

Supporting Information for Publication

**Modeling the Temperature Dependent Material Dispersion of
Imidazolium Based Ionic Liquids in the VIS-NIR**

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Table S1. Refractive index of studied ILs at different temperatures and wavelengths

IL	T (K)	λ (nm)				
		G = 430.1	F = 486.1	D = 589.6	C = 656.3	Z = 822.7
[C ₂ MIM][BF ₄]	298.15	1.4224	1.4174	1.4117	1.4095	1.4059
	303.15	1.4210	1.4159	1.4104	1.4081	1.4046
	308.15	1.4196	1.4146	1.4091	1.4069	1.4034
	313.15	1.4182	1.4132	1.4077	1.4055	1.4022
	318.15	1.4170	1.4120	1.4065	1.4043	1.4009
	323.15	1.4155	1.4106	1.4051	1.4030	1.3997
[C ₃ MIM][BF ₄]	298.15	1.4284	1.4233	1.4176	1.4152	1.4116
	303.15	1.4270	1.4219	1.4161	1.4138	1.4102
	308.15	1.4256	1.4206	1.4149	1.4126	1.4090
	313.15	1.4242	1.4191	1.4135	1.4113	1.4078
	318.15	1.4228	1.4178	1.4122	1.4099	1.4065
	323.15	1.4213	1.4163	1.4109	1.4086	1.4053
[C ₄ MIM][BF ₄]	298.15	1.4324	1.4272	1.4215	1.4192	1.4156
	303.15	1.4309	1.4257	1.4200	1.4177	1.4141
	308.15	1.4293	1.4243	1.4186	1.4164	1.4129
	313.15	1.4279	1.4229	1.4173	1.4151	1.4116
	318.15	1.4266	1.4216	1.4160	1.4138	1.4103
	323.15	1.4251	1.4201	1.4146	1.4124	1.4090
[C ₆ MIM][BF ₄]	298.15	1.4386	1.4334	1.4276	1.4253	1.4216
	303.15	1.4372	1.4321	1.4263	1.4240	1.4203
	308.15	1.4358	1.4307	1.4249	1.4225	1.4188
	313.15	1.4343	1.4292	1.4235	1.4212	1.4177
	318.15	1.4329	1.4278	1.4221	1.4199	1.4163
	323.15	1.4313	1.4263	1.4207	1.4184	1.4150
[C ₈ MIM][BF ₄]	298.15	1.4439	1.4387	1.4328	1.4305	1.4268
	303.15	1.4425	1.4373	1.4315	1.4292	1.4255
	308.15	1.4410	1.4359	1.4301	1.4278	1.4241
	313.15	1.4395	1.4343	1.4285	1.4262	1.4226
	318.15	1.4381	1.4329	1.4272	1.4249	1.4214
	323.15	1.4365	1.4314	1.4257	1.4235	1.4200

[C ₂ MIM][NTF ₂]	298.15	1.4334	1.4284	1.4226	1.4203	1.4165
	303.15	1.4319	1.4269	1.4212	1.4190	1.4154
	308.15	1.4304	1.4254	1.4199	1.4176	1.4141
	313.15	1.4289	1.4239	1.4183	1.4160	1.4125
	318.15	1.4271	1.4222	1.4167	1.4145	1.4111
	323.15	1.4257	1.4207	1.4152	1.4130	1.4095
[C ₃ MIM][NTF ₂]	298.15	1.4354	1.4303	1.4247	1.4224	1.4188
	303.15	1.4338	1.4288	1.4232	1.4210	1.4175
	308.15	1.4323	1.4273	1.4218	1.4196	1.4161
	313.15	1.4306	1.4257	1.4202	1.4180	1.4145
	318.15	1.4291	1.4241	1.4186	1.4164	1.4130
	323.15	1.4276	1.4227	1.4172	1.4150	1.4117
[C ₄ MIM][NTF ₂]	298.15	1.4370	1.4320	1.4265	1.4242	1.4208
	303.15	1.4354	1.4305	1.4250	1.4228	1.4194
	308.15	1.4338	1.4289	1.4234	1.4212	1.4179
	313.15	1.4324	1.4274	1.4219	1.4197	1.4163
	318.15	1.4308	1.4258	1.4204	1.4182	1.4149
	323.15	1.4290	1.4241	1.4188	1.4167	1.4136
[C ₆ MIM][NTF ₂]	298.15	1.4401	1.4351	1.4293	1.4270	1.4234
	303.15	1.4386	1.4336	1.4279	1.4257	1.4221
	308.15	1.4370	1.4320	1.4263	1.4240	1.4204
	313.15	1.4355	1.4305	1.4249	1.4226	1.4192
	318.15	1.4338	1.4289	1.4233	1.4211	1.4176
	323.15	1.4321	1.4272	1.4217	1.4195	1.4161
[C ₂ MIM][OTF]	298.15	1.4453	1.4399	1.4339	1.4315	1.4278
	303.15	1.4439	1.4385	1.4326	1.4303	1.4266
	308.15	1.4423	1.4370	1.4311	1.4288	1.4252
	313.15	1.4408	1.4355	1.4297	1.4274	1.4238
	318.15	1.4393	1.4341	1.4283	1.4260	1.4225
	323.15	1.4378	1.4326	1.4269	1.4246	1.4212
[C ₄ MIM][OTF]	298.15	1.4487	1.4434	1.4373	1.4348	1.4309
	303.15	1.4472	1.4418	1.4358	1.4334	1.4296

	308.15	1.4456	1.4403	1.4343	1.4319	1.4282
	313.15	1.4443	1.4389	1.4330	1.4306	1.4268
	318.15	1.4428	1.4375	1.4316	1.4292	1.4256
	323.15	1.4414	1.4361	1.4303	1.4280	1.4244

Table S2. Density (g/cm³) as a function of temperature

IL	T(K)					
	298.15	303.15	308.15	313.15	318.15	323.15
[C ₂ MiM][BF ₄]	1.2849	1.2812	1.2774	1.2736	1.2699	1.2661
[C ₃ MiM][BF ₄]	1.2371	1.2334	1.2297	1.2261	1.2225	1.2188
[C ₄ MiM][BF ₄]	1.2010	1.1975	1.1939	1.1904	1.1869	1.1834
[C ₆ MiM][BF ₄]	1.1452	1.1418	1.1384	1.1349	1.1315	1.1281
[C ₈ MiM][BF ₄]	1.1043	1.1008	1.0974	1.0941	1.0908	1.0875
[C ₂ MiM][NTf ₂]	1.5185	1.5134	1.5084	1.5034	1.4984	1.4934
[C ₃ MiM][NTf ₂]	1.4747	1.4698	1.4648	1.4600	1.4551	1.4502
[C ₄ MiM][NTf ₂]	1.4366	1.4319	1.4271	1.4223	1.4176	1.4129
[C ₆ MiM][NTf ₂]	1.3722	1.3676	1.3631	1.3585	1.3539	1.3494
[C ₂ MiM][OTf]	1.3821	1.3779	1.3737	1.3695	1.3654	1.3613
[C ₄ MiM][OTf]	1.2977	1.2937	1.2898	1.2859	1.2820	1.2781

Table S3. Coefficients of the linear fit of densities as a function of temperature

$\rho = \rho_0 + \rho_1 T$	ρ_0 (g/cm ³)*	ρ_1 (g/cm ³ K)*
[C ₂ MiM][BF ₄]	1.3037274	-7.52491 10 ⁻⁴
[C ₃ MiM][BF ₄]	1.2553258	-7.30337 10 ⁻⁴
[C ₄ MiM][BF ₄]	1.2186637	-7.05960 10 ⁻⁴
[C ₆ MiM][BF ₄]	1.1622218	-6.81731 10 ⁻⁴
[C ₈ MiM][BF ₄]	1.1209841	-6.71251 10 ⁻⁴
[C ₂ MiM][NTf ₂]	1.5435027	-1.001806 10 ⁻³
[C ₃ MiM][NTf ₂]	1.4991230	-9.78571 10 ⁻⁴
[C ₄ MiM][NTf ₂]	1.4603420	-9.49234 10 ⁻⁴
[C ₆ MiM][NTf ₂]	1.3949770	-9.11840 10 ⁻⁴
[C ₂ MiM][OTf]	1.4028434	-8.32171 10 ⁻⁴
[C ₄ MiM][OTf]	1.3172910	-7.85046 10 ⁻⁴

* Standard deviation of ρ_0 and ρ_1 are 3.7×10^{-6} and 9.6×10^{-8} , respectively.

Table S4. Molar refraction coefficients for different wavelengths and temperatures ($R = R_0 + \Delta RN_c$)

		[C _n MiM][BF ₄]		[C _n MiM][NTf ₂]	
λ (nm)	T (K)	R_0 (cm ³ /mol)	ΔR (cm ³ /mol)	R_0 (cm ³ /mol)	ΔR (cm ³ /mol)
430.1	298.15	29.743	4.7637	57.572	4.7275
486.1		29.429	4.7178	56.989	4.6836
589.6		29.074	4.6649	56.320	4.6345
656.3		28.928	4.6430	56.042	4.6152
822.7		28.702	4.6092	55.600	4.5875
589.6	298.15	29.074	4.6649	56.320	4.6345
	303.15	29.056	4.6702	56.338	4.6372
	308.15	29.061	4.6710	56.384	4.6296
	313.15	29.068	4.6703	56.367	4.6374
	318.15	29.071	4.6722	56.361	4.6408
	323.15	29.077	4.6711	56.390	4.6359

Table S5. Molar mass of the studied ILs

IL	M (g/mol)
[C ₂ MiM][BF ₄]	197.97
[C ₃ MiM][BF ₄]	212.00
[C ₄ MiM][BF ₄]	226.02
[C ₆ MiM][BF ₄]	254.08
[C ₈ MiM][BF ₄]	282.13
[C ₂ MiM][NTf ₂]	391.31
[C ₃ MiM][NTf ₂]	405.34
[C ₄ MiM][NTf ₂]	419.36
[C ₆ MiM][NTf ₂]	447.41
[C ₂ MiM][OTf]	260.23
[C ₄ MiM][OTf]	288.29

Table S6. Molar volume coefficients for different temperatures ($V_m = V_0 + \Delta VN_c$)

T(K)	[C _n MiM][BF ₄]		[C _n MiM][NTf ₂]	
	V_0 (cm ³ /mol)	ΔV (cm ³ /mol)	V_0 (cm ³ /mol)	ΔV (cm ³ /mol)
298.15	120.55	16.879	223.57	17.084
303.15	120.89	16.935	224.31	17.141
308.15	121.23	16.991	225.06	17.200
313.15	121.58	17.045	225.81	17.258
318.15	121.93	17.099	226.56	17.318
323.15	122.28	17.154	227.30	17.378