Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Effects of substituent branching and chirality on physical properties of ionic liquids based on cationic ruthenium sandwich complexes

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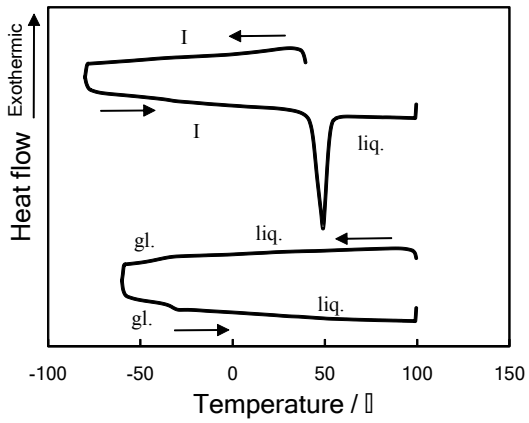
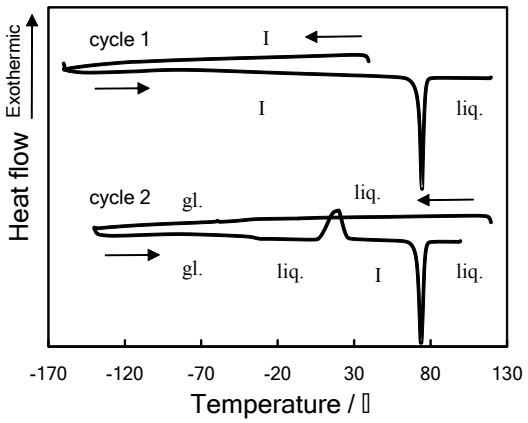
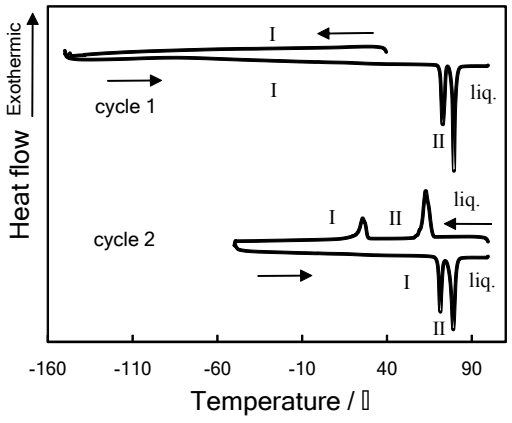
(a) *rac*-[**1**][PF_6]



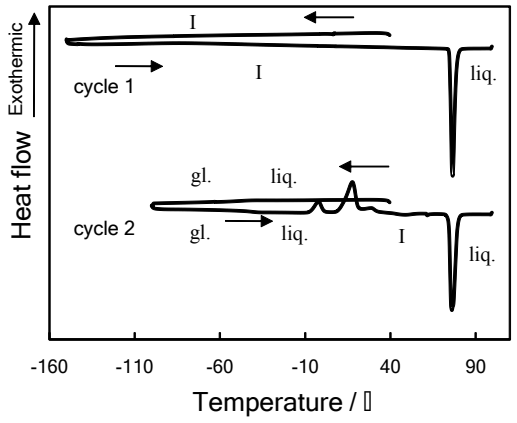
(b) *chiral*-[**1**][PF_6]



(c) [**2**][PF_6]



(d) [**3**][PF_6]



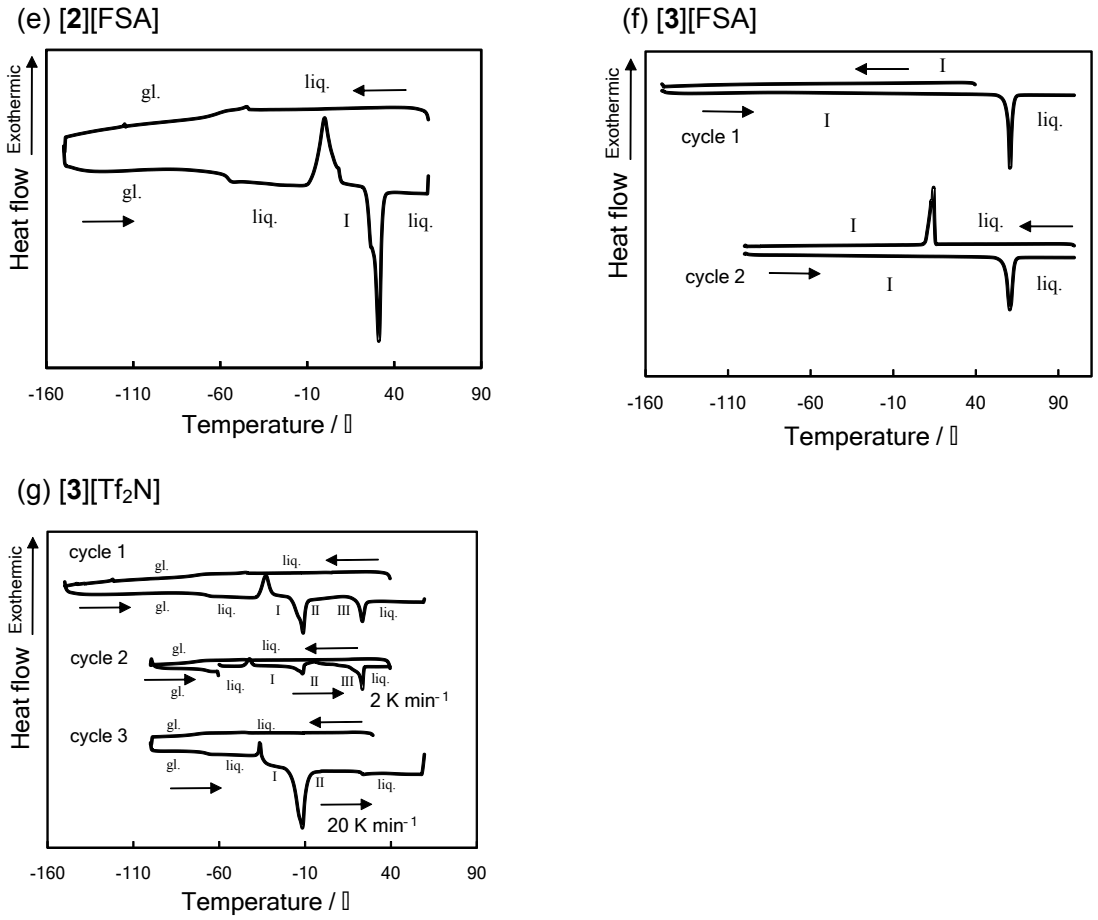


Fig. S1 DSC traces of salts that exhibited melting (*gl.*: glassy phase, *liq.*: liquid phase).

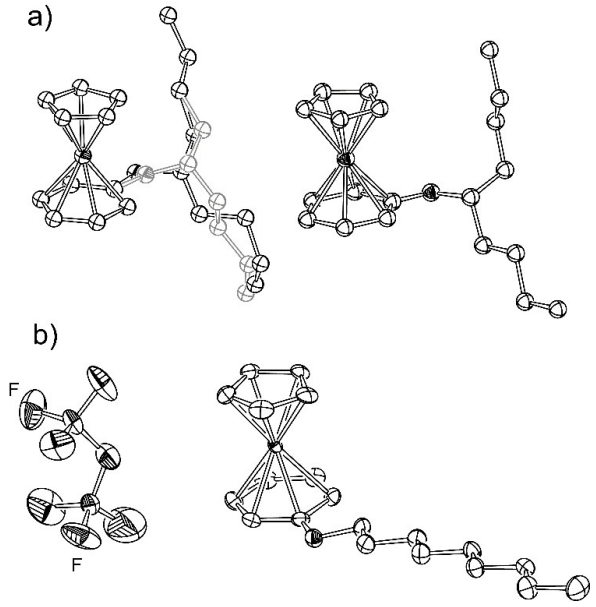


Fig. S2 Ortep diagrams of molecular structures of (a) [**2**][PF_6] and (b) [**3**][FSA]. One of the disordered parts in the substituent in [**2**][PF_6] is displayed in gray.

Table S1 Viscosity data (mPa s) for [**1**]X (X = PF_6, FSA, Tf_2N) and [**3**][Tf_2N]

°C	*rac*-[**1**][PF_6]	*rac*-[**1**][FSA]	*rac*-[**1**][Tf_2N]	[**3**][Tf_2N]
–20		40300	40300	9300
–15		23800	22200	5980
–10		13200	12100	3820
–5		7440	6850	2320
0		4710	4260	1580
5	248000	3020	2720	1090
10	118000	1970	1800	766
15	61900	1350	1220	543
20	33600	960	861	409
25	19600	700	623	312
30	11800	511	447	239
35	7420	381	336	187
40	5040	285	251	147
45	2840	221	189	115
50	1860	173	146	92

Table S2 Viscosity data (mPa s) for [**2**][FSA]

°C	[**2**][FSA]
–9	23800
–5	14700
–1	9680
5	5440
9	3790
15	2340
19	1700
25	1110
29	836
35	554
39	430
45	292
50	218

Table S3 Viscosity data (mPa s) for [**2**][Tf_2N]

°C	[**2**][Tf_2N]
–20	87200
–16	47100
–10	21100
–6	13000
0	6860
4	4260
10	2410
14	1740
20	1100
25	775
30	549
34	428
40	296
44	236
50	172

Table S4 Crystallographic parameters

	[**2**][PF_6]	[**3**][PF_6]	[**3**][FSA]
Empirical formula	$C_{20}H_{29}F_6OPRu$	$C_{20}H_{29}F_6OPRu$	$C_{20}H_{29}F_2NO_5RuS_2$
Formula weight	531.47	531.47	566.63
Crystal system	Triclinic	Triclinic	Triclinic
Space group	*P*–1	*P*–1	*P*–1
a (Å)	7.2400(9)	10.389(3)	7.928(3)
b (Å)	18.137(2)	10.393(3)	9.542(4)
c (Å)	18.786(2)	11.050(3)	16.403(6)
α (°)	114.7030(10)	84.703(4)	98.073(5)
β (°)	94.018(2)	67.159(4)	101.571(4)
γ (°)	97.896(2)	82.242(4)	103.610(4)
Volume (Å^3)	2197.4(5)	1088.4(5)	1158.3(8)
Z	4	2	2
$d_{calcd.}$ (mg m^{-3})	1.606	1.622	1.625
T (K)	100	100	100
μ (mm^{-1})	0.845	0.853	0.904
Reflections collected	10721	5053	5408
Independent reflections	7656 (R_{int} =0.0204)	3740 (R_{int} = 0.0162)	4022 (R_{int} = 0.0260)
F(000)	1080	540	580
R_1[a], wR_2[b] ($I > 2\sigma$(I))	0.0258, 0.0656	0.0256, 0.0579	0.0577, 0.1556
R_1[a], wR_2[b] (all data)	0.0286, 0.0679	0.0292, 0.0597	0.0610, 0.1629
Goodness-of-fit on F^2	1.038	1.060	1.114
Completeness to θ (%)	98.3	97.3	98.0
Parameters	587	263	281
Largest diff. peak and hole	1.040 and −0.562	0.554 and −0.473	2.362 and −1.235

[a] $R_1 = \Sigma \, ||F_o| - |F_c|| \, / \, \Sigma \, |F_o|$, b) $wR_2 = [\, \Sigma \, w(F_o^2 - F_c^2)^2 \, / \, \Sigma \, w(F_o^2)^2]^{1/2}$