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The Effect of C2 Substitution on Melting Point and Liquid Phase Dynamics of Imidazolium Based-Ionic Liquids: Insights from Molecular Dynamics Simulations

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Table 1: Calculated self-diffusion coefficients ($10^{-12}m^2/s$) at different temperatures for [BMIM][PF6].

	cation	anion
300	7.25	3.57
330	32.75	19.72
360	85.85	61.73
390	188.85	132.16
420	304.09	258.28
450	552.20	380.87

Table 2: Calculated self-diffusion coefficients ($10^{-12}m^2/s$) at different temperatures for [BMIM][PF6].

	cation	anion
300	2.09	1.73
330	5.98	3.73
360	17.15	12.48
390	57.16	43.43
420	149.72	111.91
450	302.97	268.01

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Table 3: Calculated self-diffusion coefficients ($10^{-12}m^2/s$) at different temperatures for [EMIM][PF6].

	cation	anion
350	90.63	54.18
380	198.63	129.75
410	338.22	241.05
440	593.14	419.03
470	825.80	656.65
500	1144.07	929.36

Table 4: Calculated self-diffusion coefficients ($10^{-12}m^2/s$) at different temperatures for [EMMIM][PF6].

	cation	anion
400	130.27	89.96
430	302.72	210.29
460	445.36	372.44
490	756.17	640.83
520	1087.18	927.94

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Table 5: Fitting coefficients of Vogel-Fulcher-Tamman (VFT) equation $D = Ae^{-B/(T-T_g)}$ for the self-diffusion coefficients of the studied ionic liquids. The two low temperature points in [BMMIM][PF6] were ignored in the fitting. (Units: A in $10^{-8}m^2/s$, B and T_g in K)

	cation			anion		
	A	B	T_g	A	B	T_g
$[BMIM][PF6]$	1146.93	2.75	160.58	954.63	1.43	184.94
$[BMMIM][PF6]$	1720.11	13.89	168.94	3376.09	283.68	86.14
$[EMIM][PF6]$	1228.70	3.67	145.29	1478.82	5.41	135.70
$[EMMIM][PF6]$	1000.06	2.76	212.44	1129.40	3.63	211.63