Supporting Information

Thermal Properties and Crystal Structures of Ionic Liquids from Ruthenium Sandwich Complexes with Trialkoxybenzene Ligands: Effects of Substituent Positions and Alkyl Chain Lengths

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Table S1. Crystallographic parameters.

	[**1-C2**][PF_6]	[**1-C2**][FSA]	[**1-C6**][PF_6]
Empirical formula	$C_{17}H_{23}F_6O_3P$ Ru	$C_{17}H_{23}F_2NO_7RuS_2$	$C_{29}H_{47}F_6O_3PRu$
Formula weight (g mol^{-1})	521.39	556.55	689.71
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P\ 2_1/c$	$P\ n$	$P\ 2_1/c$
Crystal size (mm^3)	0.20 × 0.18 × 0.07	0.44 ×0.16 × 0.05	0.60 × 0.30 × 0.04
a (Å)	10.5875(15)	10.3045(13)	29.936(8)
b (Å)	18.049(3)	12.2620(15)	10.558(2)
c (Å)	13.8724(14)	17.288(2)	21.067(5)
α (°)	90	90	90
β (°)	130.849(7)	95.673(2)	110.539(3)
γ (°)	90	90	90
Volume (Å^3)	2005.3(5)	2173.8(5)	6235(3)
Z	4	4	8
$d_{calcd.}$ (g cm^{-3})	1.710	1.701	1.469
λ (Å)	0.71073	0.71073	0.71073
T (K)	100	100	100
μ (mm^{-1})	0.930	0.969	0.618
Reflections collected	9660	11640	29471
Independent reflections	3534 [R_{int} = 0.0367]	6434 [R_{int} = 0.0588]	10981 [R_{int} = 0.0735]
F(000)	1048	1128	2864
R_1[a)], wR_2[b)] [$I > 2\sigma$ (I)]	0.0224, 0.0568	0.0301, 0.0770	0.0897, 0.2137
R_1[a)], wR_2[b)] (all data)	0.0227, 0.0571	0.0304, 0.0773	0.1014, 0.2240
Goodness-of-fit on F^2	1.033	1.050	1.069
Completeness to θ (%)	99.7	99.7	99.6
Parameters	303	548	728
Largest diff. peak and hole	0.724 and −0.388	0.813 and −0.794	3.063 and −1.578

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

(Continued)

	[**1-C12**][PF_6]	[**1-C18**][PF_6]
Empirical formula	$C_{47}H_{83}F_6O_3PRu$	$C_{65}H_{119}F_6O_3PRu$
Formula weight (g mol^{-1})	942.17	1194.64
Crystal system	Monoclinic	Monoclinic
Space group	$P\ 2_1/c$	$P\ 2_1/c$
Crystal size (mm^3)	0.38 × 0.28 × 0.09	0.36 × 0.22 × 0.06
a (Å)	10.3170(14)	10.283(2)
b (Å)	10.1037(14)	10.161(2)
c (Å)	48.423(7)	64.085(13)
α (°)	90	90
β (°)	98.444(3)	97.965(3)
γ (°)	90	90
Volume (Å^3)	4992.9(12)	6631(2)
Z	4	4
$d_{calcd.}$ (g cm^{-3})	1.253	1.197
λ (Å)	0.71073	0.71073
T (K)	100	100
μ (mm^{-1})	0.404	0.318
Reflections collected	23128	28440
Independent reflections	8783 [R_{int} = 0.0467]	11405 [R_{int} = 0.0345]
F(000)	2008	2584
R_1[a)], wR_2[b)] [$I > 2\sigma$ (I)]	0.0513, 0.1308	0.0611, 0.1516
R_1[a)], wR_2[b)] (all data)	0.0547, 0.1381	0.0631, 0.1585
Goodness-of-fit on F^2	1.188	1.361
Completeness to θ (%)	99.8	97.4
Parameters	572	723
Largest diff. peak and hole	1.030 and −1.928	1.116 and −2.722

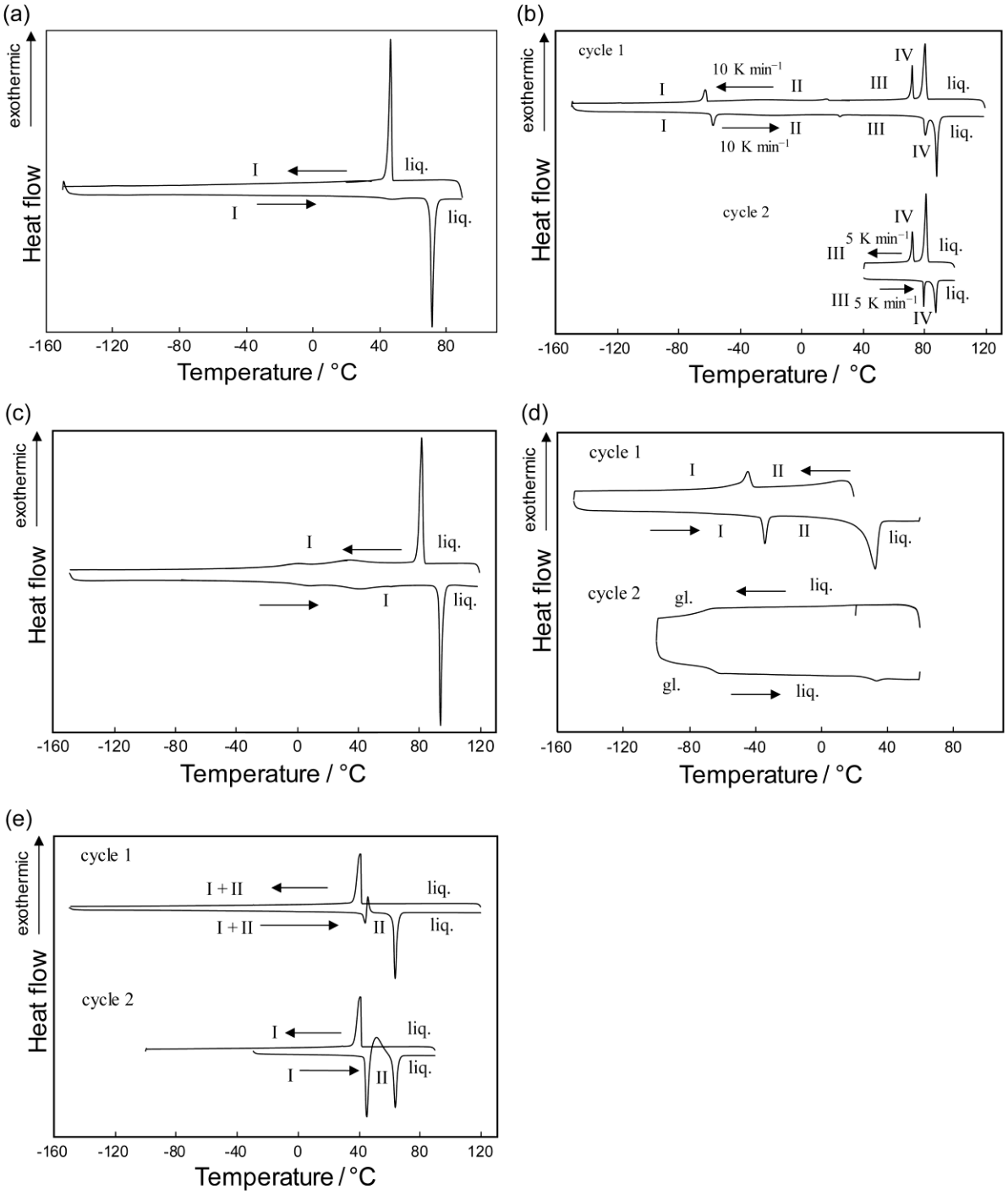

Figure S1. DSC traces of (a) [**1-C6**][PF_6], (b) [**1-C12**][PF_6], (c) [**1-C18**][FSA], (d) [**1-C6**][FSA], and (e) [**1-C18**][FSA]. Glassy state and liquid phase are indicated as gl. and liq., respectively.

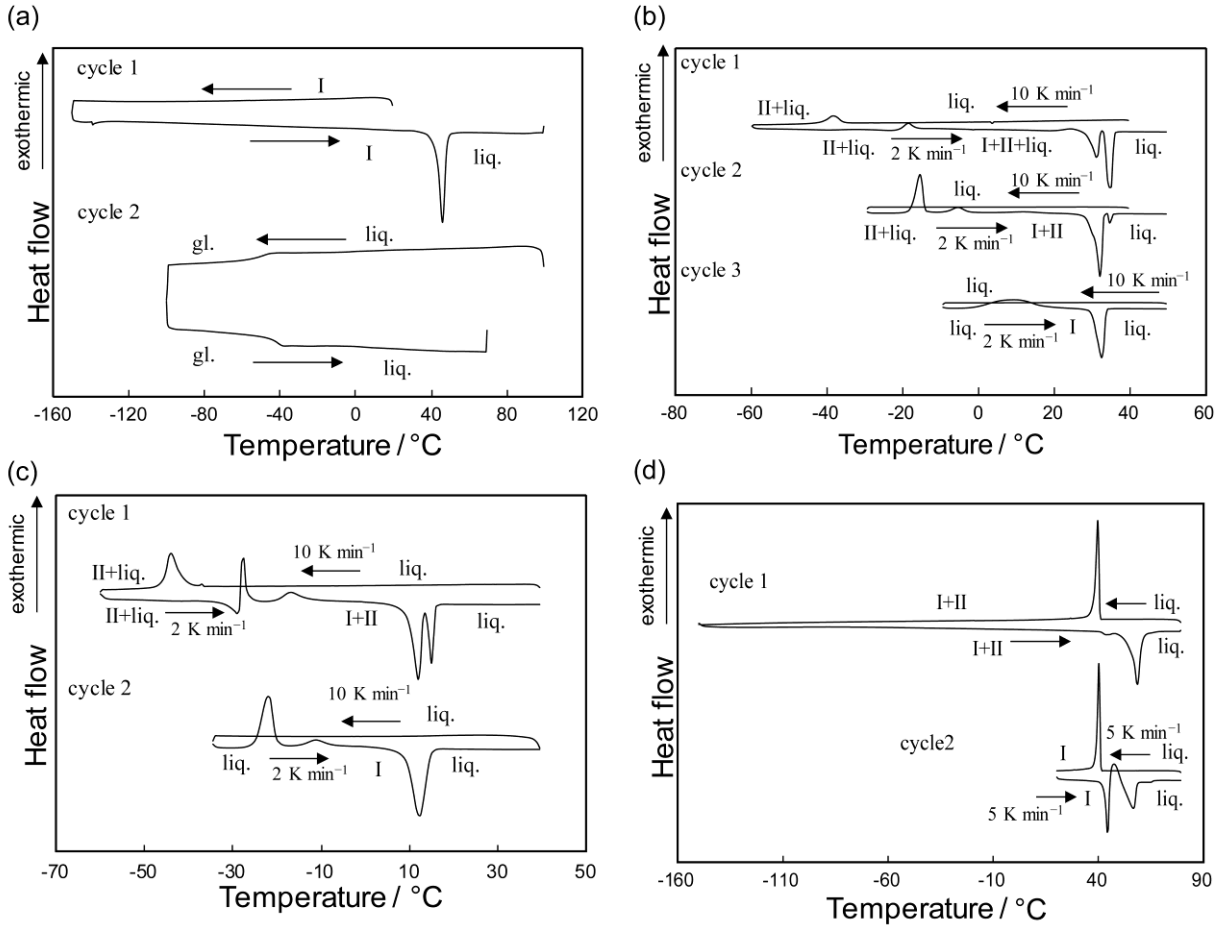

Figure S2. DSC traces of (a) [**2-C6**][PF_6], (b) [**2-C12**][PF_6], (c) [**2-C12**][FSA], and (d) [**1-C18**][FSA]. Glassy state and liquid phase are indicated as gl. and liq., respectively.

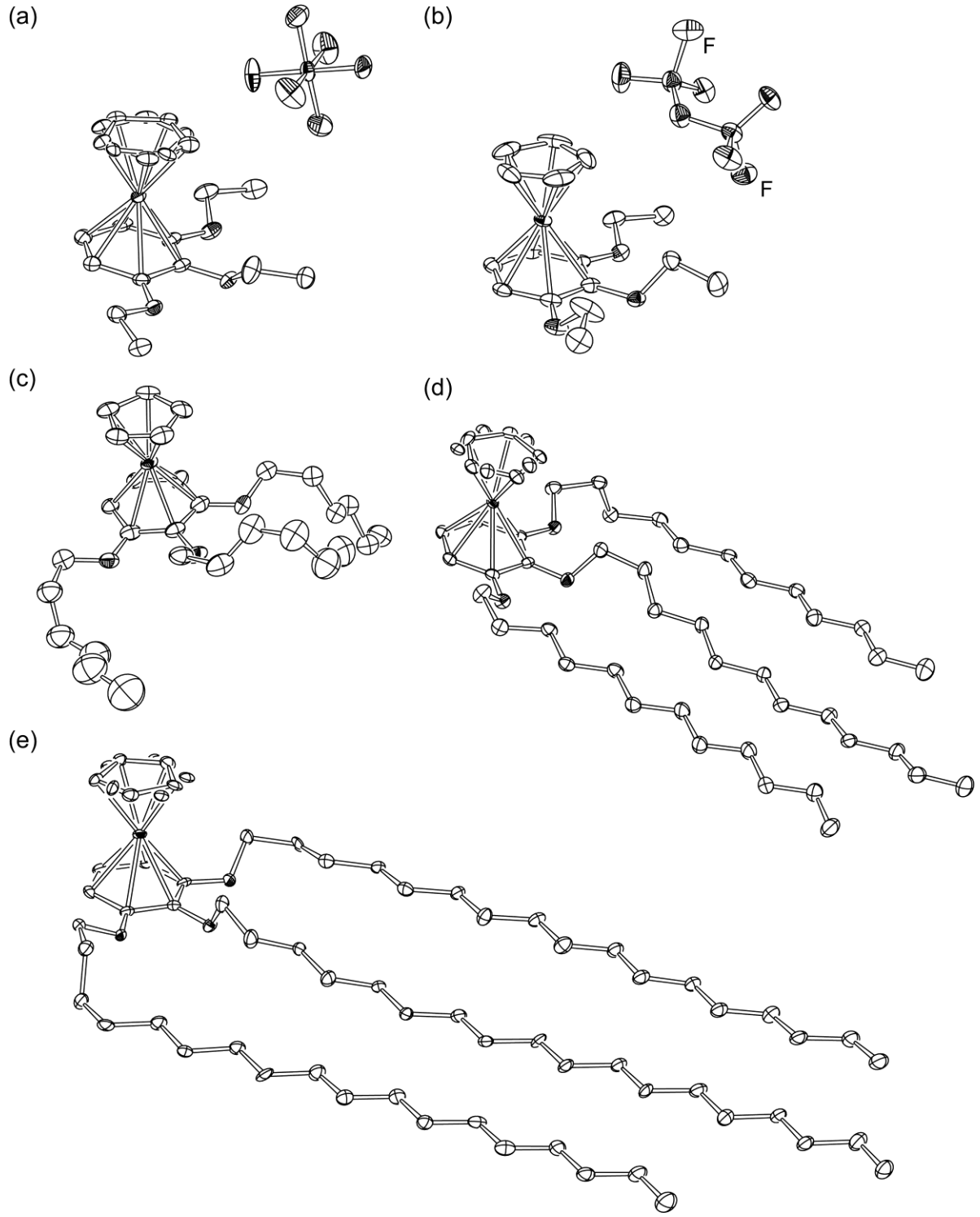

Figure S3. ORTEP drawings of the molecular structures in (a) [**1-C2**][PF_6], (b) [**1-C2**][FSA], (c) [**1-C6**][PF_6], (d) [**1-C12**][PF_6], and (e) [**1-C18**][PF_6].