Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Ionic Plastic Crystals and Ionic Liquids Containing Quaternary Cations with Alkenyl Substituents: Chemical Phase Transformations by Bromine Vapor

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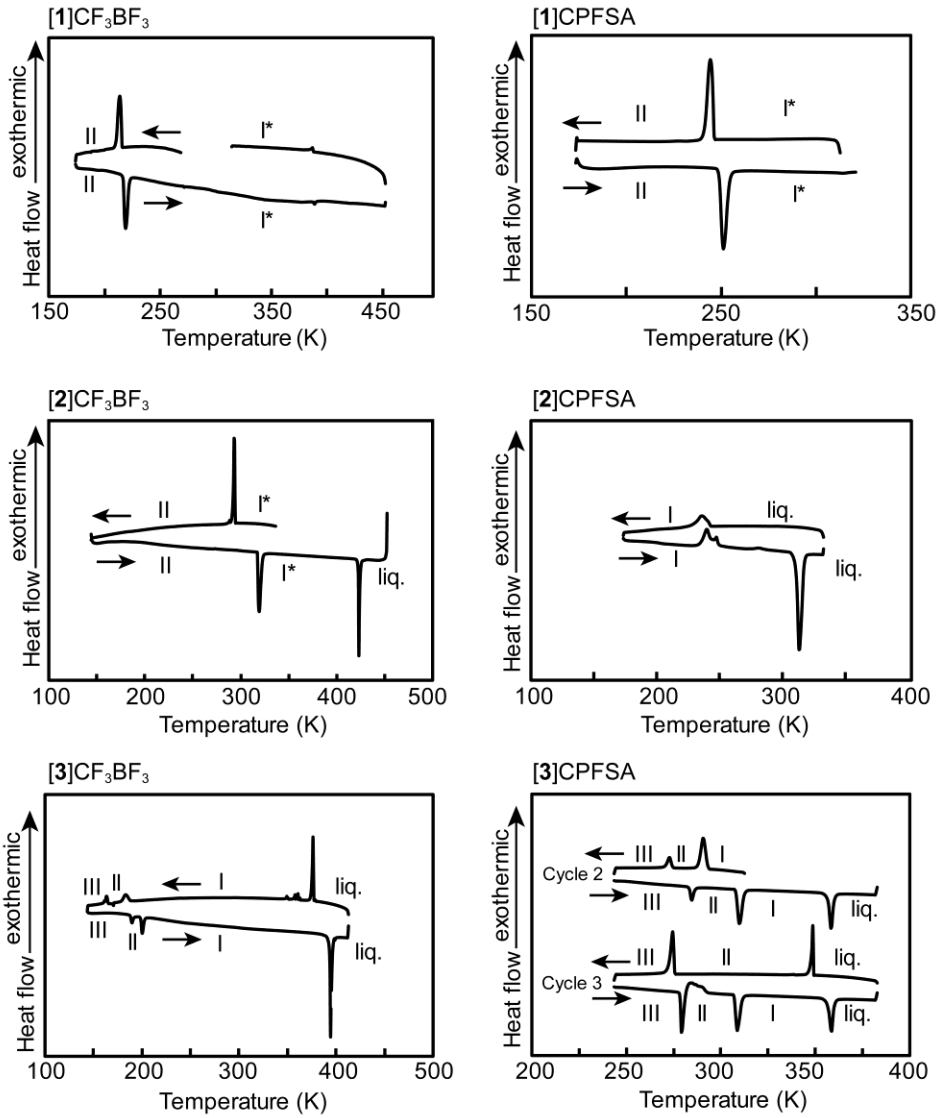


Fig. S1. DSA traces of [**1**]X–[**3**]X, where X = CPFSA or CF_3BF_3.

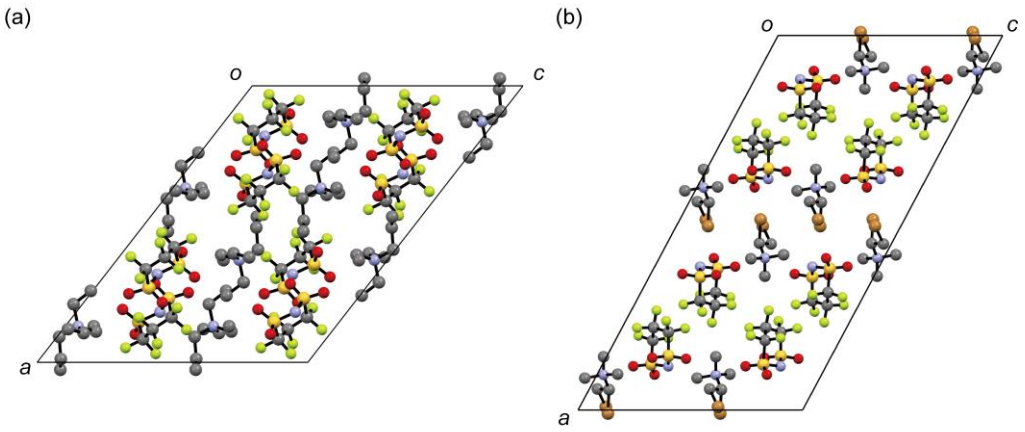


Fig. S2. Packing diagrams of (a) [**2**]CPFSA and (b) [**1-Br**]CPFSA at 90 K. Hydrogen atoms have been omitted.

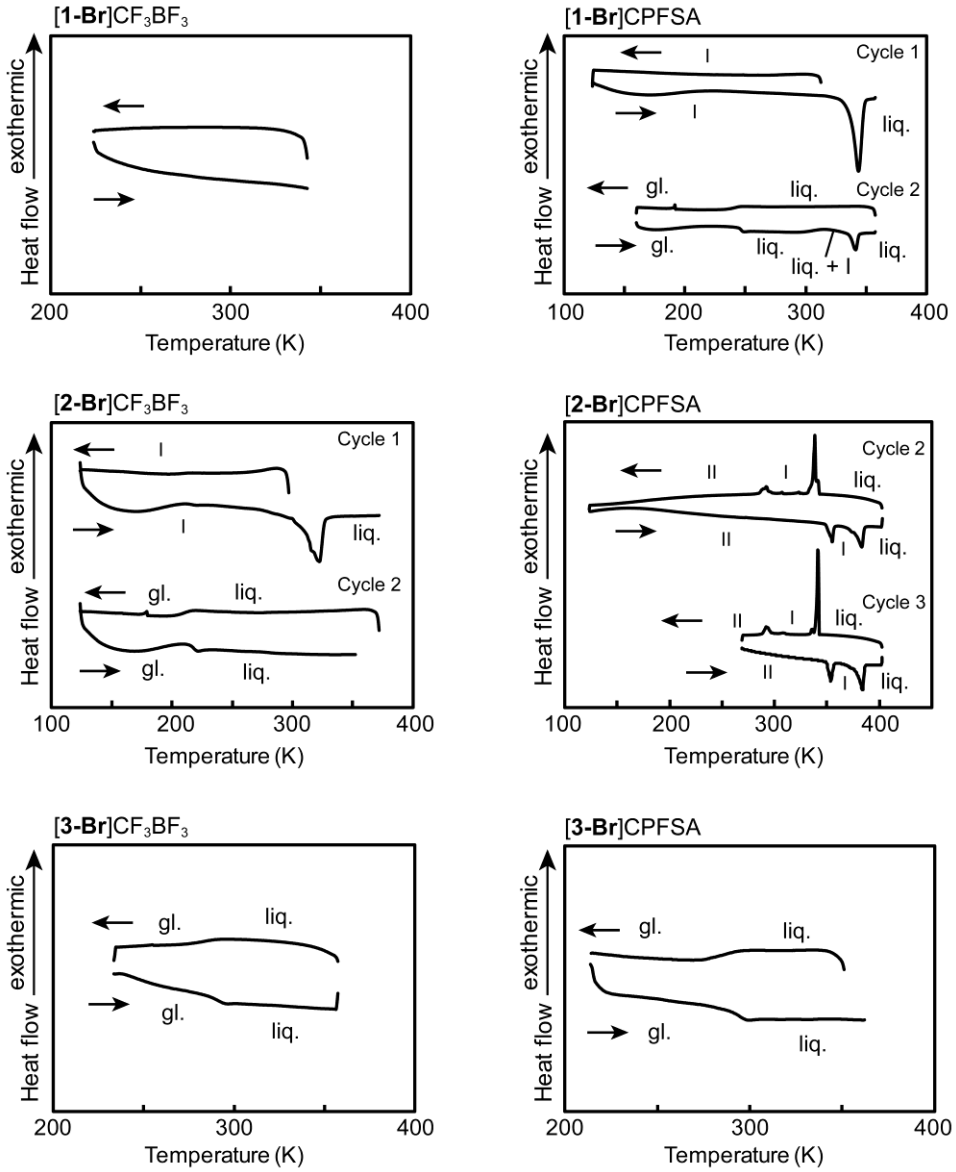


Fig. S3. DSC traces of [**1-Br**]X–[**3-Br**]X, where X = CPFSA or CF_3BF_3, and liq. and gl. are the liquid and glassy states, respectively.

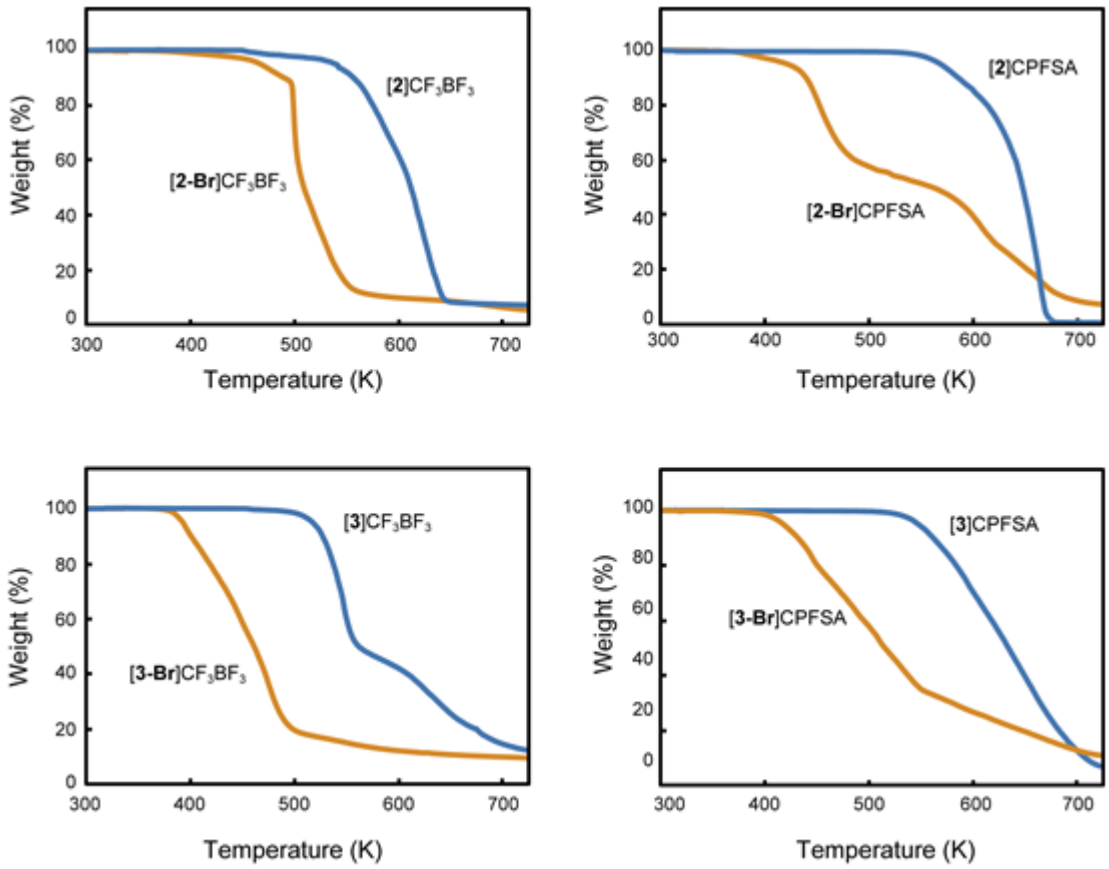
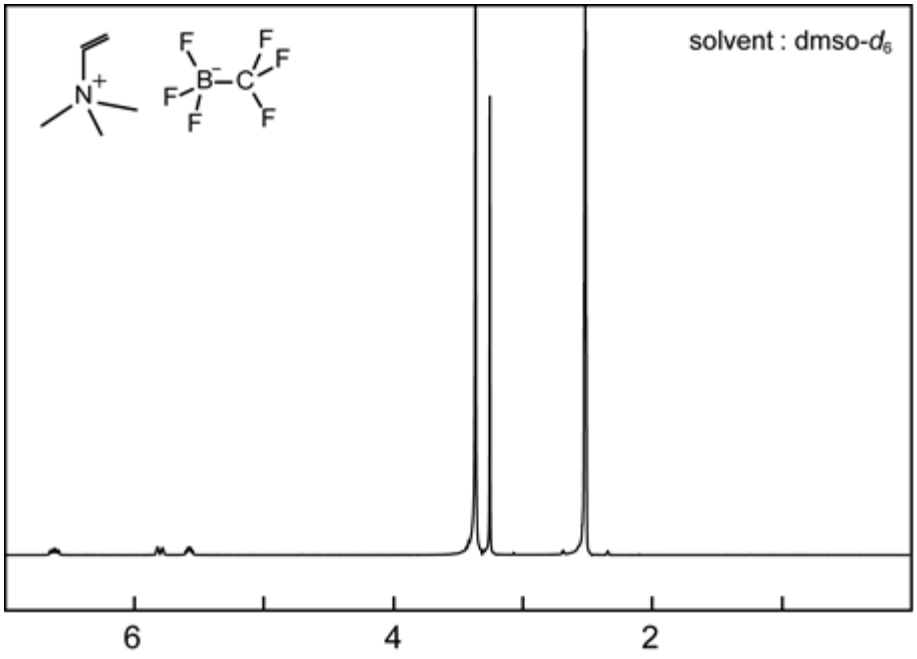


Fig. S4. TG traces of [**1**]X–[**3**]X and [**1-Br**]X–[**3-Br**]X, where X = CPFSA or CF_3BF_3 at 3 K min^{-1} under a nitrogen atmosphere.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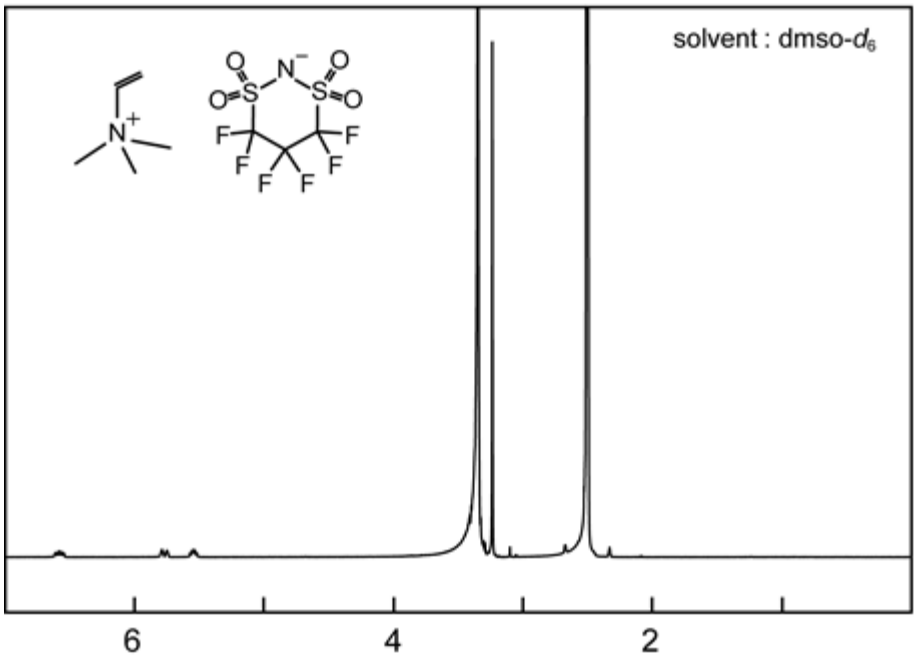
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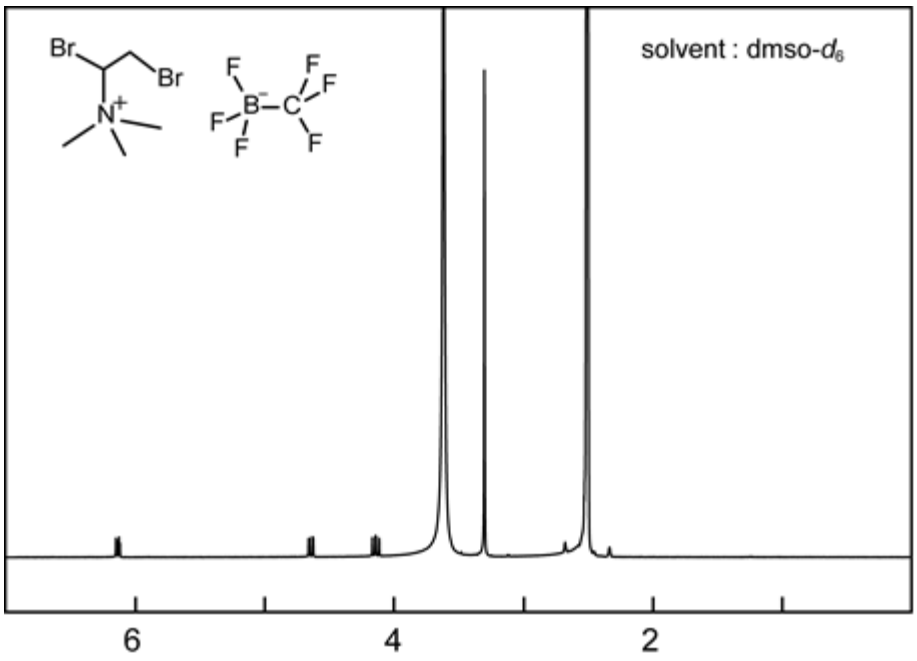
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B−
C
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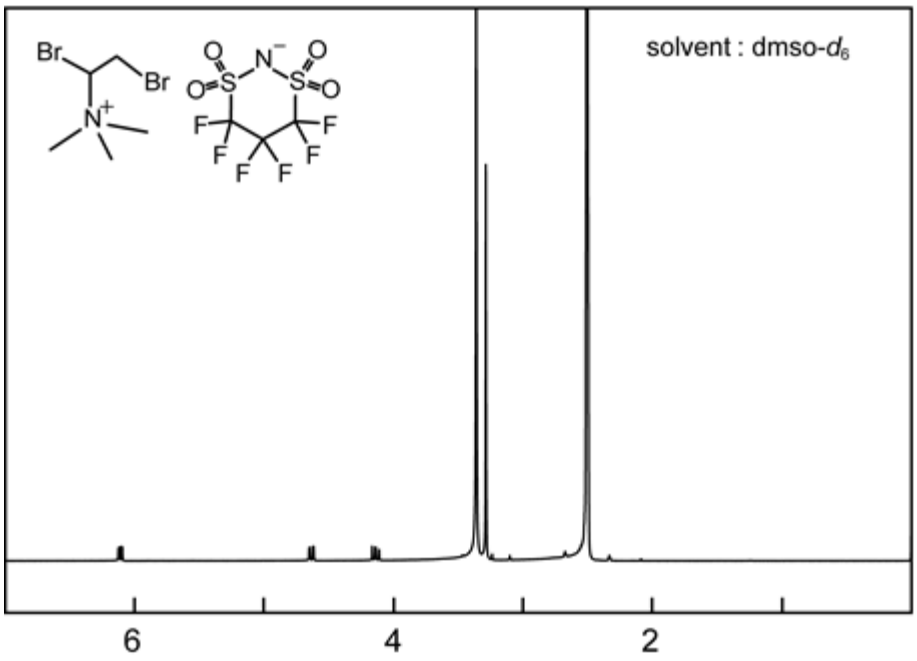
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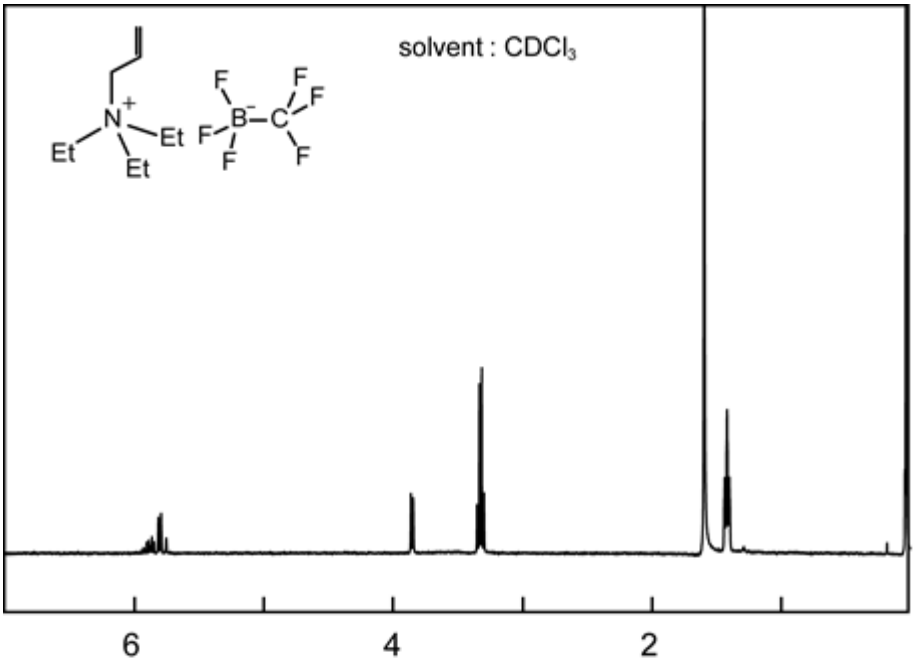
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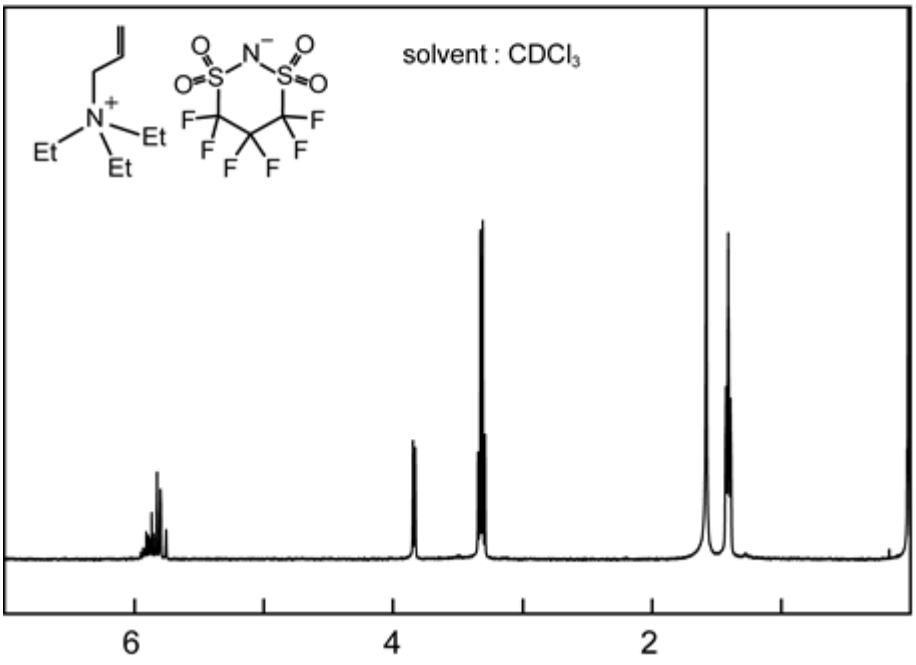
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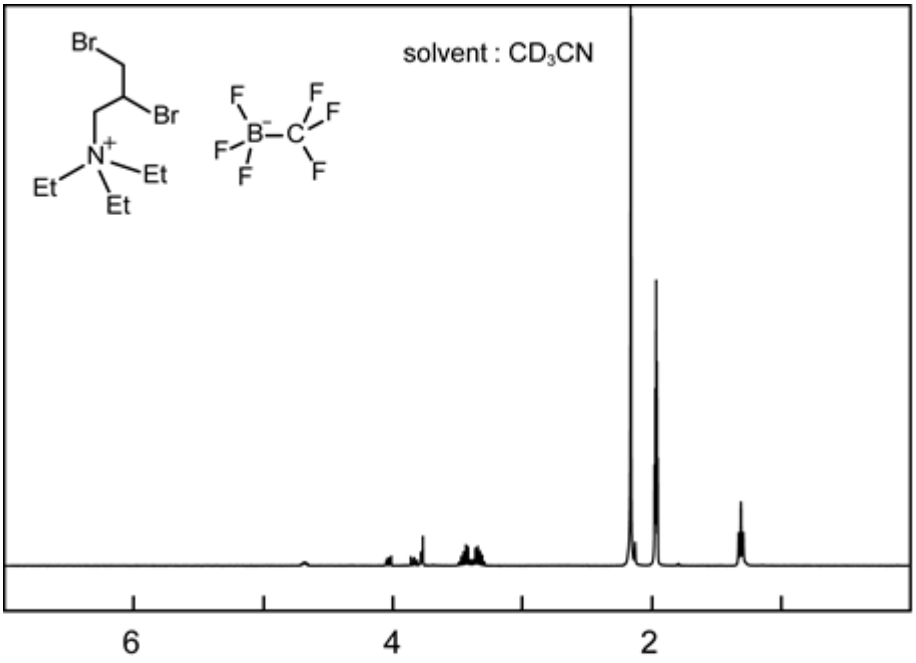
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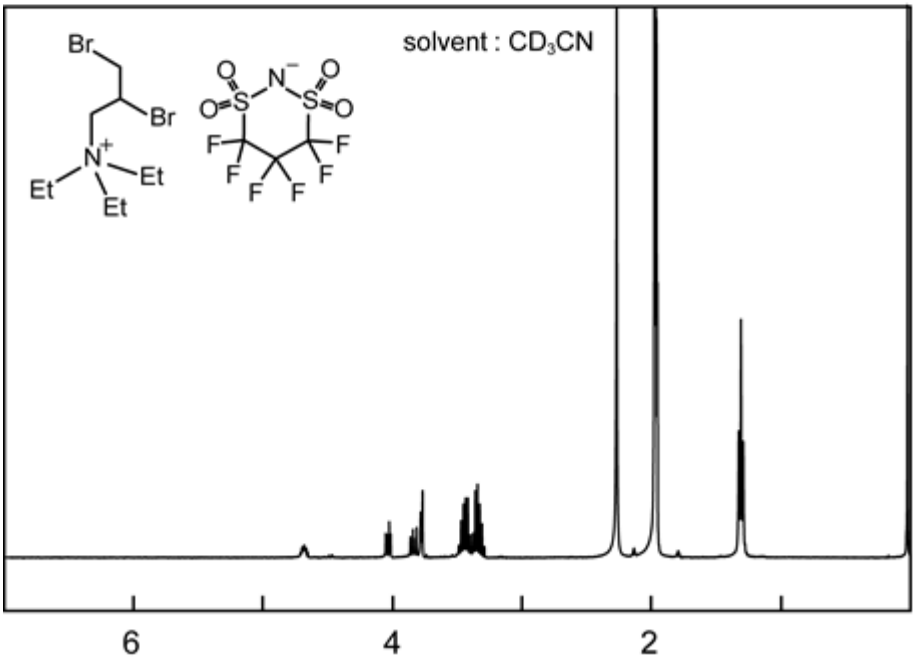
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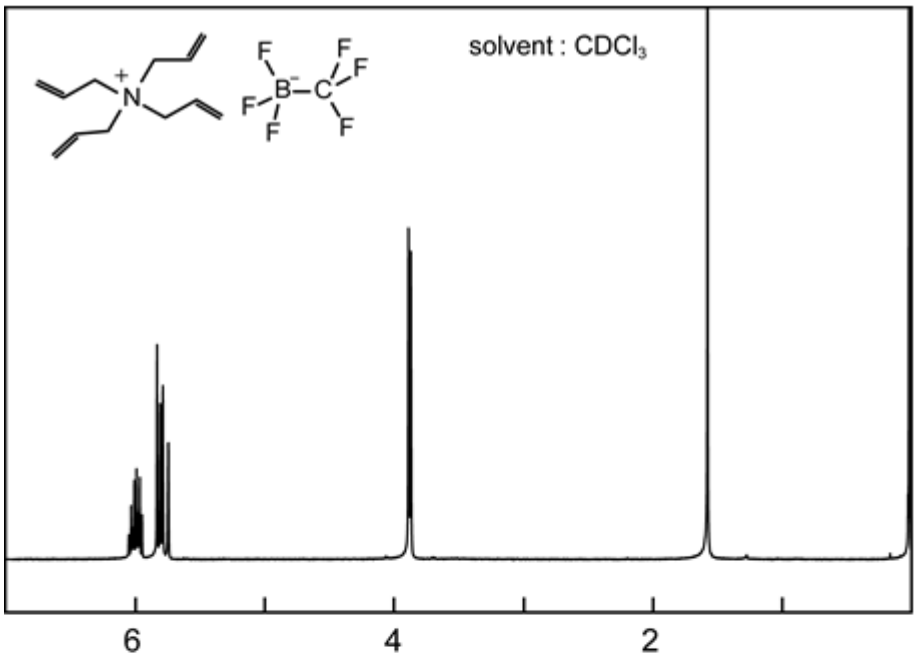
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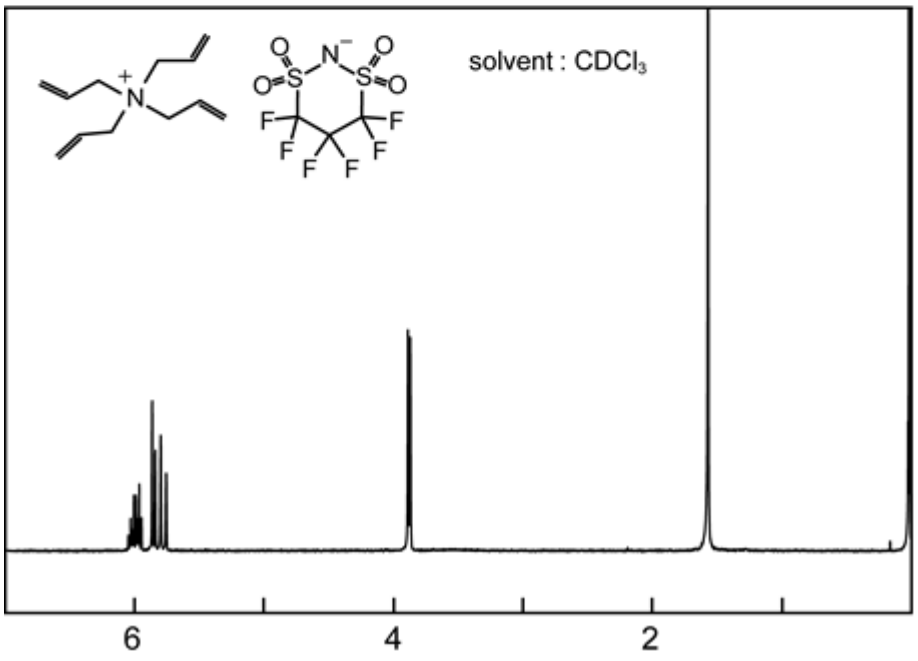
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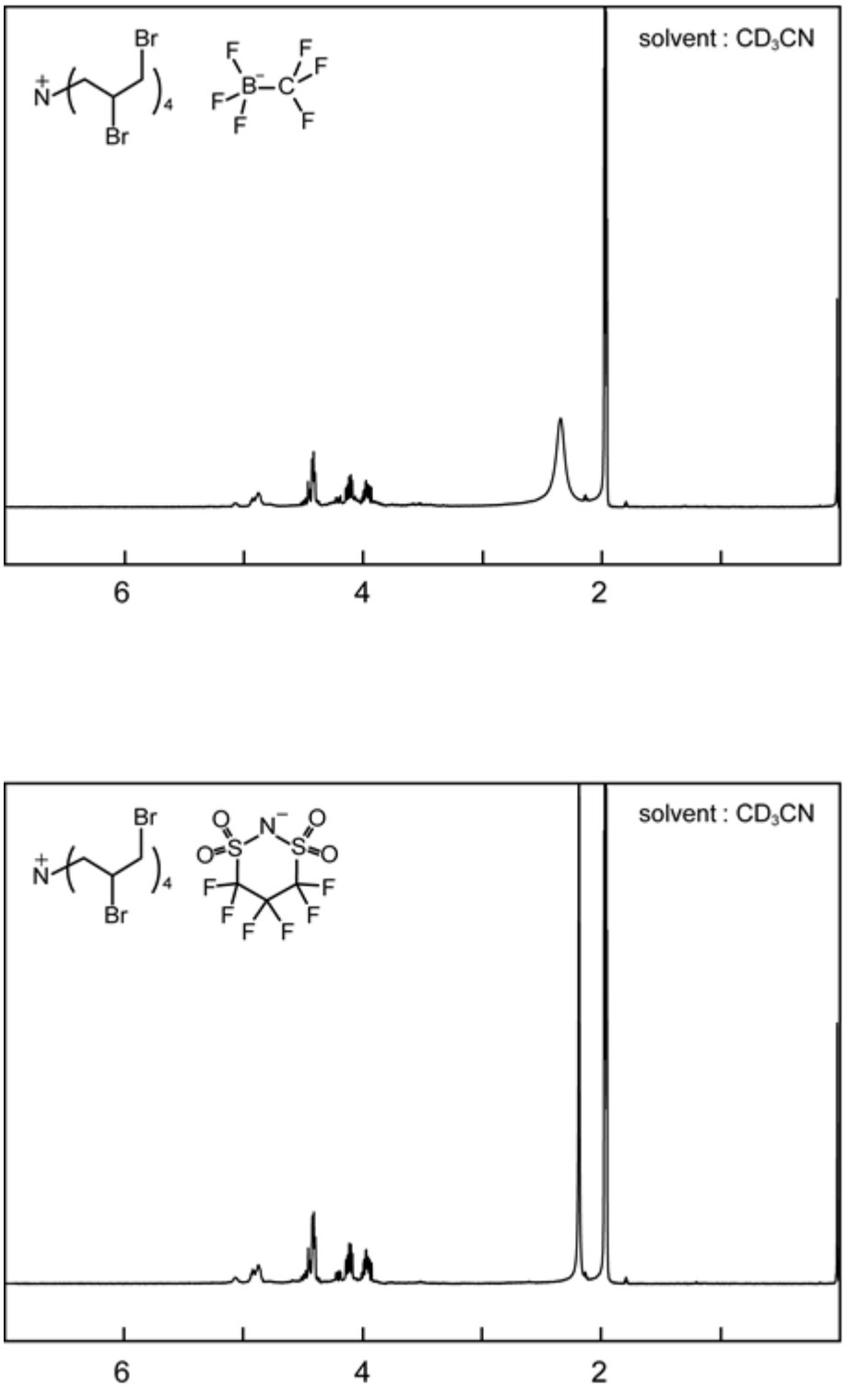

Fig. S5. ^{1}H NMR spectra of [**1**]X–[**3**]X and [**1-Br**]X–[**3-Br**]X, where X = CPFSA,) or CF_3BF_3.

Table S1. Cell parameters

	[**1**]CF_3BF_3	[**1**]CPFSA	[**2**]CF_3BF_3
	193 K (Phase II)	203 K (Phase II)	273 K (Phase II)
Crystal system	triclinic	orthorhombic	monoclinic
a (Å)	12.31(2)	24.63(13)	13.785(11)
b (Å)	14.45(2)	9.69(9)	4.863(3)
c (Å)	7.840(14)	5.92(6)	6.984(5)
α (°)	97.01(5)		
β (°)	96.56(4)		90.66(4)
γ (°)	110.97(5)		
V (Å^3)	1273(4)	1414(20)	468.2(6)
Z [a)]	4	4	1

a) Estimated from molecular volume.

Table S2. Crystallographic parameters

	[**2**]CPFSA	[**1-Br**]CPFSA
Empirical formula	$C_{12}H_{20}F_6N_2O_4S_2$	$C_8H_{12}Br_2F_6N_2O_4S_2$
Formula weight	434.42	535.85
Crystal system	monoclinic	monoclinic
Space group	*C*2/c	*C*2/c
a / Å	23.447(6)	31.144
b / Å	10.992(3)	7.460
c / Å	17.992(7)	16.328(7)
β / °	127.576(3)	117.839(5)
V / Å^3	3675(2)	3355(2)
Z	8	8
ρ_{calkd} / g cm^{-3}	1.57	2.131
F (000)	1792	2096
Reflns collected	10214	9050
Independent reflns	4189	3824
Parameters	238	220
R(int)	0.0586	0.0461
$R_1{}^a$, $R_w{}^b$ ($I > 2\sigma(I)$)	0.0498, 0.1017	0.0366, 0.0950
$R_1{}^a$, $R_w{}^b$ (all data)	0.0978, 0.1171	0.0495, 0.1006
Goodness of fit	1.009	1.105
$\Delta\rho_{max,min}$ [e Å^{-3}]	0.425, −0.615	2.272, −1.030

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