Supporting Information

Ionic Liquids Containing 1,1-Dicyano-1-acetylmethanide Anion as Potential Electrolytes

Haryo Pandu Winoto, Shalu Agarwal, Jin Kyu Im, Minserk Cheong, and Je Seung Lee*

Department of Chemistry and Research Institute of Basic Sciences, Kyung Hee University, Seoul 130-701, Korea
**E-mail: leejs70@khu.ac.kr*
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Syntheses of ionic liquids

1-Ethyl-3-methylimidazolium bromide ([EMIm]Br), 1-butyl-3-methylimidazolium bromide ([BMIm]Br), *N*-ethyl-*N*-methylmorpholinium bromide ([EMMor]Br), *N*-ethyl-pyridinium bromide ([EPy]Br), *N*-ethyl-*N*-methylpyrrolidinium bromide ([EMPyr]Br), *N*-ethyl-*N*-methylpiperidinium bromide ([EMPip]Br), 1-(ethyleneglycol monomethylether)-3-methylimidazolium methanesulfonate ($[E_1MIm][MeSO_3]$), 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ($[EMIm][Tf_2N]$), and sodium 1,1-dicyano-1-acetylmethanide ($Na[C(CN)_2(COCH_3)]$, Na[DCNAcC]) were prepared according to the literature procedures as mentioned in manuscript.

Synthesis of [EMIm][DCNAcC]. In a 100 mL one-neck flask, a solution of Na[DCNAcC] (0.7 g, 5.38 mmol) in acetone (10 mL) and a solution of [EMIm]Br (1.03 g, 5.38 mmol) in acetonitrile (25 mL) were mixed. After the mixture was stirred at room temperature for 24 h, white precipitate was filtered off and the solvents were removed by rotary evaporation. The crude product was dissolved in dichloromethane (20 mL) followed by filtration to remove the remained NaBr dissolved in [EMIm][DCNAcC]. After reducing the volumn, [EMIm][DCNAcC] was obtained as a light yellow oil by drying under vacuum for 24 h at 80 °C (Yield: 98%).

Elemental analysis calcd (%) for $C_{11}H_{14}N_4O$: C, 60.53; H, 6.47; N, 25.67; O, 7.33. Found: C, 60.99; H, 6.31; N, 25.60; O, 7.10. ^{1}H NMR (400 MHz, D_2O, 25 °C) δ 1.45 (t, 3H, CH_3); 2.04 (s, 3H, CH_3); 3.86 (s, 3H, NCH_3); 4.20 (q, 2H, NCH_2); 7.45 (d, 2H, CHN); 8.67 (s, 1H, NCHN).

Synthesis of [BMIm][DCNAcC]. [BMIm][DCNAcC] was prepared by reacting [BMIm]Cl with Na[DCNAcC] in a similar manner to that employed for the synthesis of [EMIm][DCNAcC] (Yield: 99%).

Elemental analysis calcd (%) for for $C_{13}H_{18}N_4O$: C, 63.39; H, 7.37; N, 22.75; O, 6.50. Found: C, 63.05; H, 7.69; N, 23.02; O, 6.24. ^{1}H NMR (400 MHz, D_2O, 25 °C) δ 0.78 (t, 3H, CH_3); 1.19 (m, 2H, CH_2); 1.70 (m, 2H, CH_2); 2.02 (s, 3H, CH_3); 3.73 (s, 3H, NCH_3); 4.04 (t, 2H, NCH_2); 7.32 (d, 2H, CHN); 8.57 (s, 1H, NCHN).

Synthesis of [E_1MIm][DCNAcC]. [E_1MIm][DCNAcC] was prepared by reacting [E_1MIm][$MeSO_3$] with Na[DCNAcC] in a similar manner to that employed for the synthesis of [EMIm][DCNAcC] (Yield: 92%).

Elemental analysis calcd (%) for for $C_{12}H_{16}N_4O_2$: C, 58.05; H, 6.50; N, 22.57; O, 12.89. Found: C, 57.95; H, 6.64; N, 22.89; O, 12.52. ^{1}H NMR (400 MHz, D_2O, 25 °C) δ 1.91 (s, 3H, CH_3); 3.28 (s, 3H, OCH_3); 3.73 (t, 2H, OCH_2); 3.75 (s, 3H, NCH_3); 4.30 (t, 2H, NCH_2); 7.36 (d, 2H, CHN); 8.66 (s, 1H, NCHN).

Synthesis of [EPy][DCNAcC]. [EPy][DCNAcC] was prepared by reacting [EPy]Br with Na[DCNAcC] in a similar manner to that employed for the synthesis of [EMIm][DCNAcC] (Yield: 97%).

Elemental analysis calcd (%) for $C_{12}H_{13}N_3O$: C, 66.96; H, 6.09; N, 19.52; O, 7.43. Found: C, 66.59; H, 5.92; N, 19.59; O, 7.90. ^{1}H NMR (400 MHz, D_2O, 25 °C) δ 1.59 (t, 3H, CH_3); 2.00 (s, 3H, CH_3); 4.58 (q, 2H, NCH_2); 8.02 (2H, t, Ar-H); 8.50 (t, 1H, Ar-H); 8.81 (d, 2H, Ar-H).

Synthesis of [EMPip][DCNAcC]. [EMPip][DCNAcC] was prepared by reacting [EMPip]Br with Na[DCNAcC] in a similar manner to that employed for the synthesis of [EMIm][DCNAcC] (Yield: 97%).

Elemental analysis calcd (%) for for $C_{13}H_{21}N_3O$: C, 66.35; H, 8.99; N, 17.86; O, 6.80. Found: C, 66.20; H, 8.67; N, 17.95; O, 7.18. ^{1}H NMR (400 MHz, D_2O, 25 °C) δ 1.07 (t, 3H, CH_3); 1.39 (m, 2H, CH_2); 1.56 (m, 4H, CH_2); 1.94 (s, 3H, CH_3); 2.72 (s, 3H, NCH_3); 3.10 (m, 4H, NCH_2); 3.36 (q, 2H, NCH_2).

Synthesis of [EMPyr][DCNAcC]. [EMPyr][DCNAcC] was prepared by reacting [EMPyr]Br with Na[DCNAcC] in a similar manner to that employed for the synthesis of [EMIm][DCNAcC] (Yield: 98%).

Elemental analysis calcd (%) for $C_{12}H_{19}N_3O$: C, 65.13; H, 8.65; N, 18.99; O, 7.23. Found: C, 65.25; H, 8.52; N, 18.86; O, 7.37. ^{1}H NMR (400 MHz, D_2O, 25 °C) δ 1.32 (t, 3H, CH_3); 2.03 (s, 3H, CH_3); 2.15 (m, 4H, CH_2); 2.97 (s, 3H, NCH_3); 3.34 (q, 2H, NCH_2); 3.43 (t, 4H, NCH_2).

Synthesis of [EMMor][DCNAcC]. [EMMor][DCNAcC] was prepared by reacting [EMMor]Br with Na[DCNAcC] in a similar manner to that employed for the synthesis of

[EMIm][DCNAcC] (Yield: 99%).

Elemental analysis calcd (%) for $C_{12}H_{19}N_3O_2$: C, 60.74; H, 8.07; N, 17.71; O, 13.48. Found: C, 60.92; H, 7.98; N, 17.80; O, 13.30. ^{1}H NMR (400 MHz, D_2O, 25 °C) δ 1.30 (t, 3H, CH_3); 2.02 (s, 3H, CH_3); 3.09 (s, 3H, NCH_3); 3.40 (t, 4H, NCH_2); 3.48 (q, 2H, NCH_2); 3.97 (t, 4H, OCH_2).

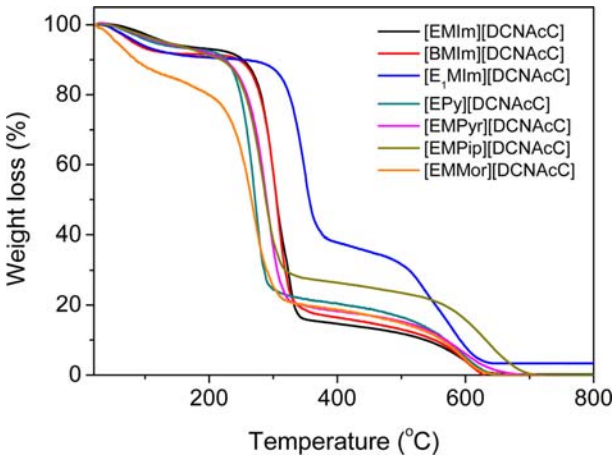

Figure S1. Thermogravimetric analysis (TGA) of various types of ILs.

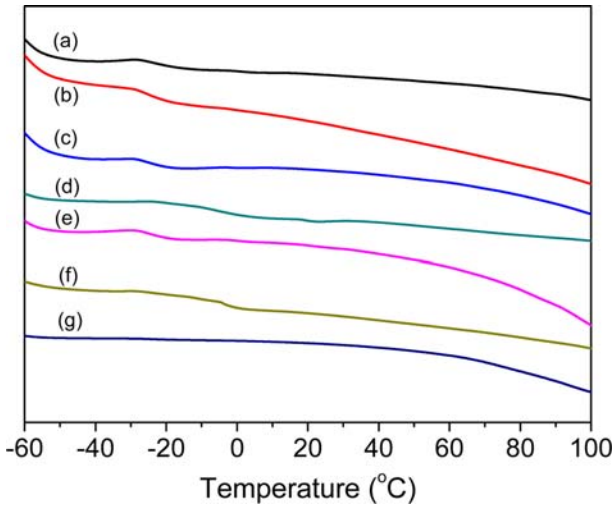

Figure S2. Differential scanning calorimetric analysis (DSC) of various types of ILs: (a) [EMIm][DCNAcC], (b) [BMIm][DCNAcC], (c) [E_1MIm][DCNAcC], (d) [EPy][DCNAcC], (e) [EMPyr][DCNAcC], (f) [EMPip][DCNAcC], and (g) [EMMor][DCNAcC].

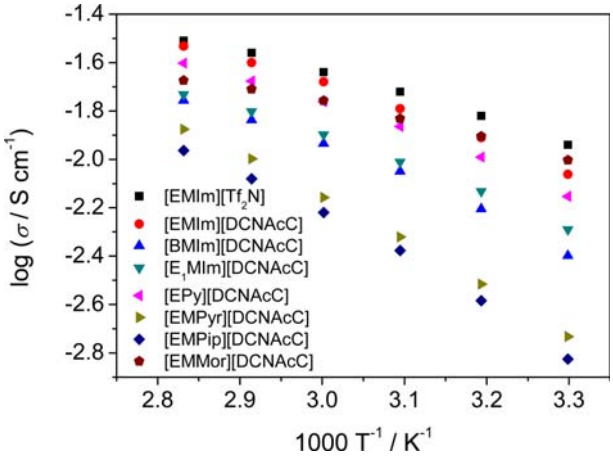

Figure S3. Ionic conductivities of ILs.