Electronic Supplementary Information:

Ionic liquid and oligomer electrolytes based on the $B(CN)_4^-$ anion; Ion association, physical and electrochemical properties.

Johan Scheers,*[a] Jagath Pitawala,[a] Frederic Thebault,[a] Jae-Kwang Kim,[a] Jou-Hyeon Ahn,[b] Aleksandar Matic[a], Patrik Johansson[a,c] and Per Jacobsson[a]

[a]*Department of Applied Physics, Chalmers University of Technology, SE-412 96 Gothenburg, Sweden.*

[b] *Department of Chemical and Biological Engineering, Engineering Research Institute , Gyeongsang National University, 900 Gajwa-dong, Jinju 660-701, Republic of Korea*

[c]*ALISTORE - European Research Institute*

*Corresponding author. Tel.: +46 31 772 3177; fax: +46 31 772 2090.
E-mail address: johan.scheers@chalmers.se

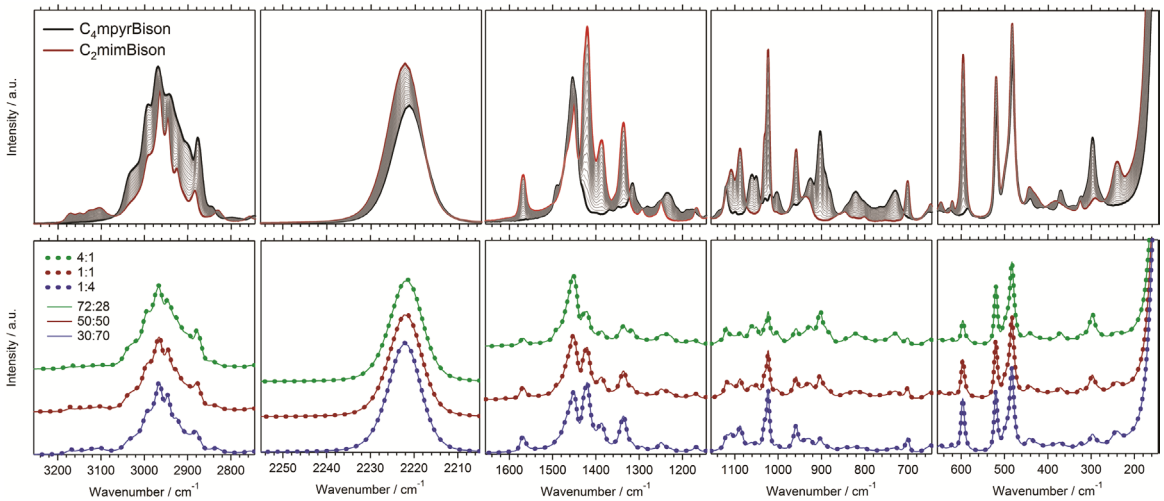

Figure S1. Raman spectra of C_2mimBison, C_4mpyrBison and twenty IL linear combinations (top), and Raman spectra of three IL mixtures (4:1, 1:1, and 1:4; by volume) and the best fits of linearly combined spectra of the neat ILs (bottom).

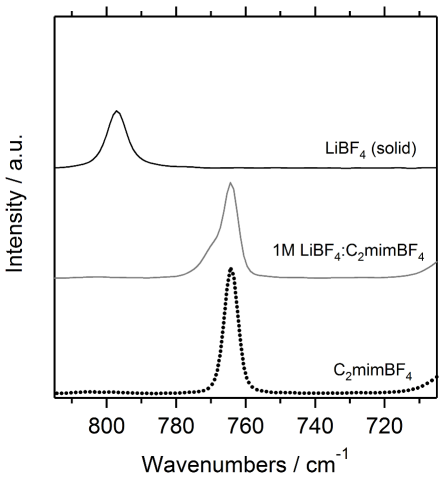

Figure S2. Raman spectroscopy results (ν_s(BF)) from a 1M $LiBF_4$:C_2mimBF_4 electrolyte with reference to the $LiBF_4$ salt (top) and C_2mimBF_4 ionic liquid (bottom).

TABLE S1. Ionic conductivity and glass transition temperatures of C_4mpyrBison, C_2mimBison, and their mixtures.

C_4mpyr^+: C_2mim^+	$\sigma_{20°C}$ / mS cm^{-1}	T_g/°C
1:0	3.43	-
9:1	5.22	-
4:1	4.65	-80
1:1	8.14	-78
1:4	10.63	-77
0:1	18.03	-76

TABLE S2. Dissociation energies for mono-, bi-, and tridentate ion pair configurations of LiBison and $LiBF_4$, as a function of computational models, and ion pair surrounding. The most stable energy for each combination is highlighted in bold.

Model:	Li^+Bison			$Li^+BF_4^-$		
	HF/6-31G(d)	MP2/6-31G(d)	B3LYP/6-311+G(d)	HF/6-31G(d)	MP2/6-31G(d)	B3LYP/6-311+G(d)
		mono/bi/tridentate			mono/bi/tridentate	
VACUUM	447/**483**/443	452/**508**/486	446/**479**/438	564′/**646**/636	582′/**676**/**676**	535′/**602**/592
CHN (ε=2.0)	**220**′/212/220′	226′/**234**′/207′	**217**′/203/–	287′/**334**/316	303′/**360**′/351	260′/**293**/275′
THF (ε=7.4)	**69**′/51/49	**75**/57′/57	**65**/42/41′	100′/**120**/97′	113′/**143**/129	76/**84**/63′
ACN (ε=36)	**28**/16/16	**34**/22/22	**23**/9/9′	47/**59**/36′	59/**82**/65′	25/**26**′/–
H_2O (ε=78)	**22**/12/17	–/18/18	**17**/5/4	39/**51**/–	51/**73**/56′	17′/**18**′/–

′One or several imaginary vibrational modes. All energies are reported in kJ mol^{-1}.

TABLE S3. Dissociation energies for mono-, bi-, and tridentate ion pair configurations of NaBison and KBison.

Model:	Na^+Bison			K^+Bison		
	HF/6-31G(d)	MP2/6-31G(d)	B3LYP/6-311+G(d)	HF/6-31G(d)	MP2/6-31G(d)	B3LYP/6-311+G(d)
		mono/bi/tridentate			mono/bi/tridentate	
VACUUM	381/**421**/404	387/**442**/441	376/**411**/394	326′/**363**/358	336/384/**388**	326′/**360**/353
ACN (ε=36)	**26**/16/16	**32**′/22/22	**22**′/9/9	**22**′/15′/15	**30**′/25/21	**19**′/8/8

′One or several imaginary vibrational modes. All energies are reported in kJ mol^{-1}.

TABLE S4. Dissociation energies (E_d) for four-coordinated Li^+, Na^+, and K^+ models.

	E_d / kJ mol^{-1}		
Structure:	HF/6-31G(d)	MP2/6-31G(d)	B3LYP/6-311+G(d)
$Li(BF_4)_4^{3-}$	341	399	261
$Li(Bison)_4^{3-}$	404	454	382
$Na(Bison)_4^{3-}$	322	359	298
$K(Bison)_4^{3-}$	243	279	223