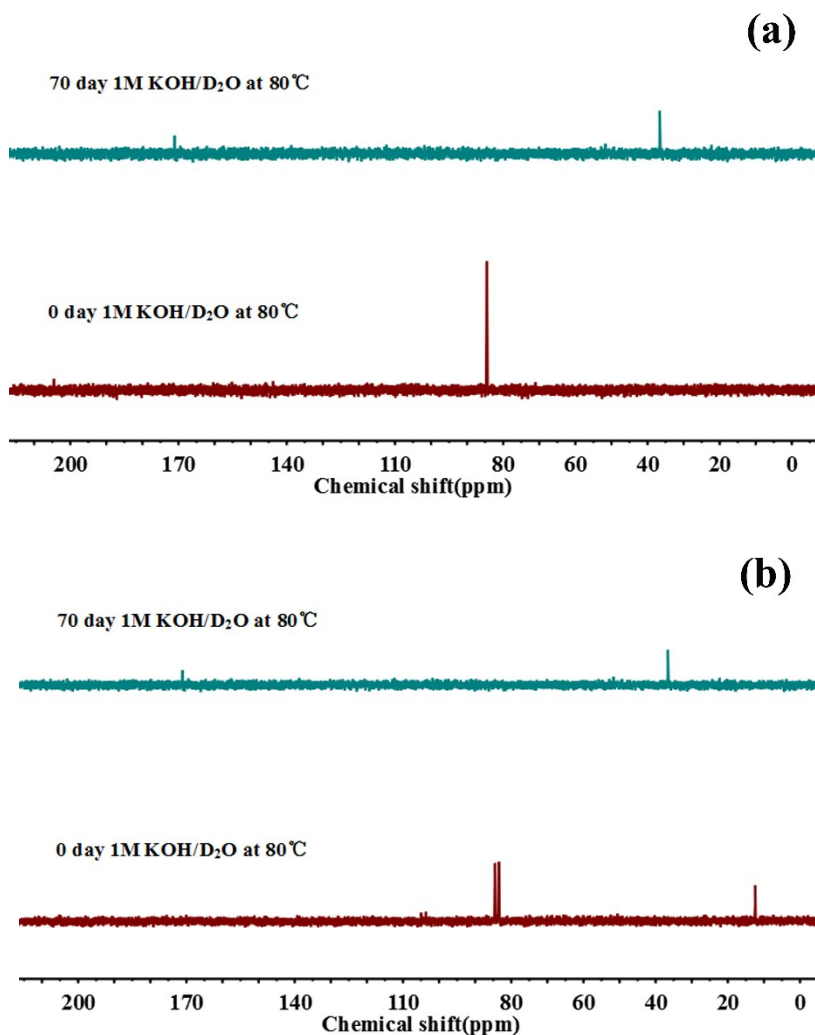


Fig. S2: ^1H NMR spectra evidence for H-D exchange of $\text{DCCp}_2\text{Co}^+\text{PF}_6^-$ in 1mol/L (a) $\text{H}_2\text{O}/\text{KOH}$ and (b) $\text{D}_2\text{O}/\text{KOH}$ at 80°C after 2 days: There is no difference between the ^1H NMR spectra in (a) and (b), indicating that there is no H-D exchange in $\text{DCCp}_2\text{Co}^+\text{PF}_6^-$



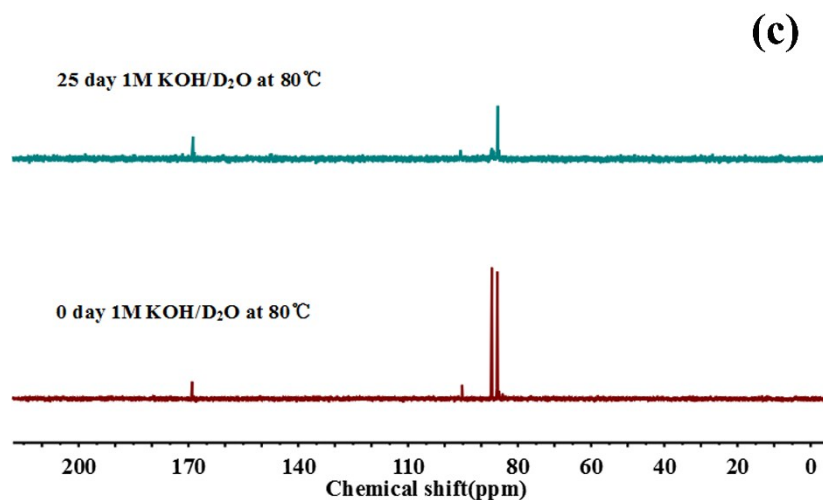
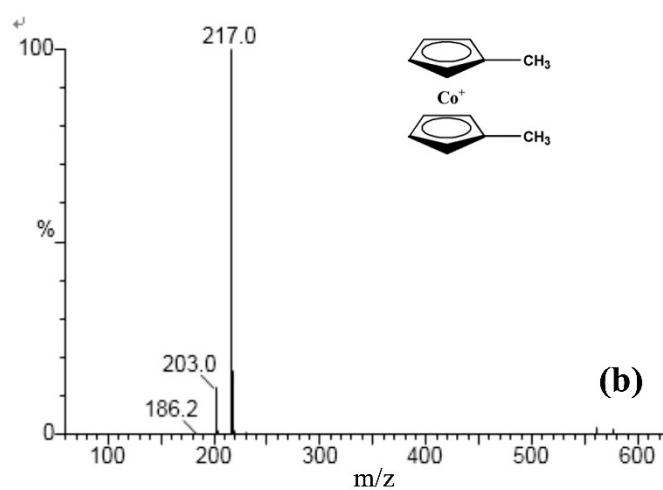
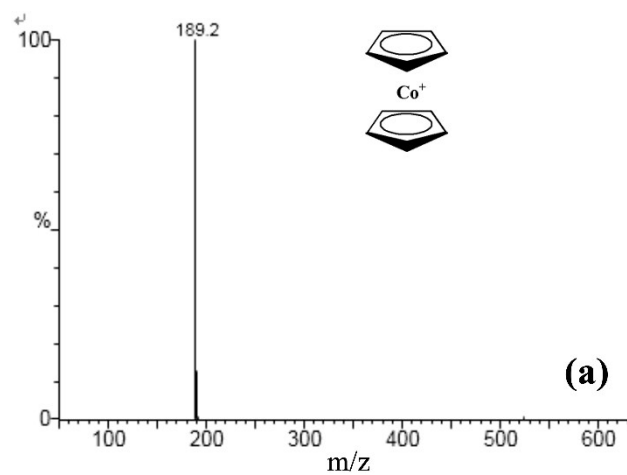


Fig. S3: ¹³CNMR spectra of (a) Cp₂Co⁺, (b) DMCp₂Co⁺PF₆⁻, and (c) DCCp₂Co⁺PF₆⁻ in 1 M KOH/D₂O at 80°C at various times.



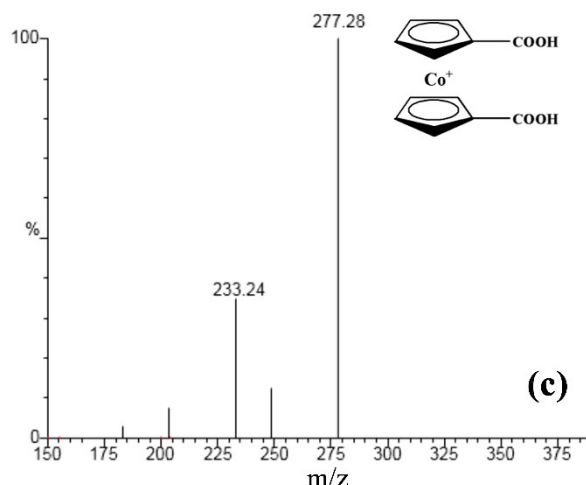


Fig. S4: Mass spectra of (a) Cp₂Co⁺, (b) DMCP₂Co⁺PF₆⁻, and (c) DCCp₂Co⁺PF₆⁻

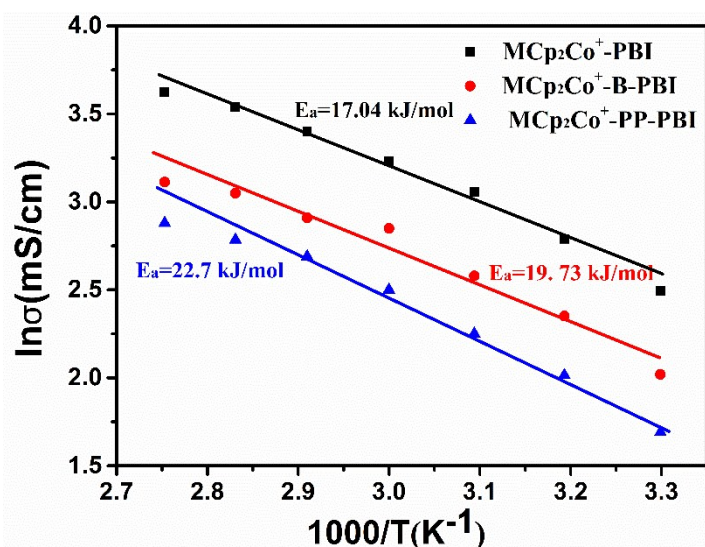


Fig. S5: Arrhenius plots of hydroxide conductivity of cobaltocenium-containing polybenzimidazole membranes.

The calculation of the degree of degradation of cobaltocenium cations in alkaline medium

The ¹H NMR spectra were used to estimate the degree of degradation of the three cobaltocenium cations in alkaline medium. For example, as shown in Fig. 3(a). The degree of degradation can be calculated by the relative integrated intensities of the indicated ¹H resonances. $(S_a + S_b + S_c + S_d + S_e) / S_1$ can be used to estimate the degree of degradation of Cp₂Co⁺ in Fig. 3(a), where S_a , S_b , S_c , S_d , S_e and S_1 are the relative integrated intensities of the peaks marked with a, b, c, d, e, and 1, respectively.

