Electronic Supplementary Information

Solvation structure and dynamics of coumarin 153 in an imidazolium-based ionic liquid with chloroform, benzene, and propylene carbonate

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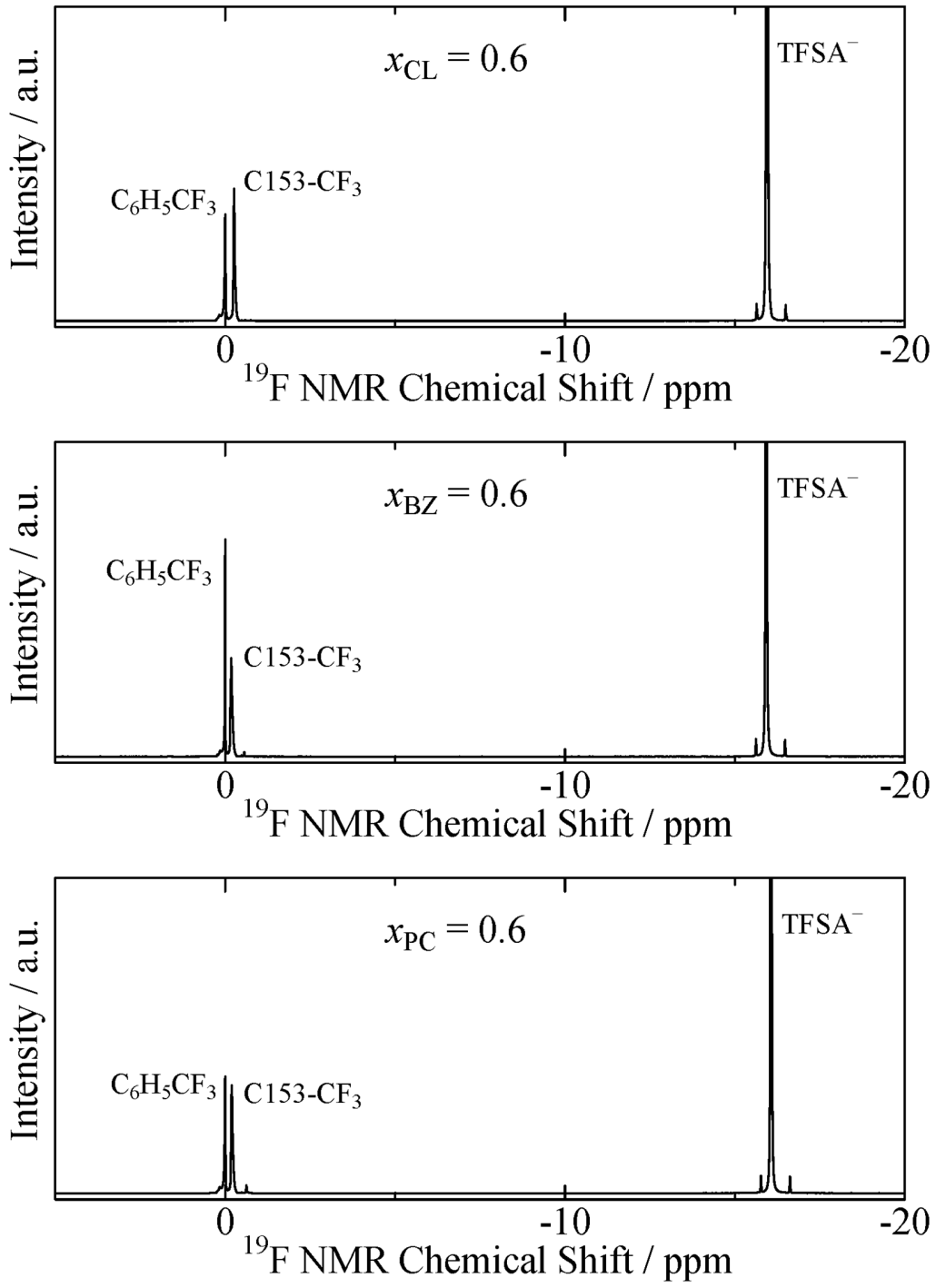

Fig. S1 Representative ^{19}F NMR spectra of C153/C_{12}mimTFSA–CL (upper), –BZ (middle), and –PC (bottom) solutions at x_{ML} = 0.6. α,α,α-Trifluorotoluene ($C_6H_5CF_3$) is the reference substance for ^{19}F atom.

Table S1 Diffusion coefficients $D/10^{-10}$ m^2 s^{-1} of chemical species in C153/C_{12}mimTFSA–CL. The values in the parentheses are the standard deviations σ.

x_{CL}	D_{cation}	D_{anion}	D_{CL}	D_{C153}
0	0.059(1)	0.073(2)		0.054(3)
0.2008	0.10(1)	0.107(7)	0.475(6)	0.099(2)
0.4000	0.14(1)	0.137(7)	1.134(1)	0.138(9)
0.5998	0.29(1)	0.302(6)	1.70(5)	0.261(1)
0.8000	0.87(8)	0.800(1)	3.99(3)	1.00(6)
0.8500	1.01(3)	1.03(3)	5.53(1)	1.45(7)
0.9000	1.76(4)	1.86(3)	10.23(7)	2.69(4)
0.9501	4.13(6)	4.192(1)	17.37(8)	7.70(6)
1			23.85(1)	13.56(1)

Table S2 Diffusion coefficients $D/10^{-10}$ m^2 s^{-1} of chemical species in C153/C_{12}mimTFSA–BZ. The values in the parentheses are the standard deviations σ.

x_{BZ}	D_{cation}	D_{anion}	D_{BZ}	D_{C153}
0	0.059(1)	0.073(2)		0.054(3)
0.1985	0.10(1)	0.126(4)	0.81(2)	0.17(6)
0.3999	0.14(1)	0.178(1)	1.076(1)	0.165(1)
0.5997	0.32(4)	0.30(6)	1.76(8)	0.321(6)
0.8000	0.78(2)	0.72(7)	4.35(3)	0.847(2)
0.8500	0.95(1)	1.051(1)	5.44(2)	1.23(1)
0.9001	1.89(1)	1.747(2)	9.57(1)	2.62(1)
0.9500	2.76(1)	3.502(1)	14.65(3)	6.01(1)
1			21.863(1)	16.37(1)

Table S3 Diffusion coefficients $D/10^{-10}$ m^2 s^{-1} of chemical species in C153/C_{12}mimTFSA–PC. The values in the parentheses are the standard deviations σ.

x_{PC}	D_{cation}	D_{anion}	D_{PC}	D_{C153}
0	0.059(1)	0.073(2)		0.054(3)
0.1992	0.097(3)	0.112(4)	0.208(7)	0.114(1)
0.4001	0.160(3)	0.144(2)	0.387(2)	0.193(1)
0.6012	0.33(6)	0.30(2)	0.73(1)	0.389(9)
0.8001	0.76(2)	0.77(10)	1.69(4)	1.018(1)
0.8501	1.04(5)	1.08(6)	2.21(7)	1.48(10)
0.8998	1.56(2)	2.010(4)	2.96(4)	1.80(9)
0.9500	1.89(2)	3.01(3)	3.50(12)	3.02(7)
1			5.170(2)	4.627(1)

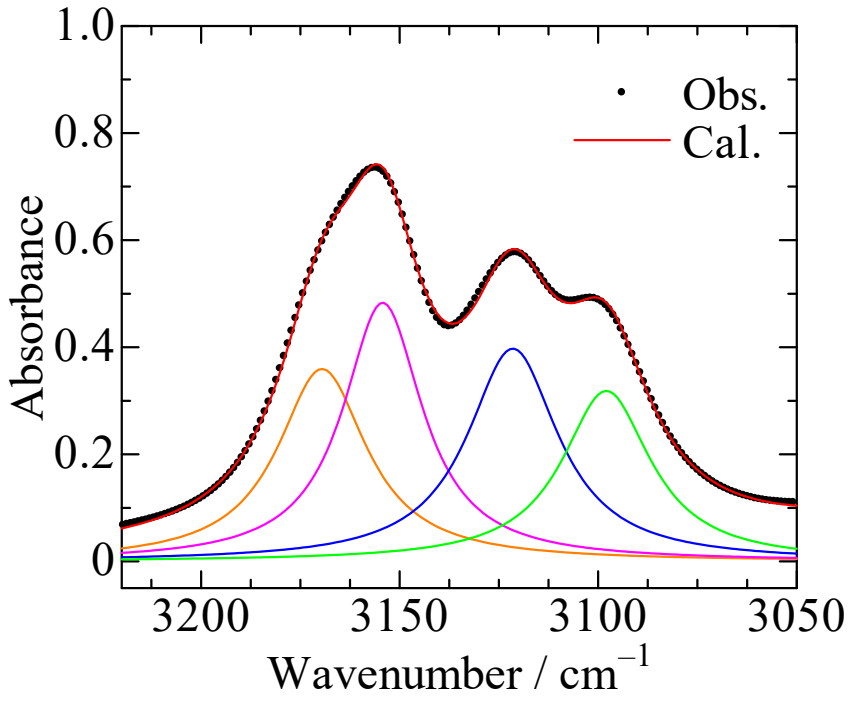

Fig. S2 Representative result of peak decomposition for IR spectrum of C_{12}mimTFSA (x_{ML} = 0). Dots and red solid line give the observed and total calculated spectra, respectively. Other colored solid lines are each component of the C–H stretching vibration of the imidazolium ring.

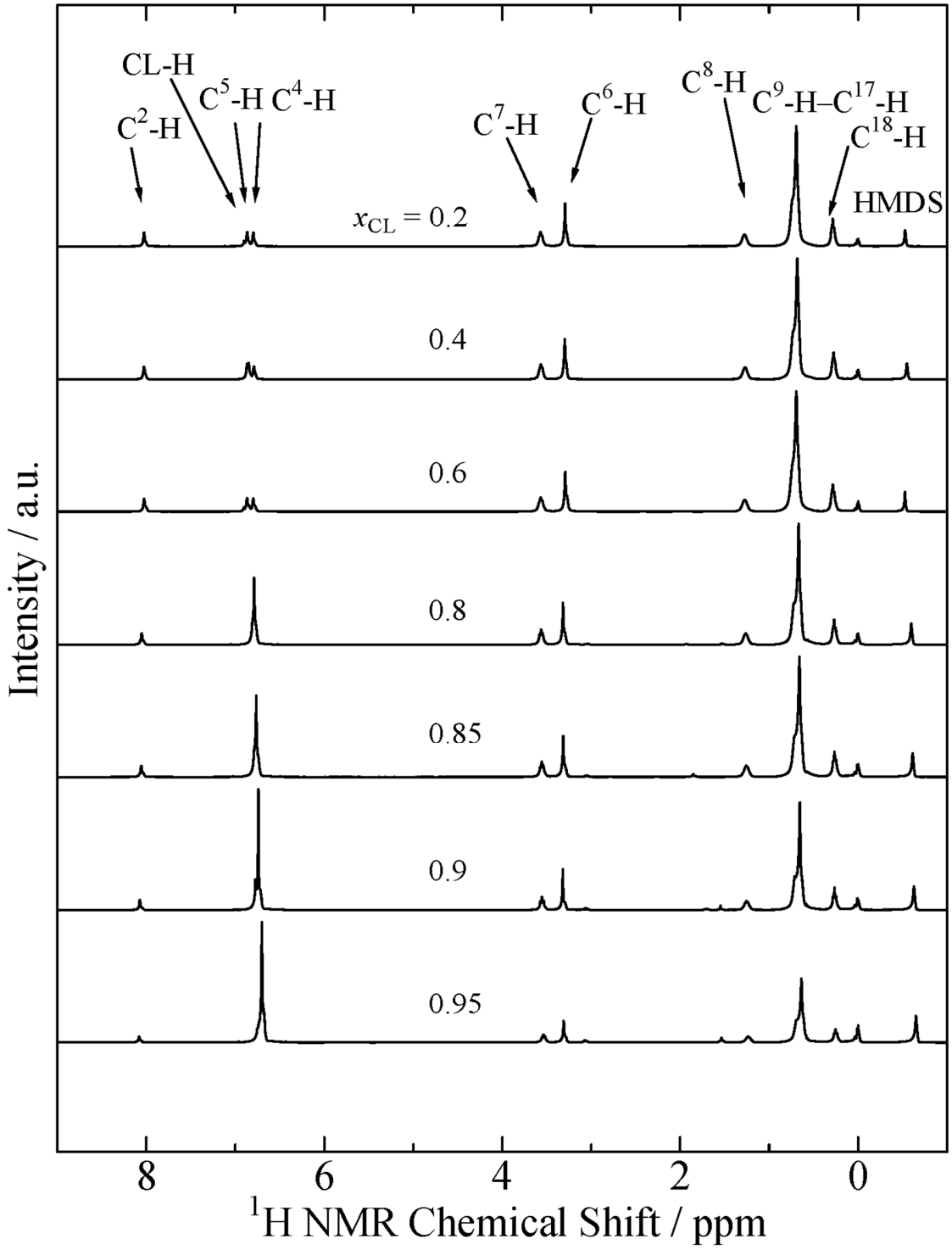

Fig. S3 ^{1}H NMR spectra of C153/C_{12}mimTFSA–CL solutions as a function of x_{CL} from 0.2 to 0.95.

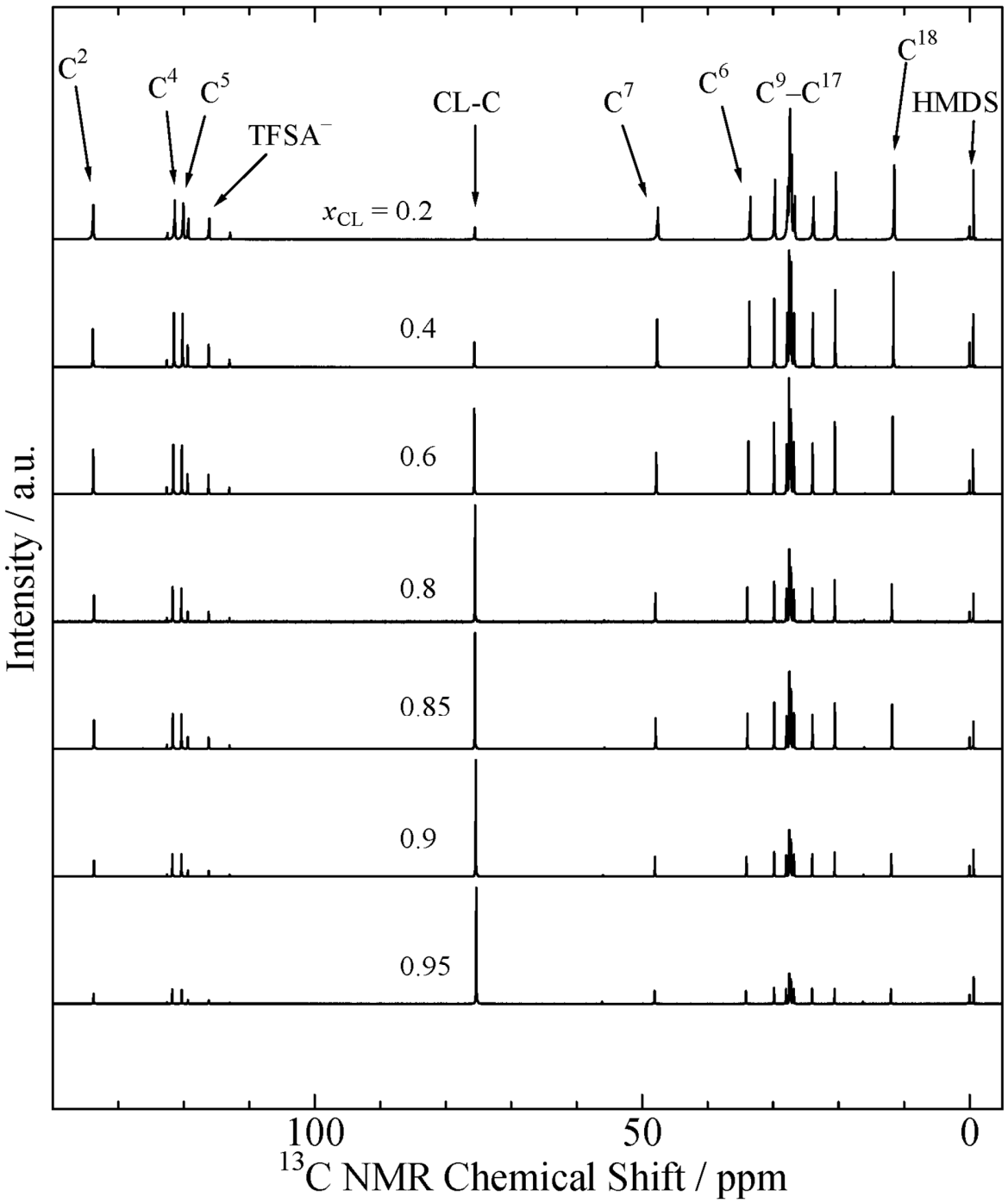

Fig. S4 ^{13}C NMR spectra of C153/C_{12}mimTFSA–CL solutions as a function of x_{CL} from 0.2 to 0.95.

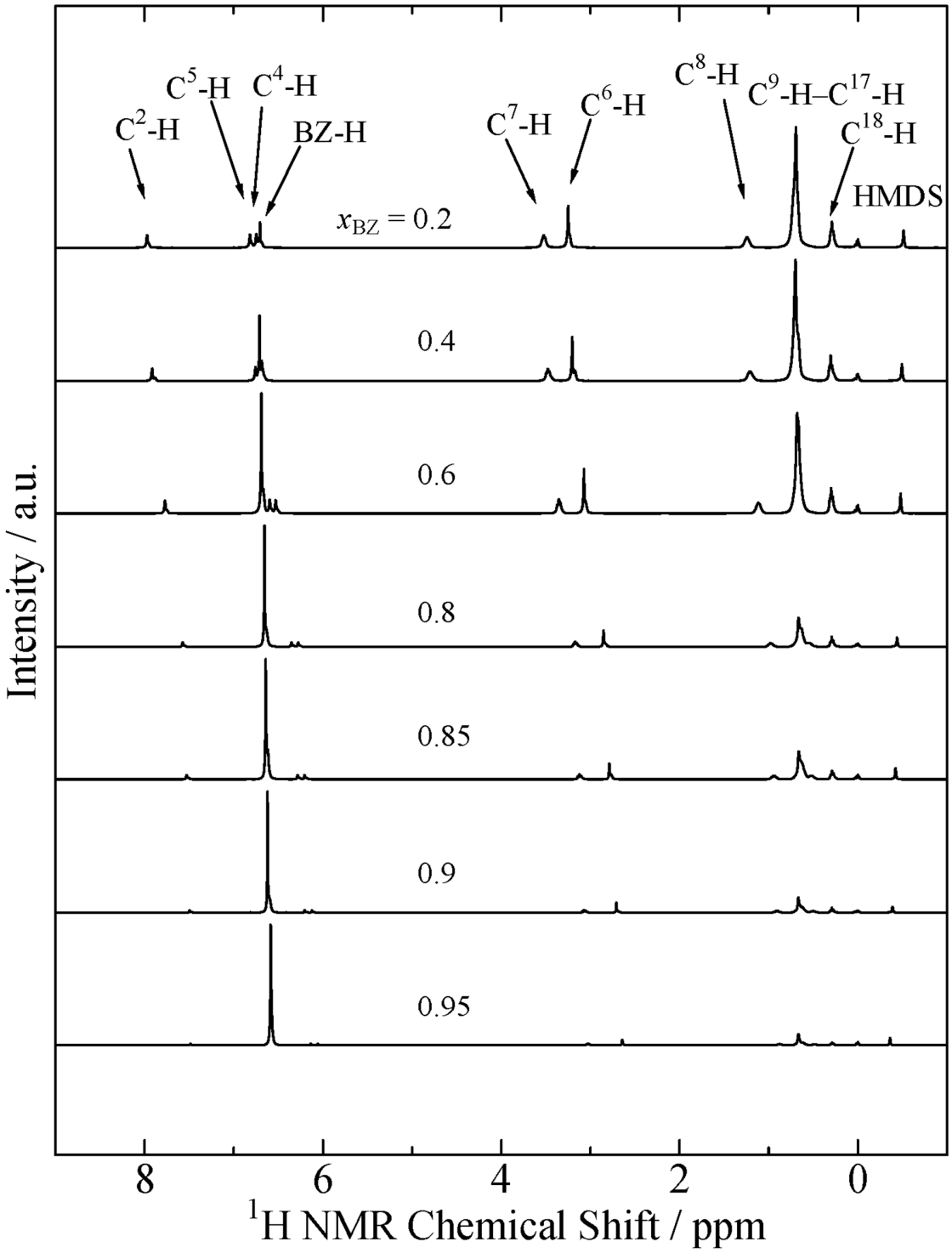

Fig. S5 ^{1}H NMR spectra of C153/C_{12}mimTFSA–BZ solutions as a function of x_{BZ} from 0.2 to 0.95.

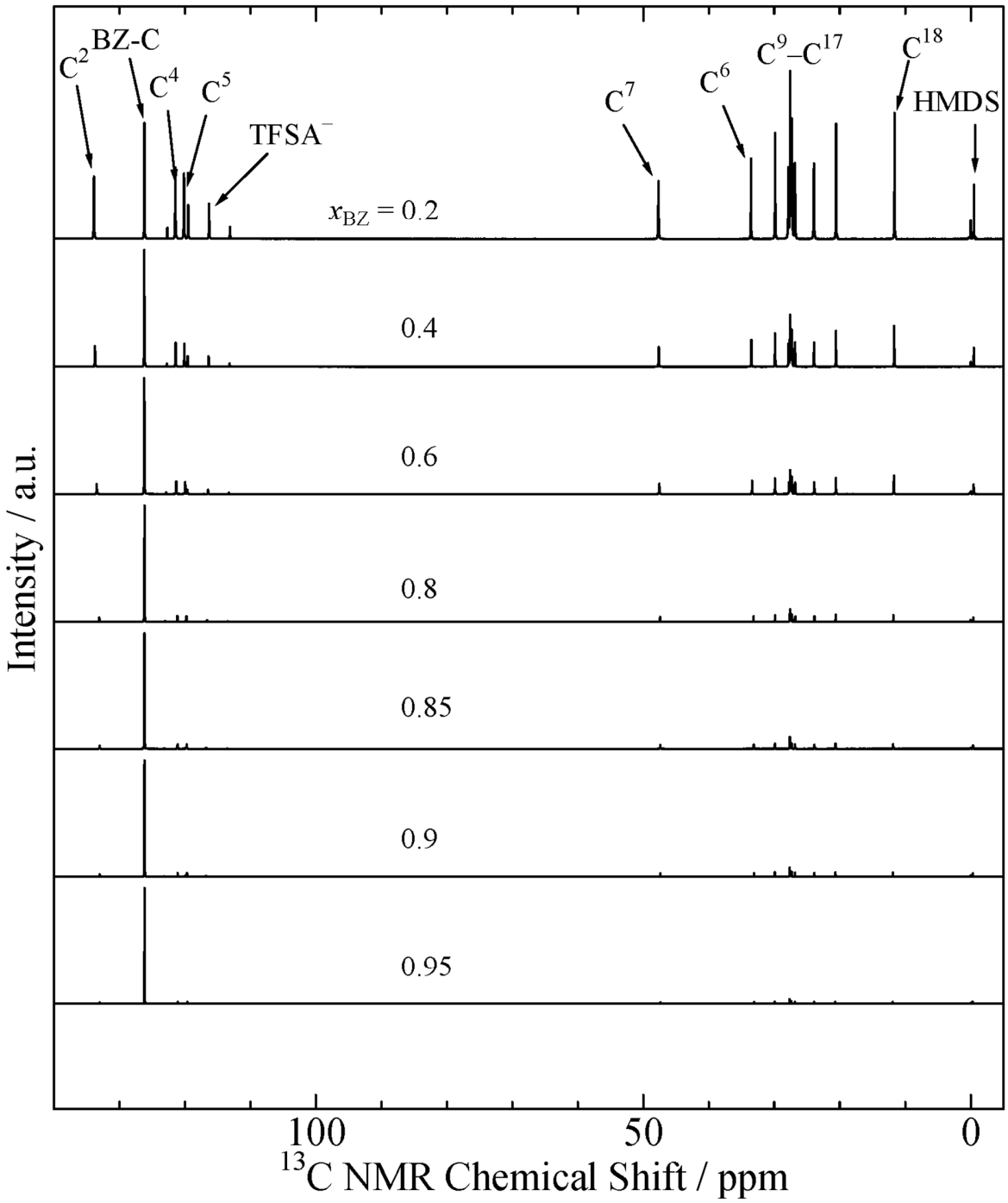

Fig. S6 ^{13}C NMR spectra of C153/C_{12}mimTFSA–BZ solutions as a function of x_{BZ} from 0.2 to 0.95.

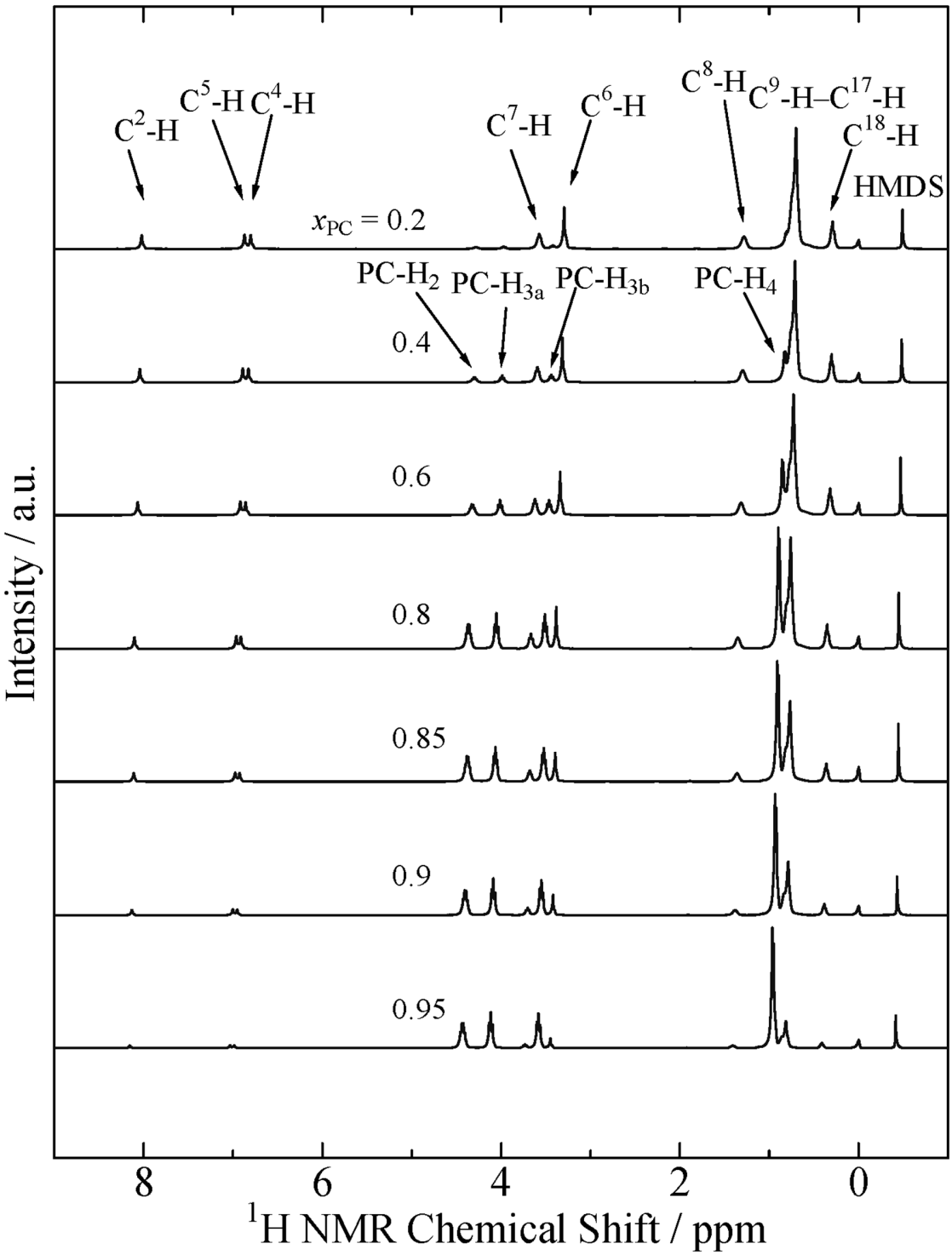

Fig. S7 ^{1}H NMR spectra of C153/C_{12}mimTFSA–PC solutions as a function of x_{PC} from 0.2 to 0.95.

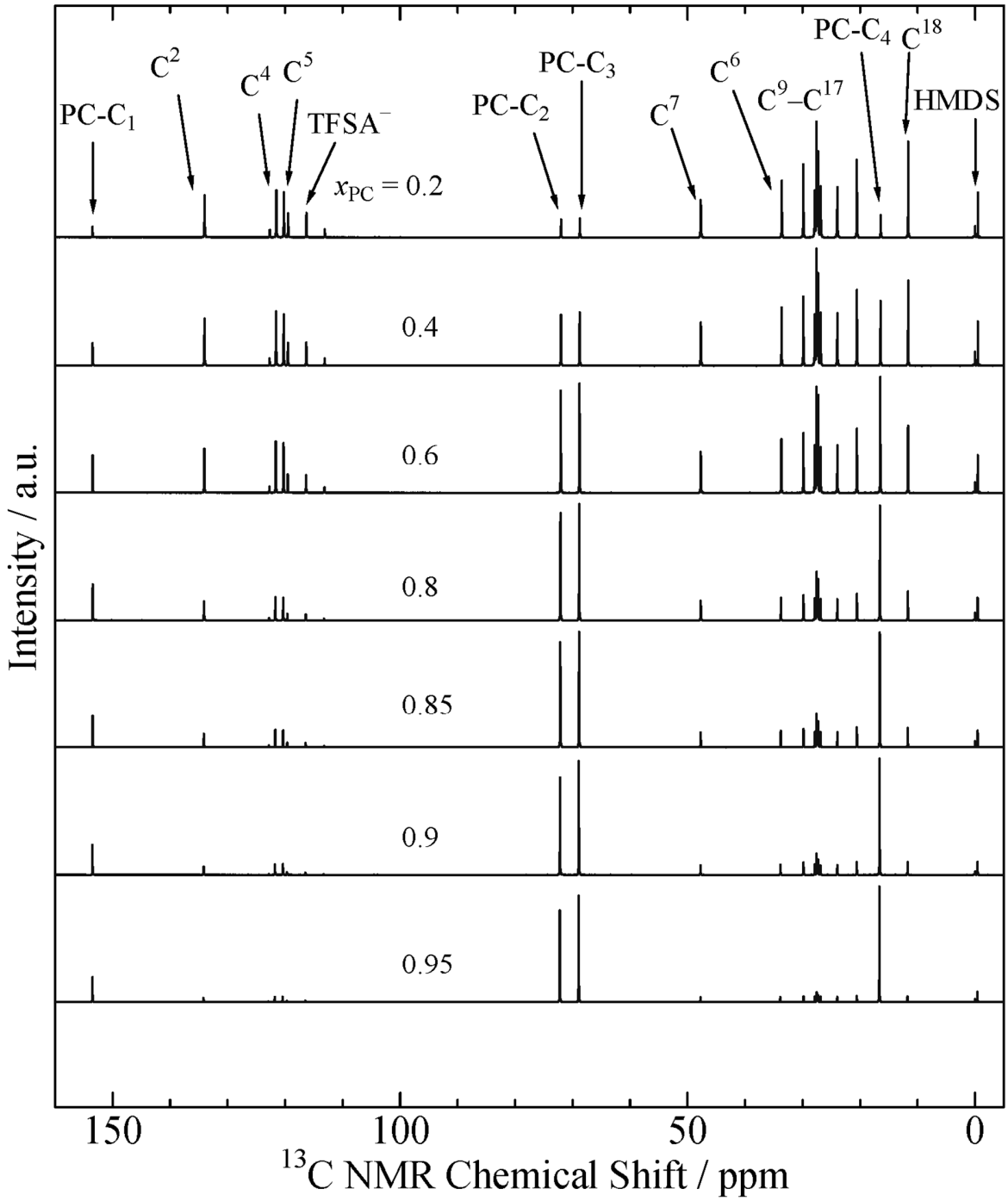

Fig. S8 ^{13}C NMR spectra of C153/C_{12}mimTFSA–PC solutions as a function of x_{PC} from 0.2 to 0.95.

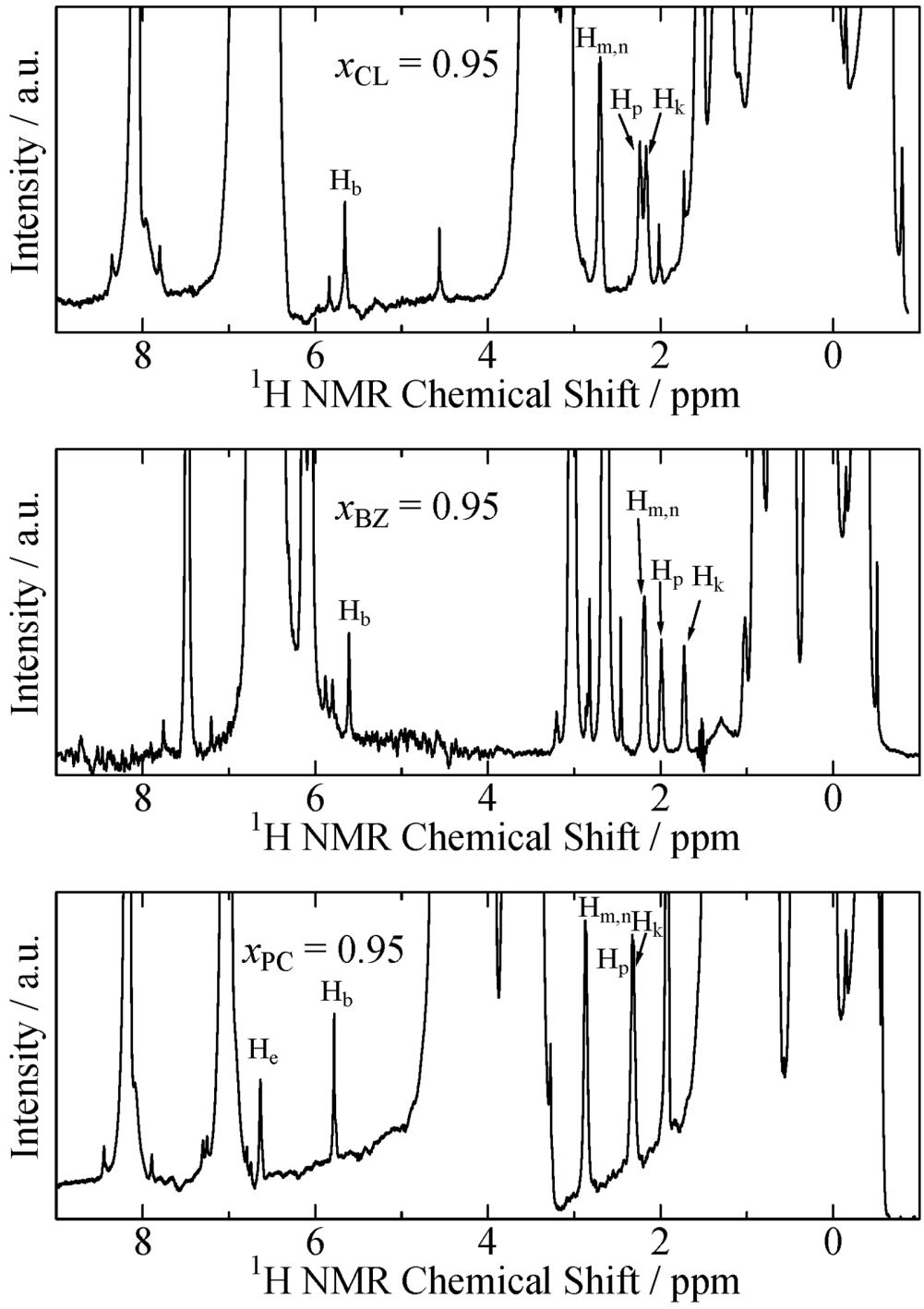

Fig. S9 Representative expanded ^{1}H NMR spectra of C153/C_{12}mimTFSA–CL (upper), –BZ (middle), and –PC (bottom) solutions at x_{ML} = 0.95.

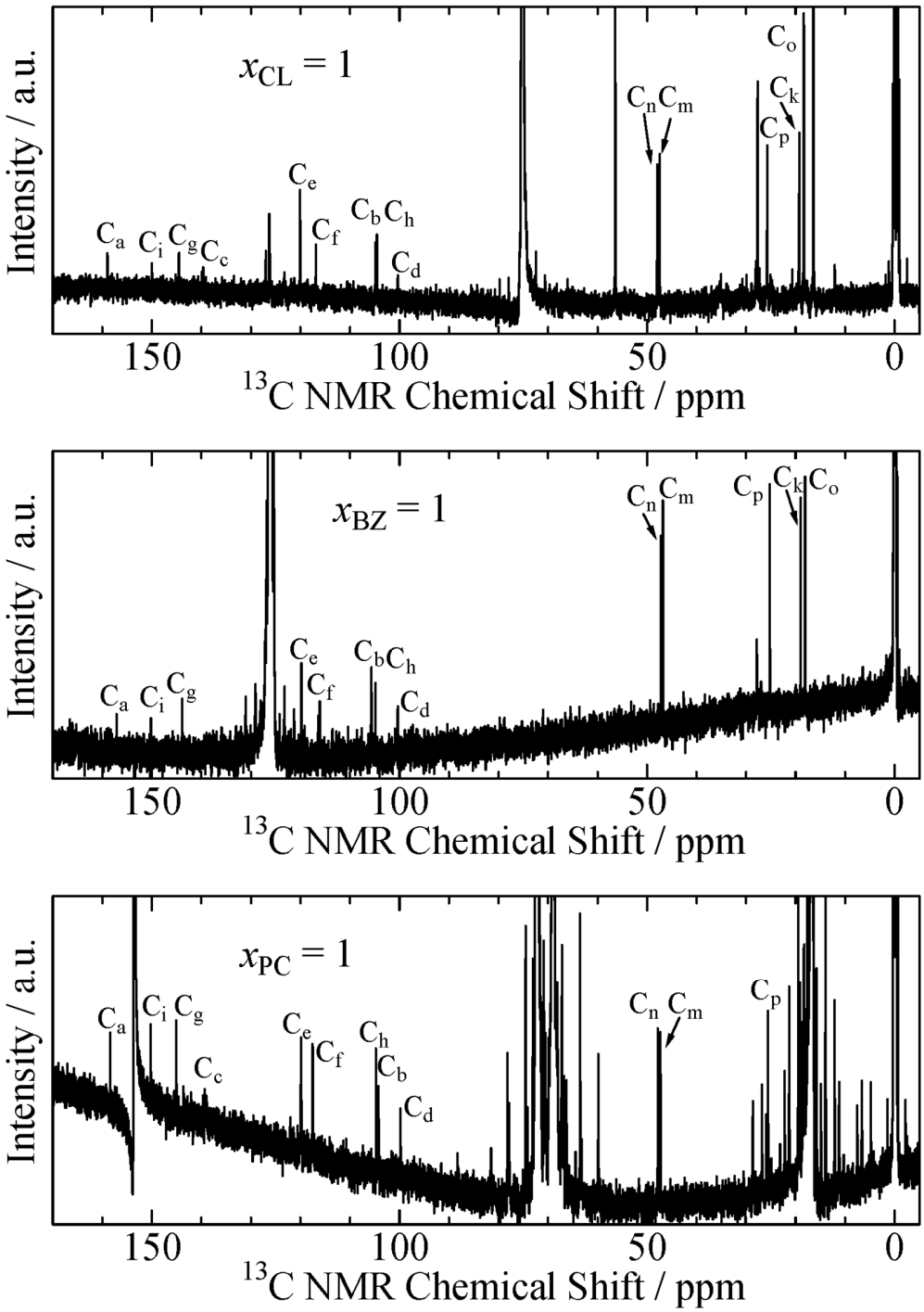

Fig. S10 Representative expanded ^{13}C NMR spectra of C153/CL (upper), BZ (middle), and PC (bottom) solutions.