

Functionalization of phenothiazine derivatives by ammonium bridge

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- p. 2-4 ¹³C{¹H} NMR data of **BA-X**.
- p. 5-7 CV of **BA-PF₆**.
- p. 8 Crystallographic data of **BA-PF₆**.

¹³C NMR data of **BA-X**

Oct-Prom-Br (CD₃OD, 100MHz) δ 144.85, 127.52, 127.26, 125.96, 122.93, 116.06, 63.26, 60.71, 50.62, 43.05, 29.04, 28.75, 25.86, 21.93, 19.77.

Oct-Prom-O-Br (CD₃OD, 100MHz) δ 138.94, 133.37, 130.29, 125.46, 122.51, 117.37, 63.69, 60.25, 49.98, 43.05, 28.95, 28.68, 25.85, 22.00, 20.56.

Oct-ClProm-Br (CD₃OD, 100MHz) δ 146.46, 144.02, 133.44, 128.00, 127.71, 127.38, 125.68, 124.68, 123.42, 122.74, 116.45, 116.16, 63.19, 60.62, 50.61, 43.23, 29.08, 28.77, 25.89, 21.96, 19.75.

Oct-ClProm-O-Br (CD₃OD, 100MHz), δ 140.12, 139.25, 138.33, 133.53, 131.75, 130.25, 125.91, 124.27, 123.09, 122.67, 117.70, 117.41, 63.63, 60.09, 50.08, 43.30, 28.98, 28.71, 25.86, 22.04, 20.57.

Ph-Prom-Br (CD₃OD, 100MHz) δ 144.80, 133.37, 129.80, 127.55, 127.28, 125.80, 122.95, 116.01, 66.75, 61.58, 49.43, 43.38, 19.97.

Ph-Prom-O-Br (CD₃OD, 100MHz) δ 138.87, 133.47, 133.21, 130.37, 129.59, 125.33, 122.56, 117.44, 67.34, 61.19, 48.81, 43.08, 20.89.

Ph-ClProm-Br (CD₃OD, 100MHz) δ 146.49, 143.86, 133.47, 133.40, 129.83, 128.00, 127.76, 127.40, 125.52, 124.46, 123.45, 122.74, 116.48, 116.14, 66.85, 61.60, 49.41, 43.59, 20.07.

Ph-ClProm-O-Br (CD₃OD, 100MHz), δ 140.12, 139.35, 138.23, 133.63, 133.21, 131.80, 130.31, 129.61, 125.81, 124.15, 123.15, 122.72, 117.80, 117.49, 67.44, 61.10, 48.83, 43.33, 20.95.

BiPh-Prom-Br (CD₃OD, 100MHz) δ 144.79, 141.88, 133.26, 127.52, 127.51, 127.17, 126.95, 125.97, 122.89, 116.06, 67.63, 61.28, 49.30, 46.94, 43.48, 20.01.

BiPh-Prom-O-Br (CD₃OD, 100MHz) δ 141.82, 138.79, 133.55, 133.31, 130.46, 127.39, 126.89, 125.04, 122.50, 117.34, 67.66, 61.46, 48.74, 43.24, 20.90.

BiPh-ClProm-Br (CD₃OD, 100MHz) δ 146.46, 143.87, 141.86, 133.46, 133.28, 127.89, 127.73, 127.52, 127.31, 126.99, 125.68, 124.62, 123.41, 122.69, 116.49, 116.19, 67.73, 61.23, 49.26, 43.65, 20.04.

BiPh-ClProm-O-Br (CD₃OD, 100MHz), δ 141.86, 140.09, 139.38, 138.23, 133.66, 133.25, 131.87, 130.37, 127.38, 126.88, 125.75, 124.07, 123.14, 122.70, 117.67, 117.39, 67.83, 61.35, 48.65, 43.43, 21.02.

Bpy-Prom-Cl (CD₃OD, 100MHz) δ 157.23, 151.57, 146.04, 138.67, 128.95, 128.86, 128.50, 127.20, 126.12, 124.26, 117.47, 68.16, 63.25, 50.93, 44.74, 21.38.

Bpy-Prom-O-Cl (CD₃OD, 100MHz) δ 155.88, 150.03, 138.81, 137.23, 133.47, 130.35, 127.60, 125.27, 124.62, 122.53, 117.28, 66.26, 61.94, 49.19, 43.07, 20.91.

Bpy-ClProm-Cl (CD₃OD, 100MHz) δ 155.76, 150.21, 146.41, 143.64, 137.30, 133.35, 127.80, 127.65, 127.58, 127.25, 125.59, 124.68, 124.45, 123.38, 122.63, 116.49, 116.19, 66.95, 61.78, 49.46, 43.49, 20.01.

Bpy-ClProm-O-Cl (CD₃OD, 100MHz), δ 155.14, 149.36, 139.39, 138.63, 137.49, 136.62, 132.95, 131.10, 129.63, 126.97, 125.17, 124.01, 123.46, 122.47, 122.02, 116.99, 116.72, 65.79, 61.16, 48.57, 42.66, 20.35.

Oct-Prom-PF₆ (CD₃CN, 100MHz), δ 144.79, 127.80, 127.538, 125.64, 123.21, 116.33, 63.57, 61.05, 51.07, 43.19, 28.97, 28.69, 25.73, 21.90, 19.83.

Oct-Prom-O-PF₆ (CD₃CN, 100MHz), δ 138.81, 132.98, 130.28, 127.08, 122.56, 117.68, 63.78, 60.22, 50.59, 43.31, 28.88, 28.63, 25.74, 21.89, 20.49.

Oct-ClProm-PF₆ (CD₃CN, 100MHz), δ 146.27, 144.09, 133.26, 128.31, 127.99, 127.62, 125.27, 124.45, 123.65, 122.88, 116.70, 116.46, 63.47, 60.91, 51.11, 43.34, 29.01, 28.73, 25.74, 21.92, 19.82.

Oct-ClProm-O-PF₆ (CD₃CN, 100MHz), δ 139.92, 138.39, 138.28, 133.20, 131.79, 130.27, 127.24, 125.78, 123.12, 122.59, 117.94, 117.73, 63.79, 60.16, 50.65, 43.53, 28.89, 28.64, 25.74, 21.91, 20.51.

Ph-Prom-PF₆ (acetone-*d*₆, 100MHz), δ 144.89, 133.69, 130.09, 127.77, 127.47, 125.41, 123.12, 116.15, 66.94, 62.34, 49.90, 43.63, 20.33.

Ph-Prom-O-PF₆ (CD₃CN, 100MHz), δ 138.82, 133.21, 133.10, 130.32, 129.37, 126.95, 122.65,

117.78, 67.27, 61.25, 49.24, 43.39, 20.88.

Ph-ClProm-PF₆ (acetone-*d*₆, 100MHz), δ 146.60, 144.05, 133.73, 133.24, 130.12, 128.29, 127.99, 127.57, 125.07, 124.24, 123.61, 122.80, 116.65, 116.22, 67.04, 62.25, 49.83, 43.82, 20.42.

Ph-ClProm-O-PF₆ (acetone-*d*₆, 100MHz), δ 140.25, 138.36, 133.34, 133.28, 131.78, 130.19, 129.74, 127.68, 126.23, 123.20, 122.61, 118.17, 117.83, 67.73, 61.28, 49.19, 43.72, 21.16.

BiPh-Prom-PF₆ (acetone-*d*₆, 100MHz), δ 144.92, 141.56, 133.76, 127.76, 127.58, 127.51, 127.39, 125.37, 123.03, 116.18, 67.47, 61.76, 49.71, 43.67, 20.33.

BiPh-Prom-O-PF₆ (acetone-*d*₆, 100MHz), δ 141.48, 139.02, 133.61, 133.03, 130.26, 127.53, 127.45, 127.29, 122.57, 117.79, 67.83, 49.12, 43.60, 21.14.

BiPh-ClProm-PF₆ (acetone-*d*₆, 100MHz), δ 146.60, 144.08, 141.64, 133.73, 133.24, 128.26, 127.95, 127.64, 127.56, 127.42, 125.25, 124.39, 123.61, 122.81, 116.64, 116.27, 67.88, 62.00, 49.87, 43.93, 20.47.

BiPh-ClProm-O-PF₆ (CD₃CN, 100MHz), δ 141.39, 139.96, 138.53, 138.25, 133.47, 133.31, 131.90, 130.38, 127.44, 127.19, 126.88, 125.68, 123.19, 122.66, 117.96, 117.77, 67.97, 61.19, 49.35, 43.72, 20.96.

Bpy-Prom-PF₆ (acetone-*d*₆, 100MHz), δ 156.02, 150.36, 144.86, 137.43, 127.89, 127.71, 127.42, 125.44, 124.58, 123.07, 116.13, 66.50, 62.76, 50.17, 43.62, 20.42.

Bpy-Prom-O-PF₆ (acetone-*d*₆, 100MHz), δ 155.89, 150.14, 138.99, 137.25, 132.97, 130.12, 127.80, 127.68, 124.37, 122.57, 117.79, 66.46, 62.22, 49.57, 43.50, 21.20.

Bpy-ClProm-PF₆ (acetone-*d*₆, 100MHz), δ 156.00, 150.36, 146.59, 143.99, 137.43, 133.18, 128.23, 127.94, 127.53, 125.15, 124.56, 124.28, 123.59, 122.76, 116.61, 116.20, 66.66, 62.73, 50.14, 43.82, 20.48.

Bpy-ClProm-O-PF₆ (acetone-*d*₆, 100MHz), δ 155.89, 150.16, 140.20, 138.33, 138.26, 137.21, 133.20, 131.68, 130.09, 127.87, 127.80, 126.36, 124.37, 123.16, 122.59, 118.06, 117.74, 66.64, 62.15, 49.65, 43.73, 21.24.

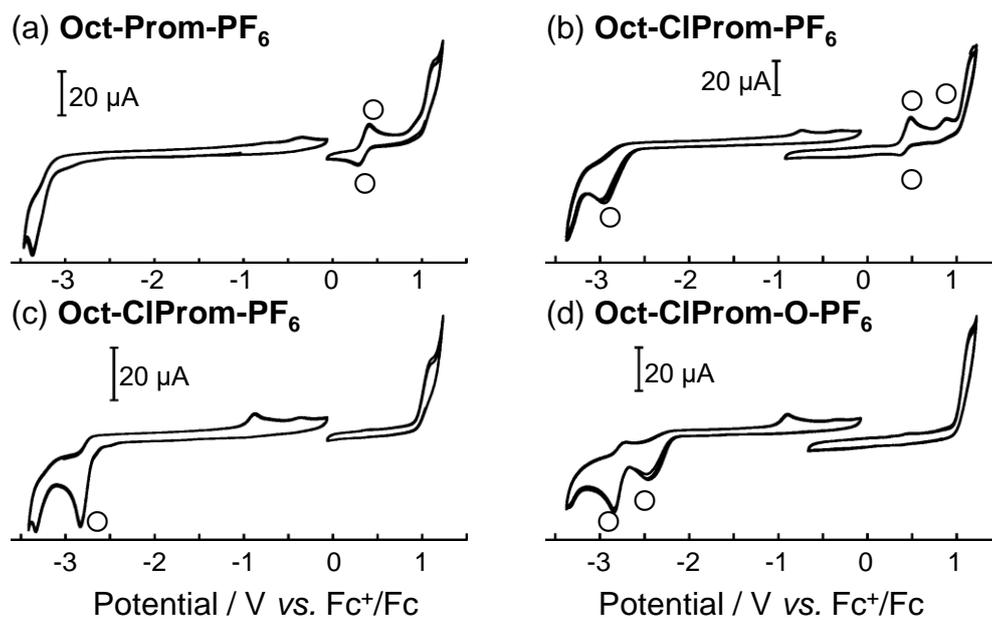


Figure S1. CV of Oct-containing BA-PF₆. DMF was used as the solvent.

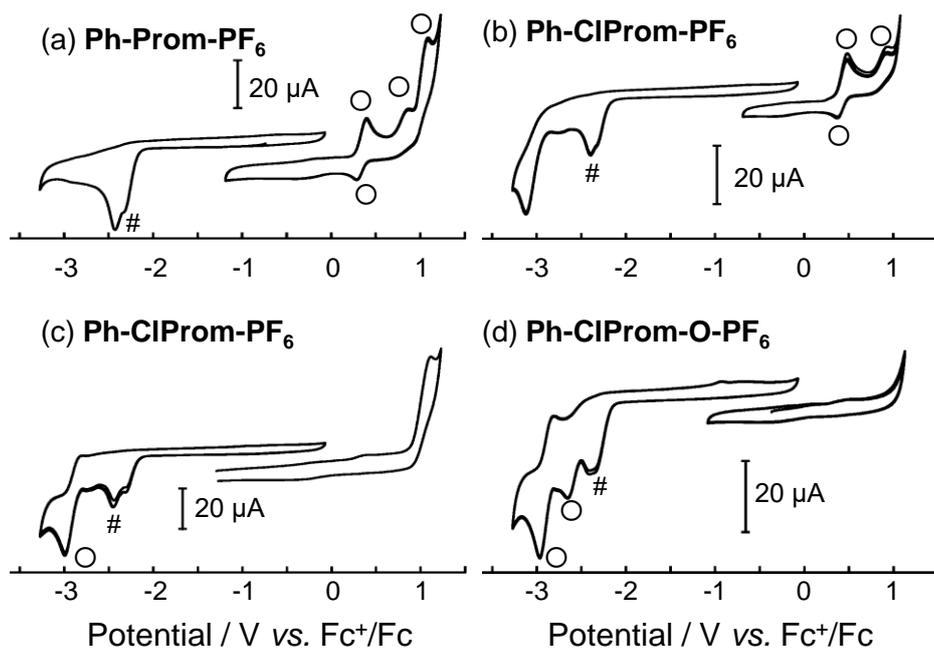


Figure S2. CV of **Ph**-containing **BA-PF₆**. DMF was used as the solvent.

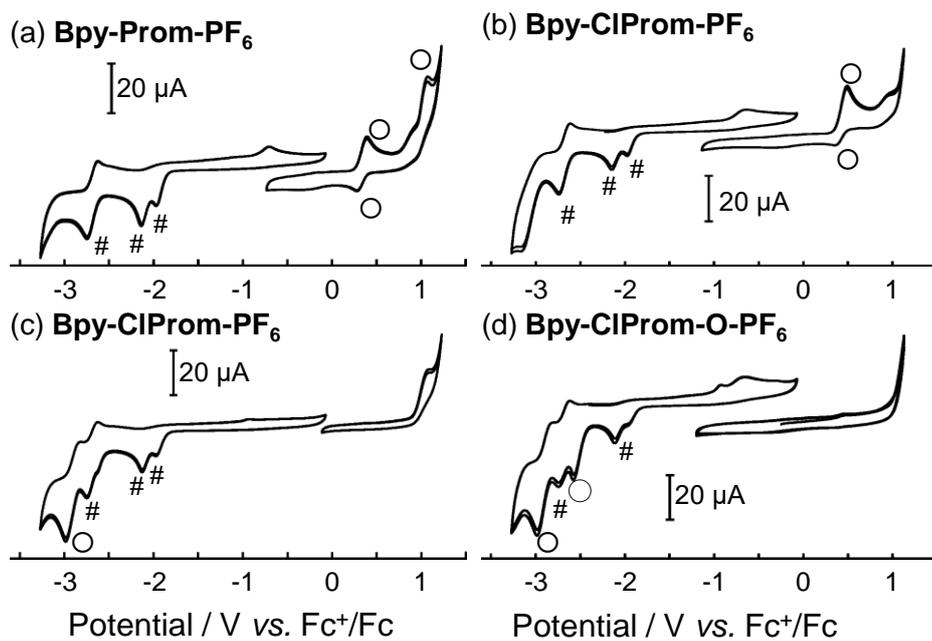


Figure S3. CV of **Bpy**-containing **BA-PF₆**. DMF was used as the solvent.

Table S1. Crystallographic data of **BA-PF₆**.

	Oct-Prom-O-PF₆	Oct-ClProm-O-PF₆	Bpy-Prom-PF₆
Formula	C ₄₄ H ₆₀ F ₁₂ N ₄ O ₂ P ₂ S ₂	C ₄₈ H ₆₄ Cl ₂ F ₁₂ N ₆ O ₂ P ₂ S ₂	C ₄₆ H ₅₀ F ₁₂ N ₆ P ₂ S ₂
Molecular Weight	1031.05	1182.01	1040.98
Crystal System	monoclinic	monoclinic	monoclinic
Space Group	<i>P</i> 2 ₁ / <i>c</i> (No. 14)	<i>P</i> 2 ₁ / <i>c</i> (No. 14)	<i>P</i> 2 ₁ / <i>c</i> (No. 14)
<i>a</i> / Å	7.94370(10)	8.1802(3)	14.4936(7)
<i>b</i> / Å	24.9032(5)	26.8118(13)	10.4801(4)
<i>c</i> / Å	12.6480(3)	12.3031(5)	15.5709(5)
α / °	90	90	90
β / °	107.689(2)	97.880(4)	99.993(4)
γ / °	90	90	90
<i>V</i> / Å ³	2383.77(8)	2672.9(2)	2329.25(16)
<i>Z</i>	2	2	2
μ /mm ⁻¹	2.431	3.155	2.480
<i>F</i> (000)	1082.40	1228.00	1076.00
<i>T</i> / K	113(2)	113(2)	113(2)
<i>D_c</i> / g cm ⁻³	1.4364	1.469	1.484
No. total reflns	8601	5356	15402
No. unique reflns	4166	4574	4672
No. variables	355	530	346
<i>R</i> (<i>R</i> ₁) ^a	0.0608 (0.0565)	0.0751 (0.0667)	0.0548 (0.0603)
<i>wR</i> 2 ^b (all data)	0.1700	0.1901	0.1507
CCDC No.	2257042	2257043	2257044