Vapor composition and vaporization thermodynamics of 1-ethyl-3-methylimidazolium hexafluorophosphate ionic liquid

A.M. Dunaev, V.B. Motalov, M.A. Korobov, D.N. Govorov, V.V. Aleksandriiskii, L.S. Kudin
Corresponding author: amdunaev@ro.ru

Supplementary materials

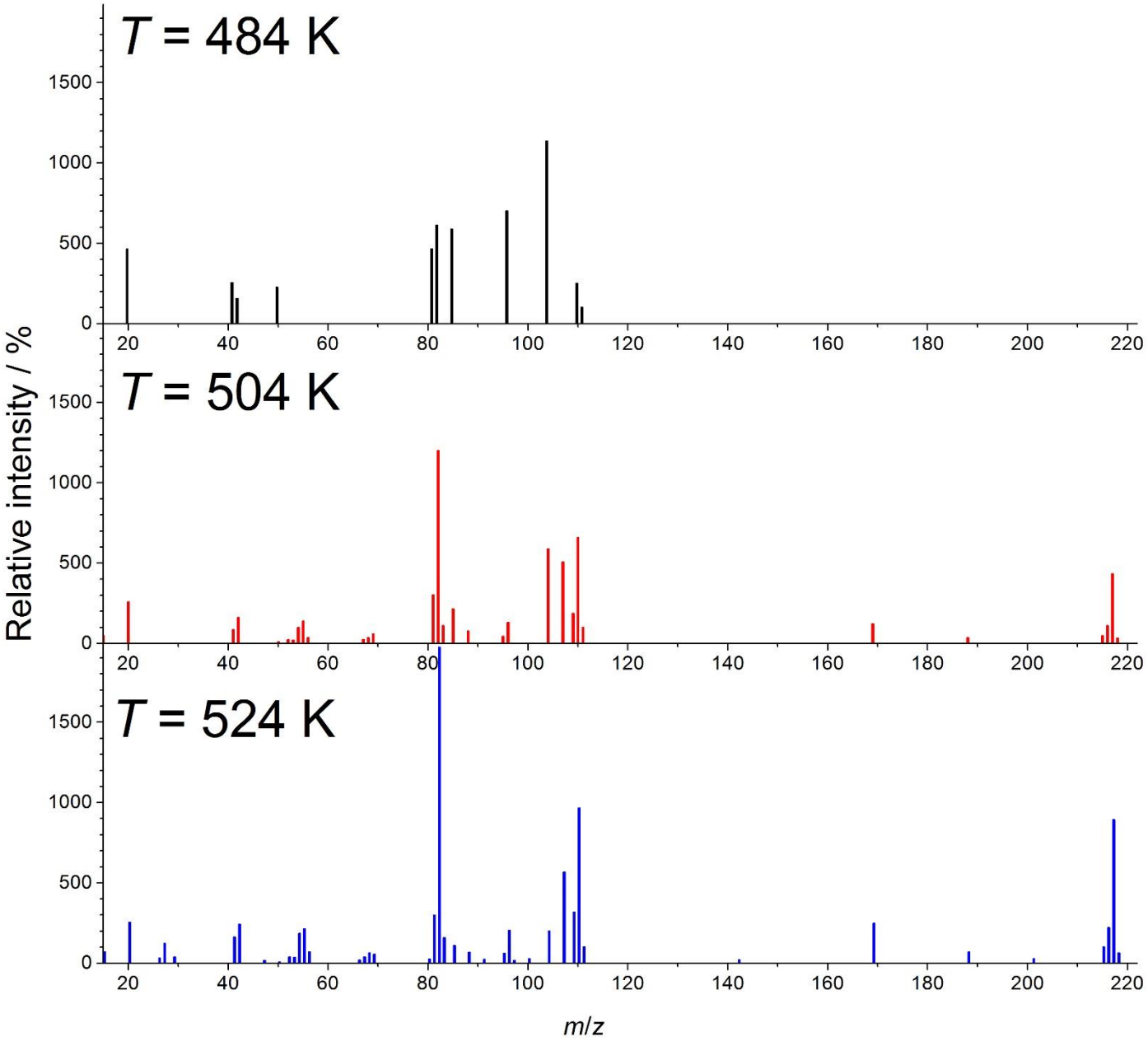

Figure S1. Full-scale background subtracted electron ionization mass spectra of $EMImPF_6$ under EC-I conditions relative to the intensity of the parent cation (m/z = 111)

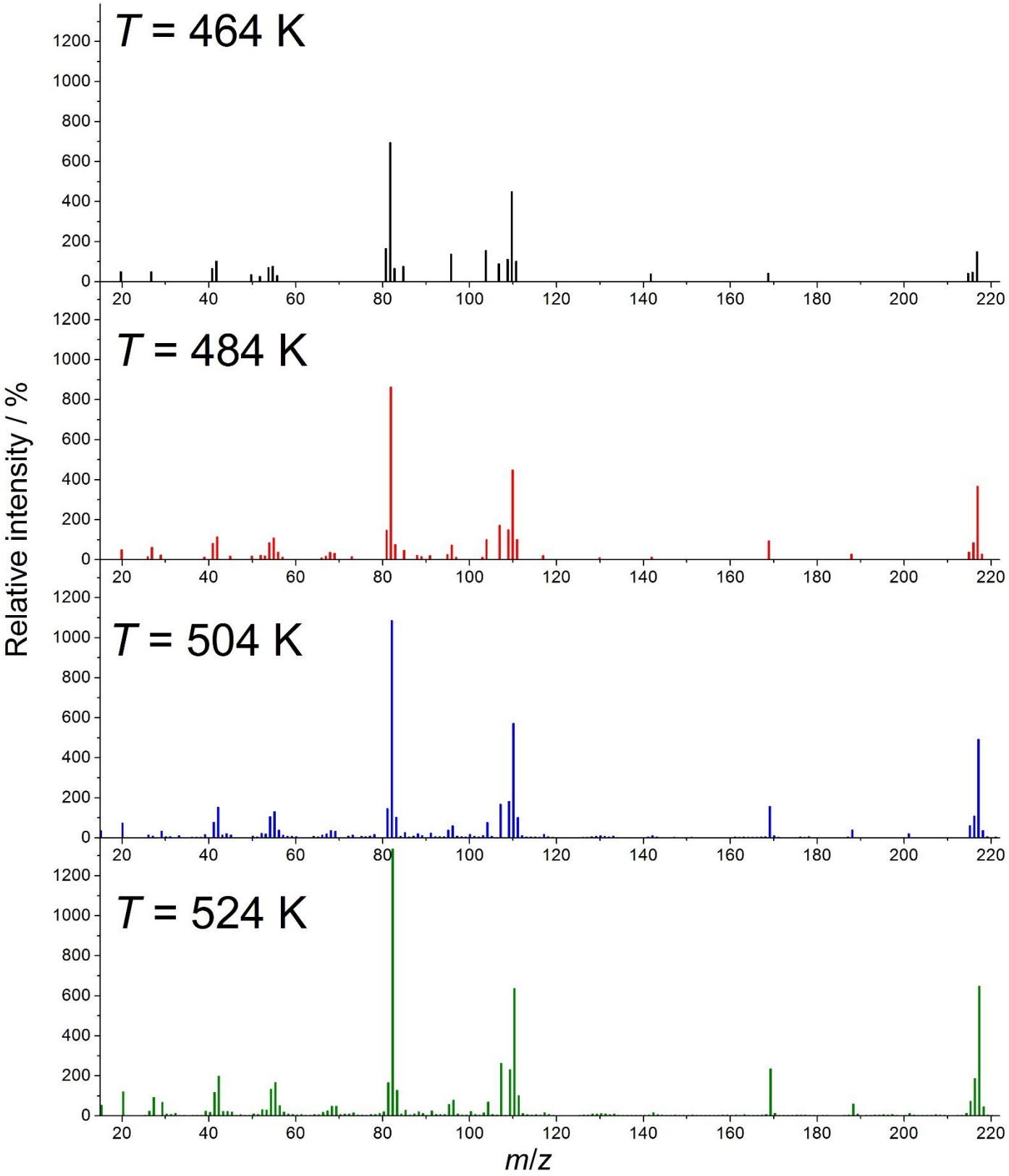

Figure S2. Full-scale background subtracted electron ionization mass spectra of $EMImPF_6$ under EC-II conditions relative to the intensity of the parent cation (m/z = 111)

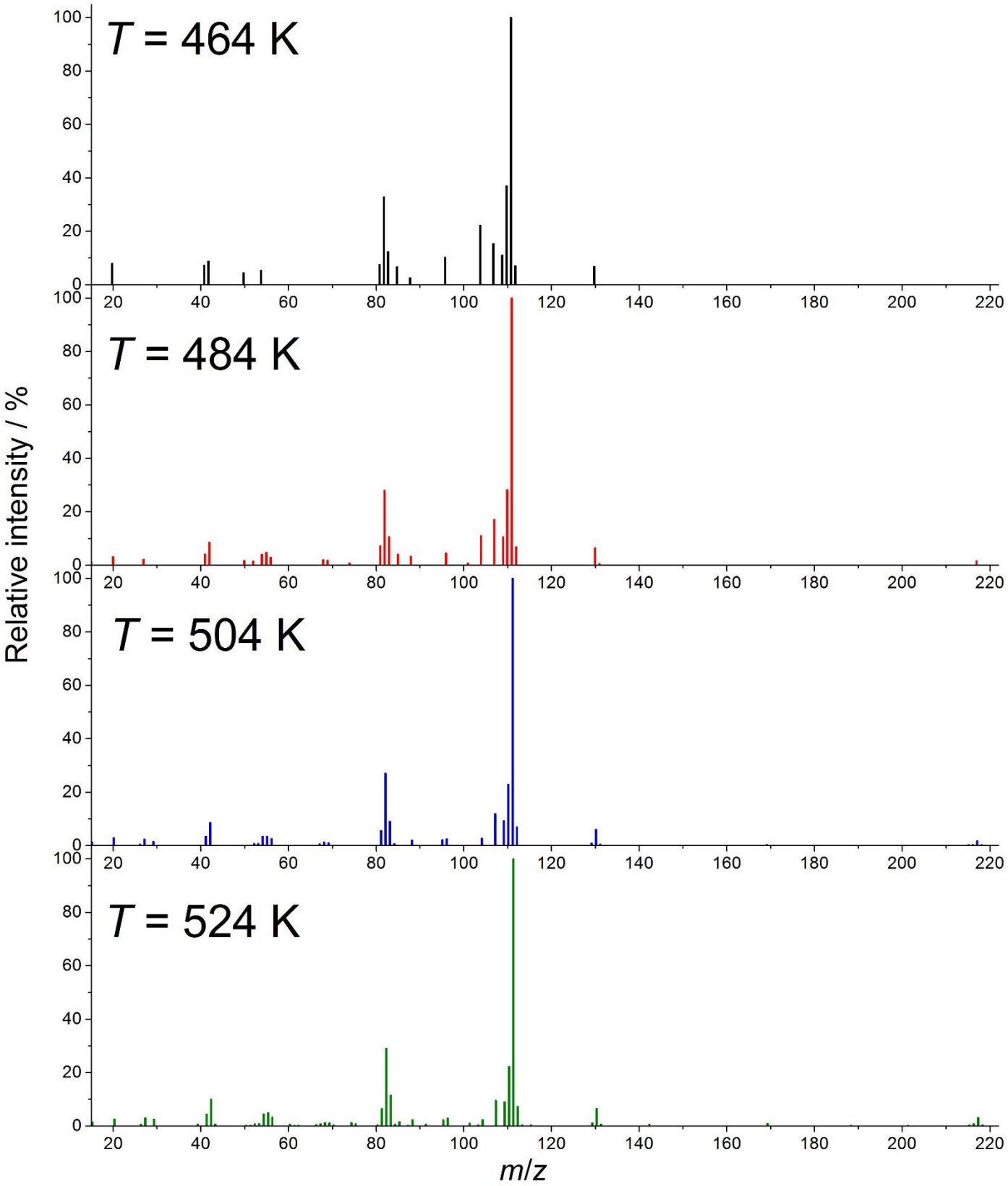

Figure S3. Full-scale background subtracted electron ionization mass spectra of $EMImPF_6$ under OC conditions relative to the intensity of the parent cation (m/z = 111)

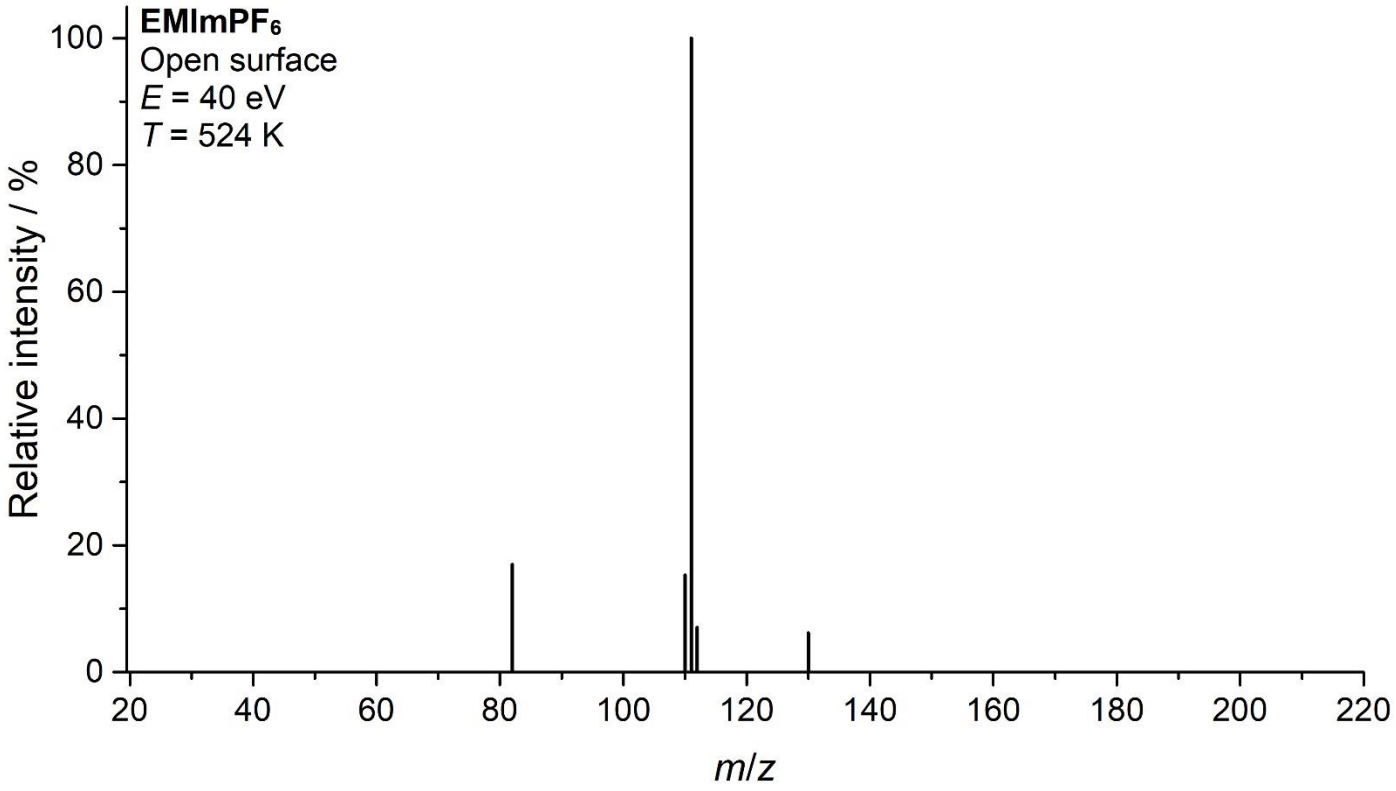

Figure S4. Full-scale background subtracted electron ionization mass spectra of $EMImPF_6$ under OS conditions relative to the intensity of the parent cation (m/z = 111)

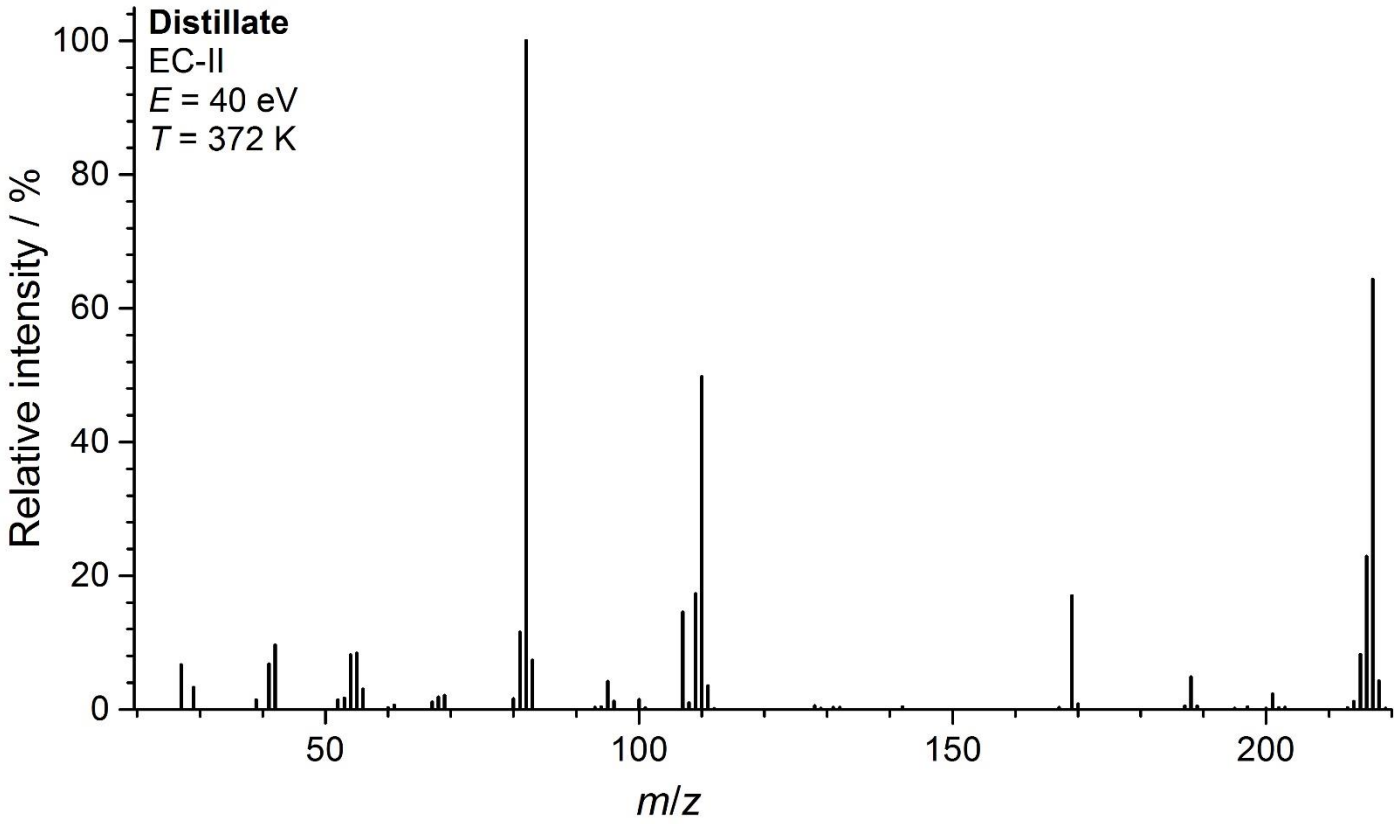

Figure S5. Full-scale background subtracted electron ionization mass spectra of IL distillate under EC-II conditions relative to the intensity of an ion with m/z = 82

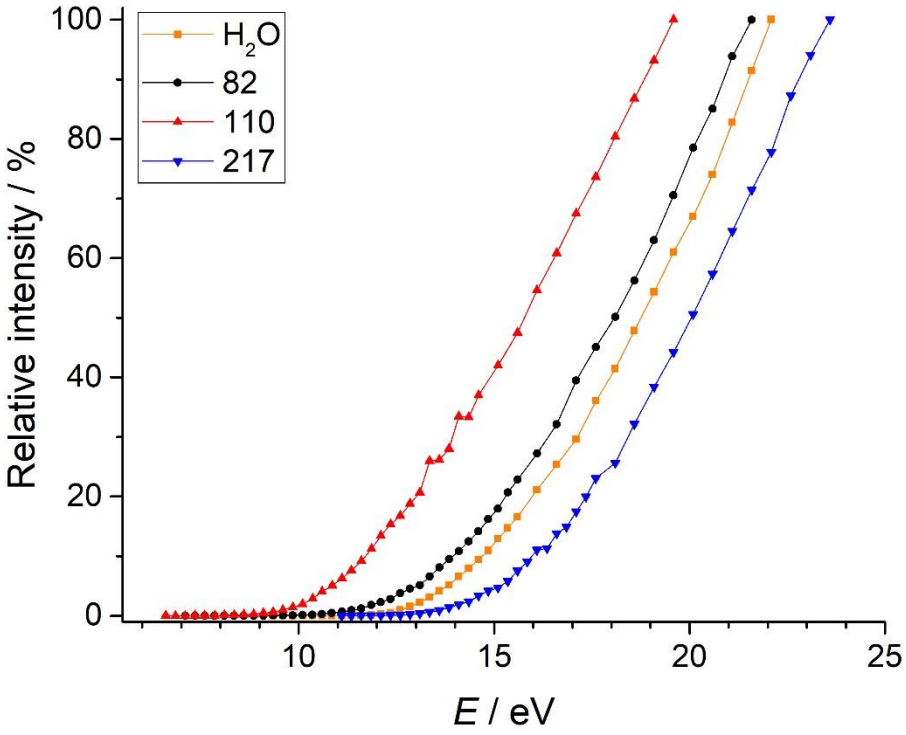

Figure S6. Ionization efficiency curves of the ions of IL distillate (90% is $C_6N_2H_{10}PF_5$) under EC-II conditions at 374 K

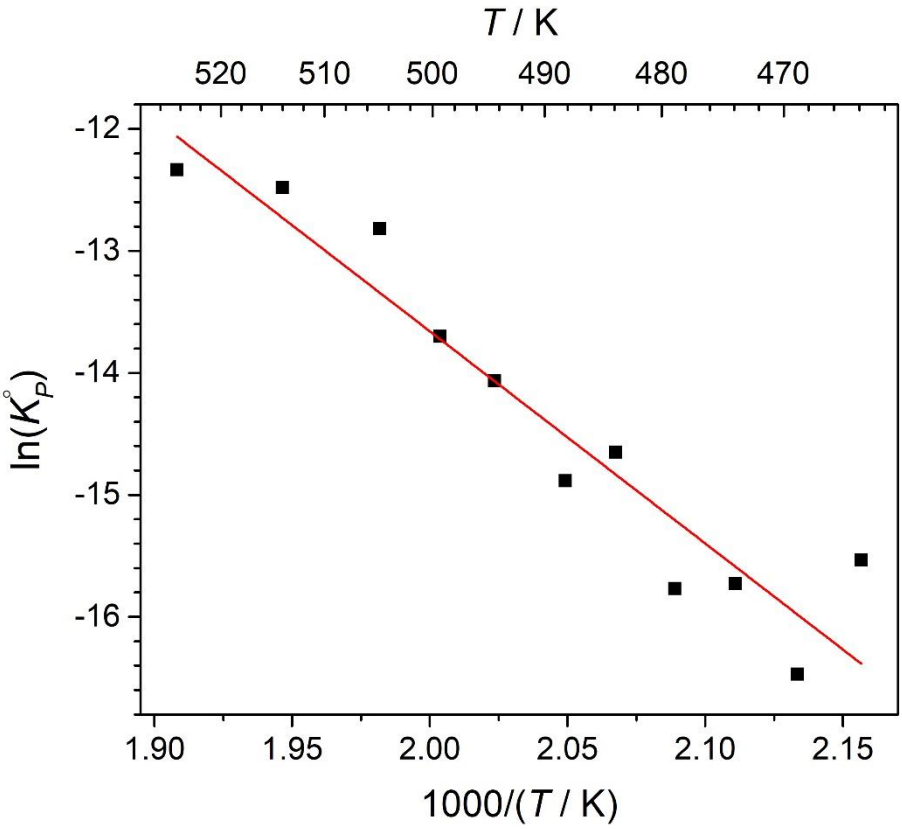

Figure S7. Temperature dependence of equilibrium constant of reaction I

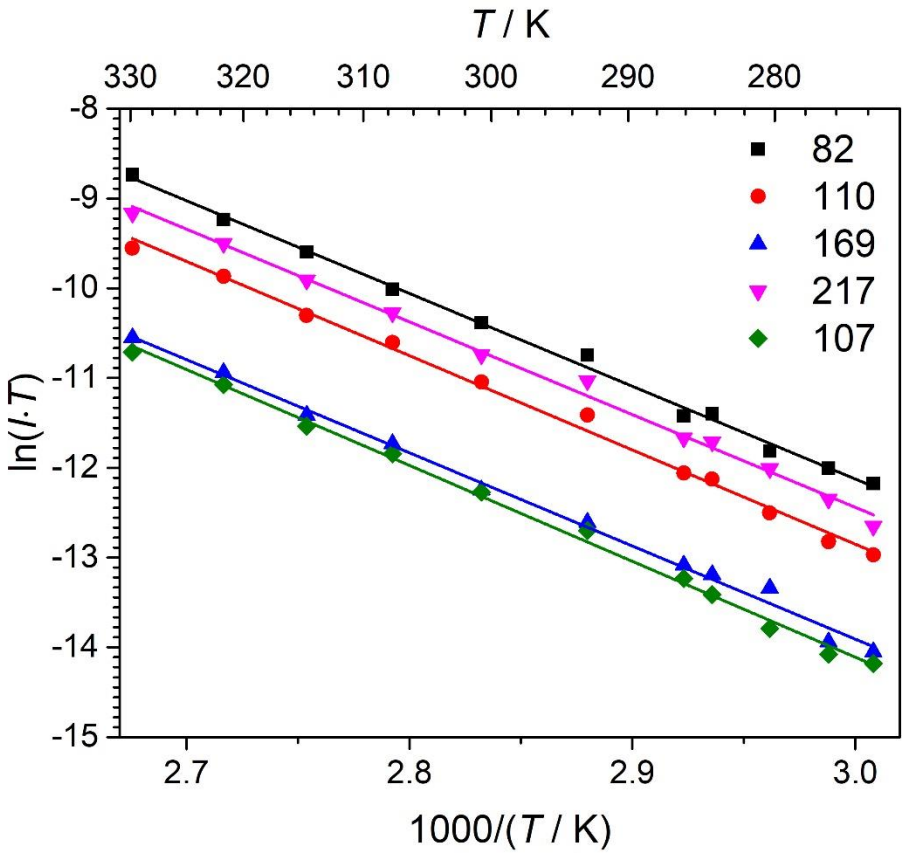

Figure S8. Temperature dependencies of ion currents over IL distillate (90% is $C_6N_2H_{10}PF_5$) obtained under EC-II conditions

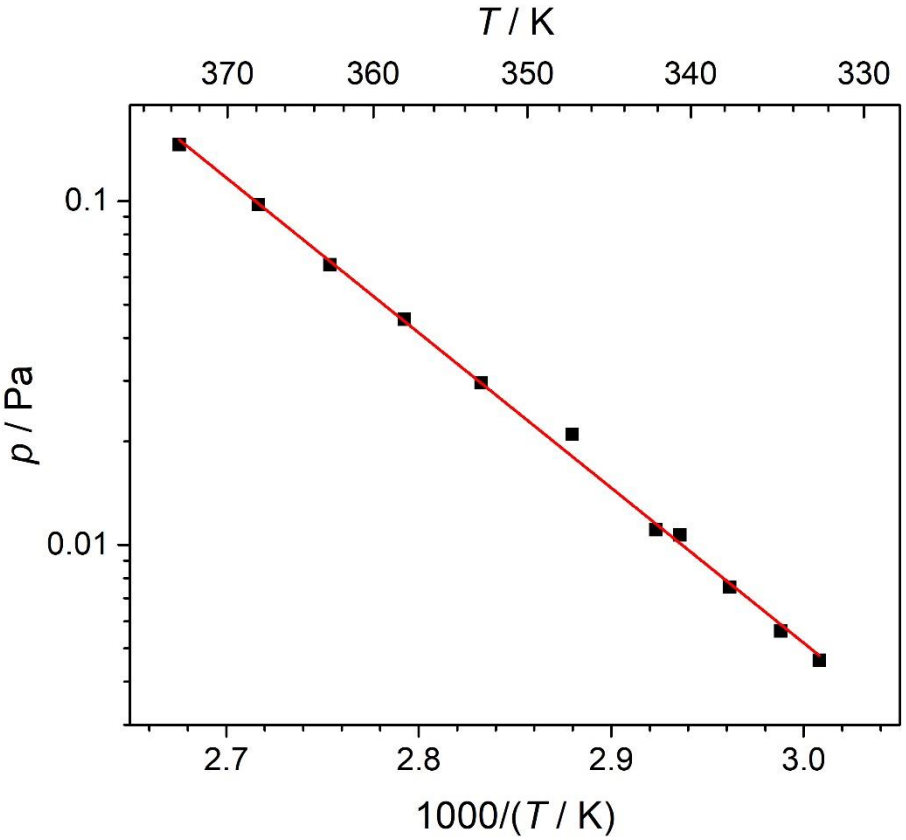

Figure S9. Temperature dependence of $C_6N_2H_{10}PF_5$ vapor pressure over IL distillate (90% is $C_6N_2H_{10}PF_5$) under EC-II conditions

Table S1. List of isogyric reactions used for determination of $\Delta_f H°$(EMImPF$_{6,\,g}$, 298.15 K)

Reaction	$\Delta_r H°$ / kJ·mol^{-1}	$\Delta_f H°$ / kJ·mol^{-1}
$EMImPF_6=EMIm^+ + PF_6^-$	343.6	-1933.4
$EMImPF_6+H_2+H^-=Im+CH_4+C_2H_6+PF_6^-$	-494.7	-1934.1
$EMImPF_6+H^-=Im+CH_3^{\cdot}+C_2H_5^{\cdot}+PF_6^-$	-73.6	-1943.2
$EMImPF_6+HF=Im+CH_3F+C_2H_5F+PF_5$	241.7	-1938.8
$EMImPF_6+H_2=Im+CH_4+C_2H_5F+PF_5$	131.6	-1929.6
$EMImPF_6+H_2=Im+CH_3F+C_2H_5F+PF_3+HF$	329.1	-1937.9
$EMImPF_6+H_2+H^-=Pyr+CH_4+C_2H_6+PF_6^-$	-448.7	1935.5
$EMImPF_6+H^-=MIm+C_2H_6+PF_6^-$	-465.2	-1932.0
$EMImPF_6+H=MIm+C_2H_6+PF_5+F$	210.2	-1936.3
$EMImPF_6+H=MIm+C_2H_5^{\cdot}+HF+PF_5$	60.8	-1948.6
$EMImPF_6=MIm+C_2H_4+HF+PF_5$	211.0	-1935.4
$EMImPF_6=MIm+C_2H_5F+PF_5$	161.0	-1927.5
$EMImPF_6+H^-=EIm+CH_4+PF_6^-$	-475.4	-1933.9
$EMImPF_6+H=EIm+CH_4+PF_5+F$	200.1	-1938.3
$EMImPF_6+H=EIm+CH_3^{\cdot}+HF+PF_5$	66.6	-1936.6
$EMImPF_6=EIm+CH_3F+PF_5$	176.8	-1948.8
$EMImPF_6=EMIm+HF+PF_5$	100.7	-1941.5
	AVERAGE:	-1937±3

Table S2. Calculated partial vapor pressures under EC conditions and sublimation enthalpies obtained in the framework of the third law method

T / K	p / ×10^4 Pa	$\Delta_s H^o$(NIP, 298.15 K)
524	16.0	152.5
514	10.3	152.0
505	6.60	151.7
494	3.51	151.8
484	1.73	152.1
474	0.93	152.1
464	0.37	153.0
469	0.63	152.3
479	1.30	152.0
488	2.51	151.7
499	4.44	152.1
478	4.54	134.91
463	1.55	135.33