

Supporting Information

Thermal Properties, Crystal Structures, and Phase Diagrams of Ionic Plastic Crystals and Ionic Liquids Containing a Chiral Cationic Sandwich Complex

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Fig. S5. ¹H NMR spectrum of (*S*)-[1]PF₆ (400 MHz, Solvent: CDCl₃).

Table S1. Crystallographic parameters.

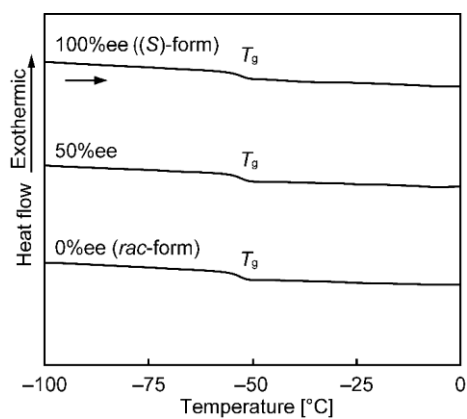


Fig. S1. DSC traces of [1]CPFSA (100% ee, 50% ee, and 0% ee).

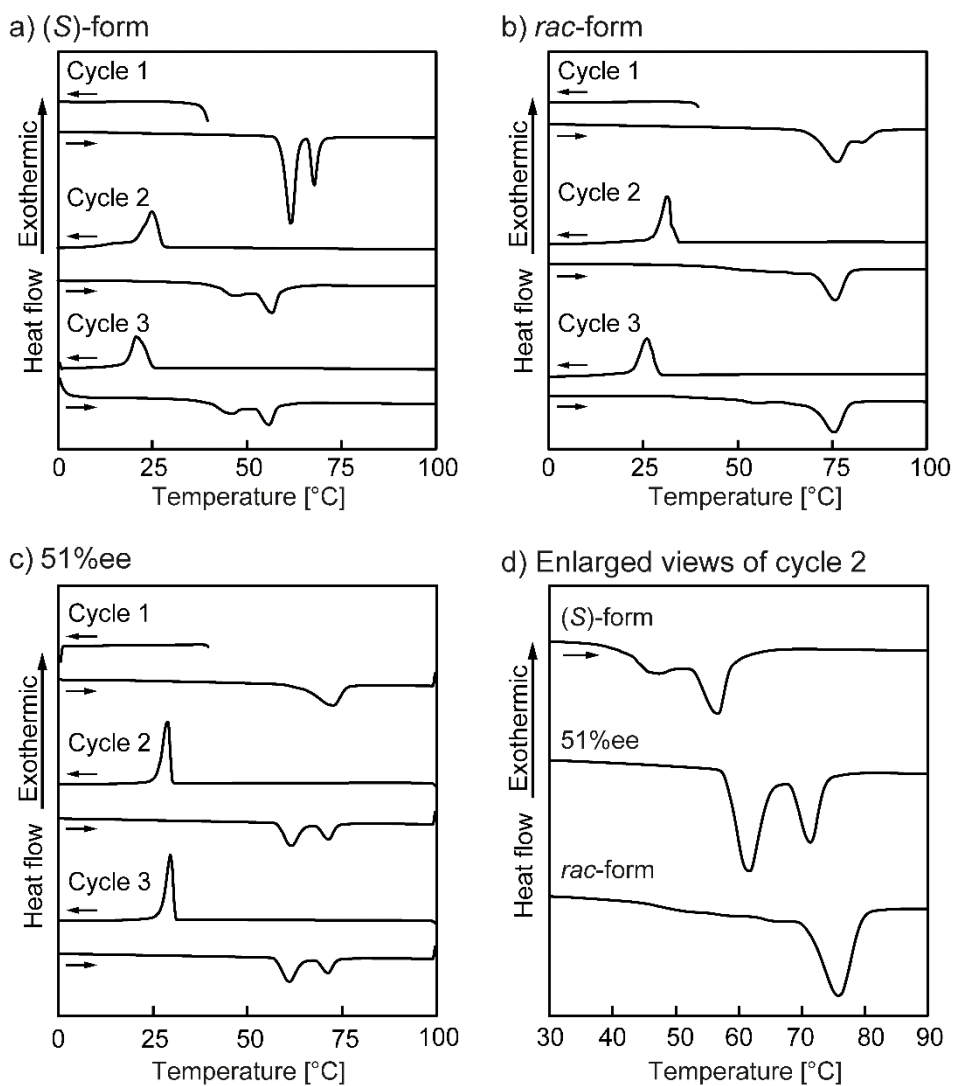


Fig. S2. DSC traces of [1]CB₁₁H₁₂ (100% ee, 51% ee, and 0% ee).

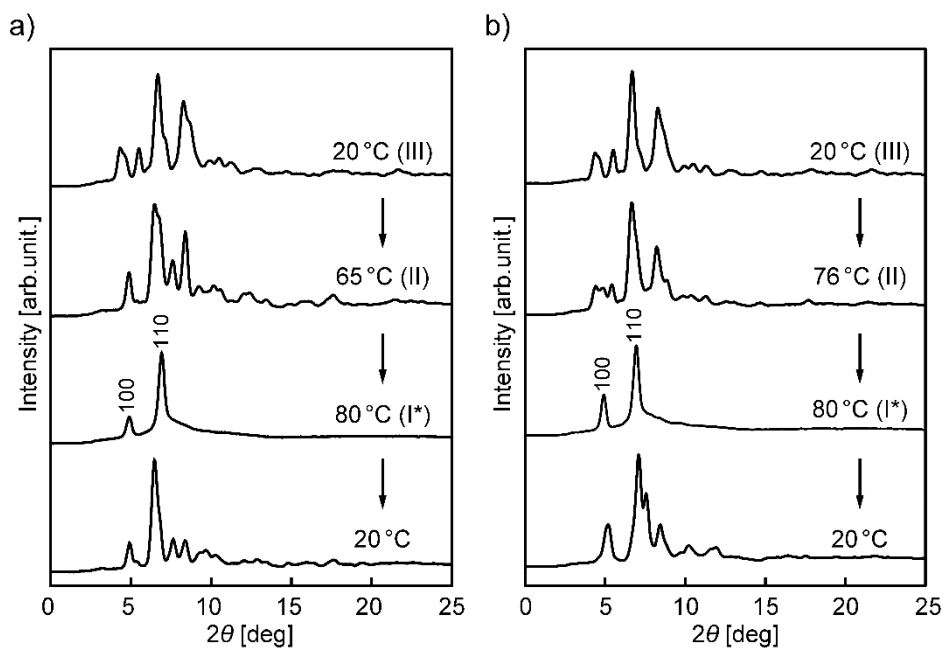


Fig. S3. PXRD patterns of (a) (*S*)- and (b) *rac*-[1]CB₁₁H₁₂ at 20 and 80 °C (MoK α radiation).

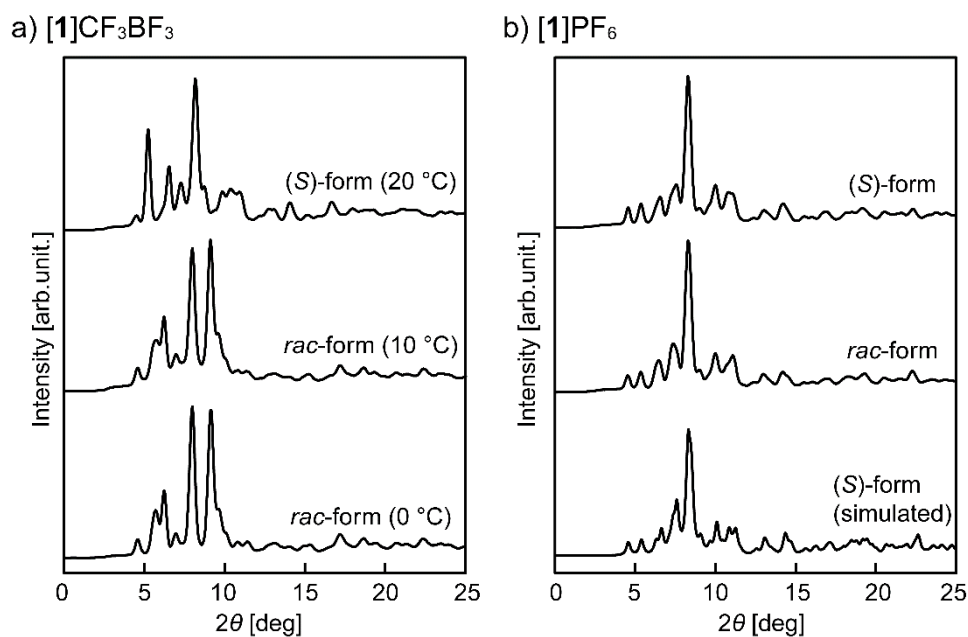


Fig. S4. PXRD patterns: (a) (*S*)-[1]CF₃BF₃ (20 °C) and *rac*-[1]CF₃BF₃ (10, 0 °C). (b) (*S*)-[1]PF₆ (20 °C), *rac*-[1]PF₆ (20 °C), and (*S*)-[1]PF₆ (simulated, MoK α radiation).

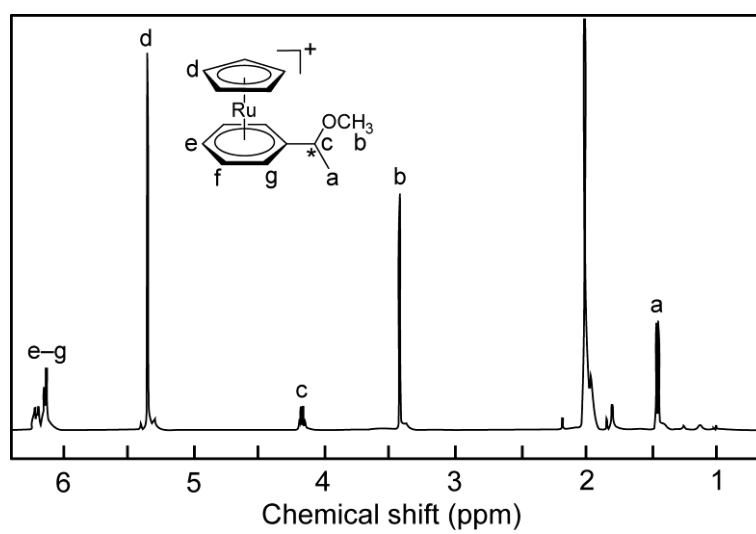


Fig. S5. ¹H NMR spectrum of (S)-[1]PF₆ (400 MHz, Solvent: CDCl₃).

Table S1. Crystallographic parameters of *S*-[**1**]PF₆ and *rac*-[**1**]CB₁₁H₁₂.

	<i>S</i> -[1]PF ₆	<i>rac</i> - α -[1]CB ₁₁ H ₁₂	<i>rac</i> - β -[1]CB ₁₁ H ₁₂
Empirical formula	C ₁₄ H ₁₇ F ₆ OPRu	C ₁₅ H ₂₉ B ₁₁ ORu	C ₁₅ H ₂₉ B ₁₁ ORu
Formula weight	447.31	445.36	445.36
Crystal system	Orthorhombic	monoclinic	triclinic
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> -1
<i>a</i> [Å]	9.5873(6)	9.590(2)	8.7042(10)
<i>b</i> [Å]	12.2766(8)	22.809(5)	10.1448(12)
<i>c</i> [Å]	12.9471(8)	9.636(2)	12.0722(14)
α [°]	90	90	99.0460(10)
β [°]	90	94.756(3)	95.8930(10)
γ [°]	90	90	96.4770(10)
<i>V</i> [Å ³]	1523.87(17)	2100.5(9)	1038.1(2)
<i>Z</i>	4	4	2
ρ_{calcd} [g cm ⁻³]	1.950	1.408	1.425
<i>F</i> (000)	888	904	452
Temperature [K]	90	90	90
Reflns collected	8801	11884	5300
Independent reflns	3494	4862	3865
Parameters	210	285	259
<i>R</i> _{int}	0.0197	0.0514	0.0157
<i>R</i> ₁ ^{<i>a</i>} , <i>R</i> _w ^{<i>b</i>} (<i>I</i> > 2 σ)	0.0144, 0.0364	0.0527, 0.0963	0.0201, 0.0532
<i>R</i> ₁ ^{<i>a</i>} , <i>R</i> _w ^{<i>b</i>} (all data)	0.0145, 0.0364	0.0852, 0.1059	0.0203, 0.0533
Goodness of fit	1.147	1.102	1.089
$\Delta\rho_{\text{max,min}}$ [e Å ⁻³]	0.301, -0.785	1.090, -1.354	0.330, -0.557
Flack parameter	0.037	–	–

$${}^a R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|. \quad {}^b R_w = [\sum w (F_o^2 - F_c^2)^2 / \sum w (F_o^2)^2]^{1/2}$$