

# Voltammetry and Spectroelectrochemistry of TCNQ in Acetonitrile/RTIL Mixtures

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Table S1. Cyclic voltammetry of TCNQ in mixtures of acetonitrile and BMImPF<sub>6</sub> or BMImBF<sub>4</sub>. Acetonitrile solutions contained 0.10 M TBAP

Cyclic voltammetry of TCNQ in acetonitrile/BMImPF<sub>6</sub>

%BMImPF <sub>6</sub>	E° <sub>1</sub> , V vs Ag/AgNO <sub>3</sub>	E° <sub>2</sub> , V vs Ag/AgNO <sub>3</sub>	ΔE°, mV
0	-0.101	-0.650	549
5	-0.113	-0.642	530
10	-0.109	-0.631	523
20	-0.106	-0.615	509
33	-0.105	-0.596	491
75	-0.102	--	--
100	-0.102	-0.541	439

Cyclic voltammetry of TCNQ in acetonitrile/BMImBF<sub>4</sub>

%BMImBF <sub>4</sub>	E° <sub>1</sub> , V vs Ag/AgNO <sub>3</sub>	E° <sub>2</sub> , V vs Ag/AgNO <sub>3</sub>	ΔE°, mV
0	-0.096	-0.645	549
5	-0.101	-0.635	534
10	-0.103	-0.626	524
20	-0.102	-0.610	508
33	-0.100	-0.593	494
50	-0.101	-0.576	476
75	-0.101	-0.557	456
100	-0.096	-0.523	427

Figure S1. Mixture of acetonitrile with 60% (v/v) BMImPF<sub>6</sub>. Red: BMIm<sup>+</sup>, Green: PF<sub>6</sub><sup>-</sup>, Blue/white: acetonitrile. Adapted with permission from Acc. Chem. Res. (2007) 40, 1087-1096.  
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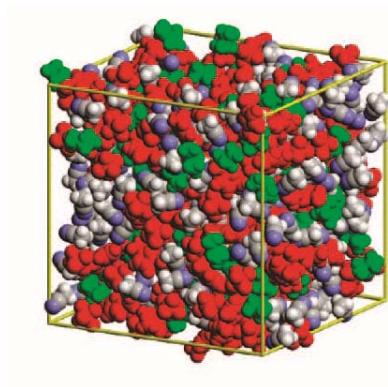


Figure S2. Cyclic voltammetry of TCNQ in AmNTf<sub>2</sub>, BMImBF<sub>4</sub>, BMImPF<sub>6</sub>, BMImNTf<sub>2</sub> and acetonitrile. Scan rate: 100 mV/s. Working electrode: Platinum. Acetonitrile contained 0.10 M TBAP

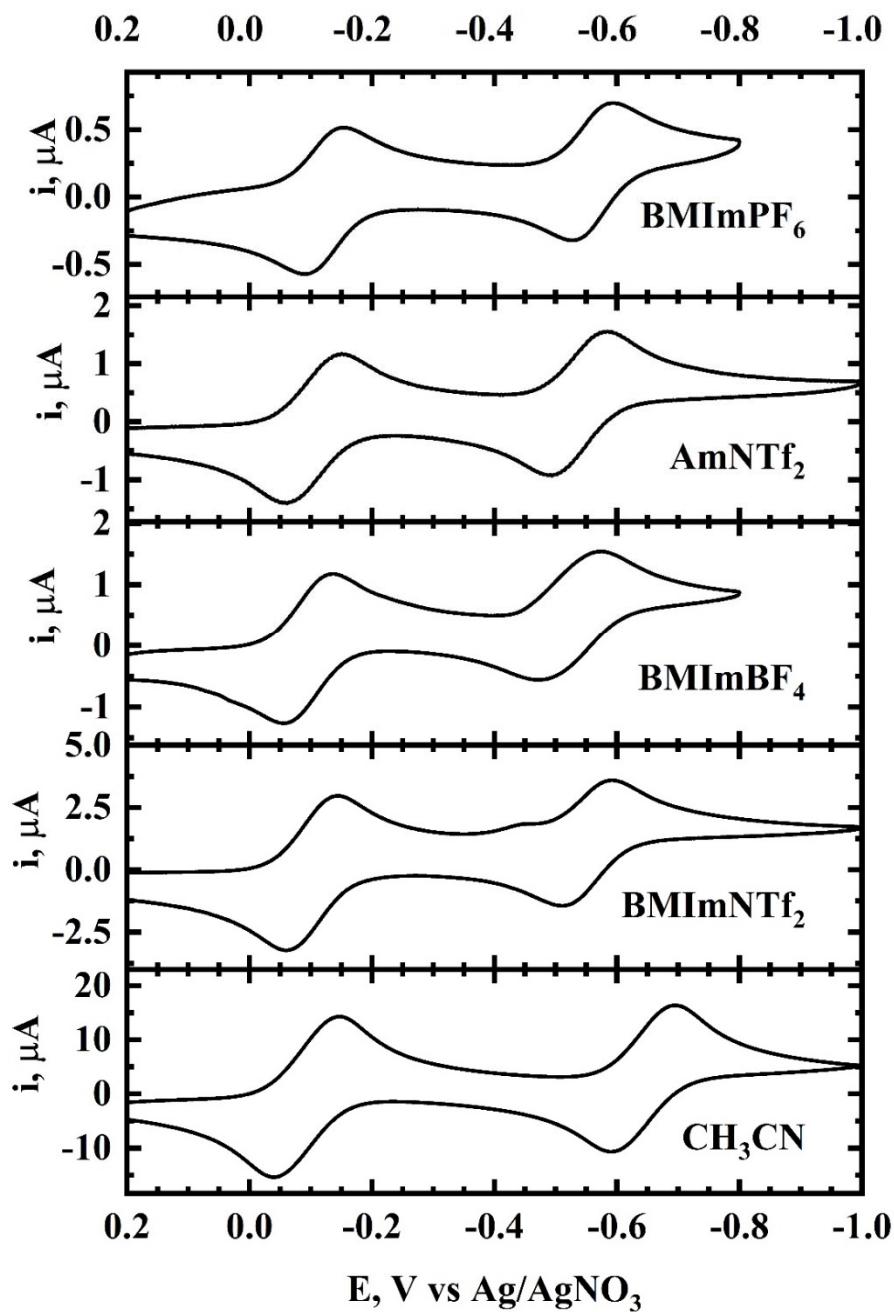
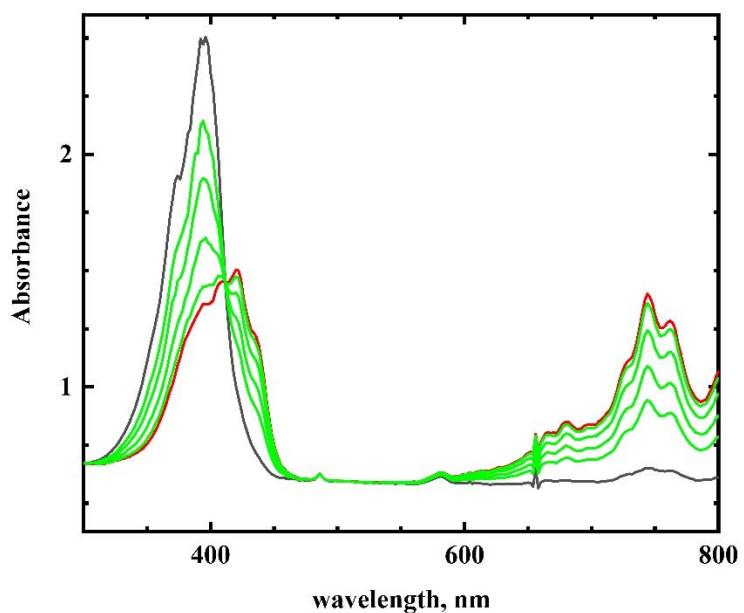
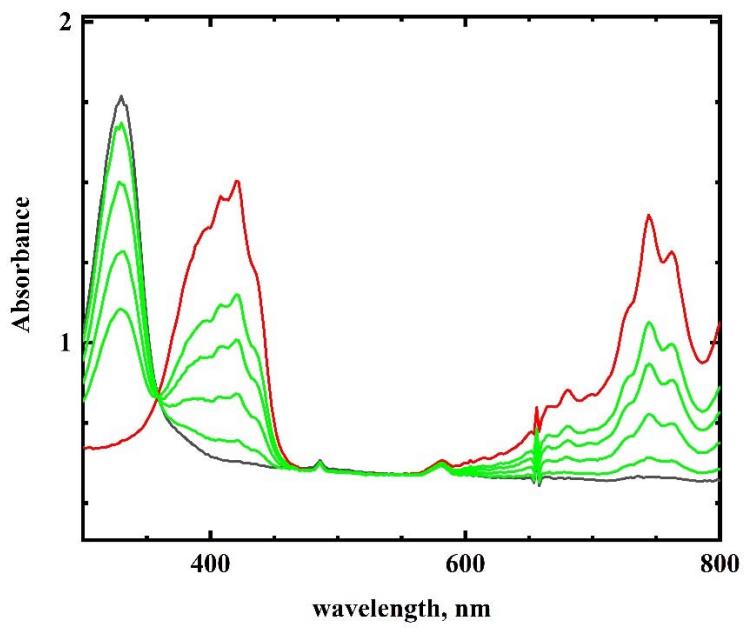


Figure S3. Visible spectroelectrochemistry of TCNQ in acetonitrile. A. First wave. B. Second wave. Electrolyte: 0.10 M TBAP



A



B

Figure S4. Infrared spectroelectrochemistry of TCNQ in THF. Initial difference spectrum (black);  $\text{TCNQ}^-$  (blue);  $\text{TCNQ}^{2-}$  (green); end of scan (red). Electrolyte: 0.10 M TBAP

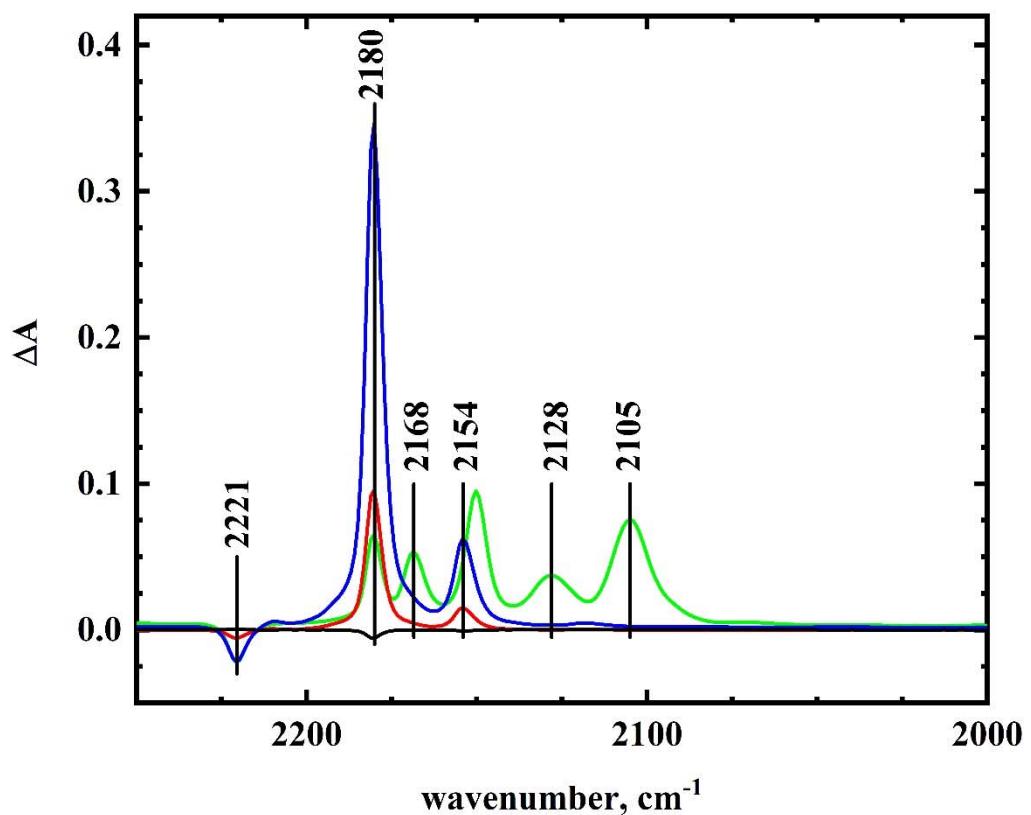


Figure S5. DFT structure of the tetramethylammonium-TCNQ<sup>2-</sup> ion pair. Gaussian 16.

