

**Table 1S** Scaling factors for the force fields of the ion pair.

scaling factor		value
stretch	C-C	0.9207 <sup>a</sup>
stretch	C-H	0.889 <sup>b</sup>
stretch	C-P	1.040 <sup>c</sup>
stretch	B-F	1.00 <sup>d</sup>
bend	C-C-C	1.0144 <sup>a</sup>
bend	C-C-H	0.95 <sup>a</sup>
bend	H-C-H	0.9016 <sup>a</sup>
bend	C-P-C	1.070 <sup>c</sup>
bend	C-C-P	1.0144 <sup>a</sup>
bend	F-B-F	1.0144 <sup>d</sup>
torsion	all	0.9523 <sup>a</sup>

<sup>a</sup> J.Baker, A.Jarzecki, P.Pulay, *J.Phys.Chem.A*, **1998**, *102*, 1412.

<sup>b</sup> S.A.Katsyuba, J.Grunenberg, R.Schmutzler, *J.Mol.Struct.*, **2001**, *559*, 315-320.

<sup>c</sup> S.A.Katsyuba, E.E.Vandyukova. *Chem. Phys. Lett.*, **2003**, *377*, No. 5-6, 658-662.

<sup>d</sup> S.A.Katsyuba, E.E.Zvereva, P.J.Dyson, A.Vidiš, *J. Phys. Chem. A*, **2007**, *111*, 352.

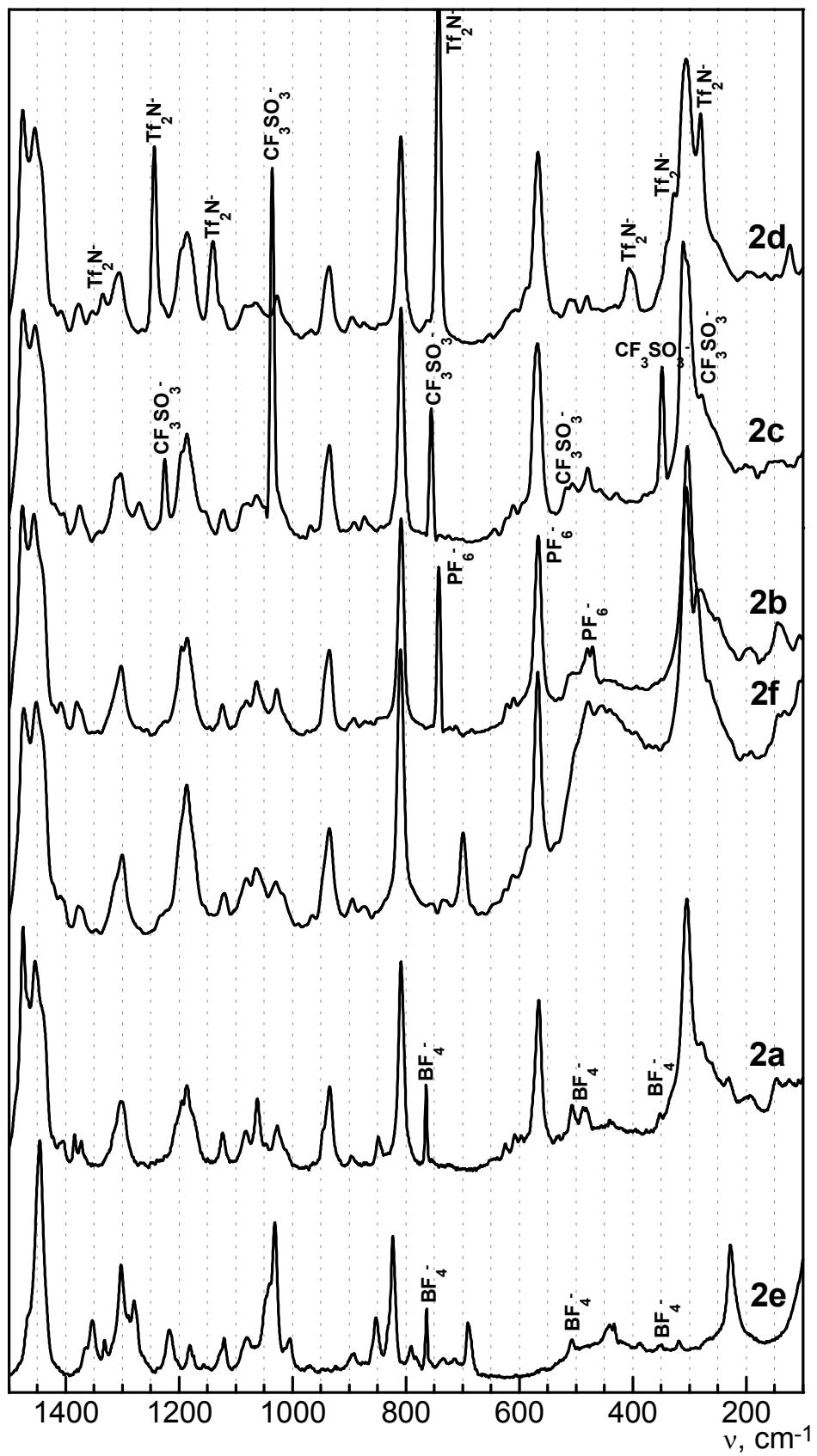


Fig.1S. Raman spectra of the ionic liquids studied. The bands of different anions are marked.

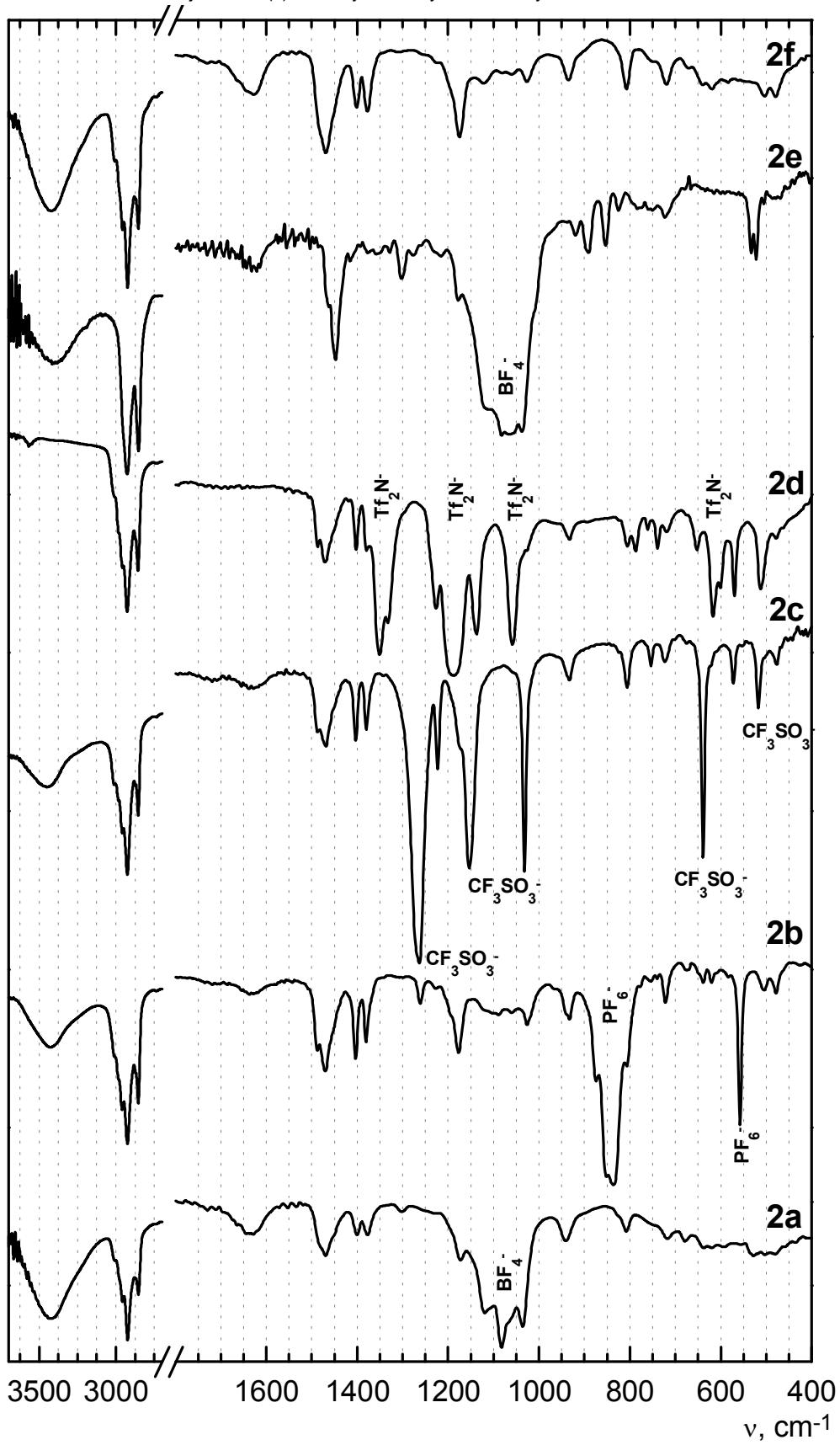


Fig.2S. IR spectra of the ionic liquids studied. The bands of different anions are marked.