SUPPORTING INFORMATION

An experimental and computational study to explore the ion-solvent interactions between selected ionic liquids and dimethylformamide

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Table S1: Molality (), , , and for (ILs + DMF) at different temperatures.

m (mol.kg^{-1})	ρ (kg.m^{-3})	u (m.s^{-1})	(cm^3.mol^{-1})	$10^{-5}\times$ (cm^3.mol^{-1}. Pa^{-1})
		[Bmim][Cl] + DMF		
		T = 293.15 K		
0.0823	954.67	1480.0	182.944	8.75
0.1680	956.61	1484.7	182.570	8.66
0.2527	958.69	1488.4	182.173	8.57
0.3267	960.83	1492.6	181.765	8.49
0.4162	963.54	1498.7	181.252	8.37
0.5009	965.76	1502.1	180.836	8.29
0.6612	969.62	1508.6	180.116	8.16
0.8708	974.69	1517.5	179.179	7.98
1.2272	983.63	1538.1	177.550	7.63
		T = 303.15 K		
0.0823	945.22	1441.9	184.772	9.40
0.1680	947.21	1446.6	184.381	9.30
0.2527	949.33	1450.5	183.968	9.21
0.3267	951.55	1454.8	183.537	9.11
0.4162	954.34	1461.0	182.999	8.98
0.5009	956.61	1465.1	182.564	8.89
0.6612	960.56	1472.3	181.814	8.73
0.8708	965.87	1480.5	180.814	8.54
1.2272	975.10	1501.9	179.103	8.14
		T = 313.15 K		
0.0823	935.71	1404.0	186.648	10.12
0.1680	937.78	1408.6	186.234	10.00
0.2527	939.90	1412.7	185.813	9.90
0.3267	942.25	1417.2	185.347	9.79
0.4162	945.10	1423.6	184.786	9.64
0.5009	947.44	1428.3	184.330	9.53
0.6612	951.52	1435.2	183.540	9.36
0.8708	956.99	1443.9	182.491	9.14
1.2272	966.44	1466.0	180.706	8.70
		T = 323.15 K		
0.0823	926.14	1367.0	188.575	11.66
0.1680	928.29	1371.5	188.136	11.14
0.2527	930.49	1375.7	187.690	10.90
0.3267	932.90	1380.1	187.203	10.72
0.4162	935.81	1386.4	186.619	10.52
0.5009	938.23	1390.8	186.138	10.38
0.6612	942.38	1398.0	185.319	10.15
0.8708	947.99	1407.3	184.222	9.88
1.2272	957.78	1430.3	182.339	9.35
		T = 343.15 K		
0.0823	906.80	1292.7	192.594	12.71

0.1680	909.10	1297.3	192.105	12.55
0.2527	911.48	1302.0	191.602	12.39
0.3267	914.00	1306.5	191.071	12.24
0.4162	917.04	1312.9	190.436	12.04
0.5009	919.63	1317.2	189.900	11.89
0.6612	924.01	1324.8	189.000	11.65
0.8708	929.97	1335.4	187.789	11.32
1.2272	940.24	1360.1	185.738	10.67
		[Bmpym][Cl] + DMF		
		T = 293.15 K		
0.0844	954.51	1486.0	186.162	8.83
0.1607	955.88	1489.5	185.894	8.76
0.2458	957.52	1494.3	185.575	8.68
0.3243	959.16	1498.4	185.256	8.59
0.4048	960.89	1505.1	184.922	8.51
0.4845	962.47	1509.4	184.620	8.43
0.6418	965.25	1516.9	184.088	8.28
0.8415	968.70	1528.0	183.432	8.11
1.2079	974.53	1544.6	182.336	7.83
		T = 303.15 K		
0.0844	945.06	1447.8	188.021	9.50
0.1607	946.48	1451.3	187.740	9.41
0.2458	948.22	1456.3	187.393	9.31
0.3243	949.92	1460.4	187.058	9.22
0.4048	951.81	1467.3	186.686	9.12
0.4845	953.43	1471.7	186.368	9.03
0.6418	956.38	1479.4	185.793	8.86
0.8415	960.00	1490.7	185.094	8.67
1.2079	966.12	1507.7	183.922	8.34
		T = 313.15 K		
0.0844	935.57	1409.7	189.929	10.23
0.1607	937.05	1413.2	189.628	10.13
0.2458	938.89	1418.3	189.255	10.01
0.3243	940.62	1422.7	188.905	9.91
0.4048	942.64	1429.6	188.500	9.80
0.4845	944.33	1434.1	188.162	9.70
0.6418	947.43	1442.0	187.546	9.51
0.8415	951.23	1453.6	186.799	9.29
1.2079	957.62	1471.0	185.553	8.92
		T = 323.15 K		
0.0844	926.00	1371.8	191.889	11.02
0.1607	927.57	1375.4	191.564	10.91
0.2458	929.48	1380.7	191.170	10.78
0.3243	931.30	1385.2	190.794	10.66
0.4048	933.39	1392.3	190.365	10.54
0.4845	935.16	1396.8	190.006	10.43
0.6418	938.42	1404.9	189.346	10.22
0.8415	942.39	1416.8	188.549	9.96

1.2079	949.07	1434.6	187.222	9.54
		T = 343.15 K		
0.0844	906.68	1296.9	195.976	12.87
0.1607	908.40	1300.8	195.604	12.72
0.2458	910.48	1306.3	195.155	12.56
0.3243	912.47	1311.0	194.729	12.41
0.4048	914.73	1318.4	194.246	12.26
0.4845	916.68	1323.1	193.834	12.11
0.6418	920.26	1331.7	193.080	11.84
0.8415	924.60	1344.1	192.174	11.52
1.2079	931.94	1362.8	190.662	10.97
		[Bmim][SCN] + DMF		
		T = 293.15 K		
0.0752	954.24	1480.6	206.746	9.88
0.1519	955.87	1488.1	206.390	9.75
0.2181	957.40	1490.7	206.058	9.68
0.2916	959.17	1494.1	205.676	9.60
0.3686	961.83	1501.1	205.104	9.46
0.4333	963.89	1506.2	204.665	9.36
0.5840	967.41	1514.2	203.920	9.19
0.7337	970.78	1521.4	203.213	9.04
1.0917	977.90	1538.1	201.735	8.72
		T = 303.15 K		
0.0752	944.78	1442.4	208.815	10.62
0.1519	946.49	1450.1	208.434	10.47
0.2181	948.08	1452.8	208.082	10.39
0.2916	949.92	1456.3	207.678	10.30
0.3686	952.65	1463.5	207.079	10.14
0.4333	954.65	1468.7	206.644	10.03
0.5840	958.39	1477.1	205.838	9.84
0.7337	961.86	1484.5	205.096	9.67
1.0917	969.20	1501.9	203.544	9.30
		T = 313.15 K		
0.0752	935.29	1404.3	210.932	11.43
0.1519	937.09	1412.1	210.523	11.26
0.2181	938.73	1415.1	210.153	11.17
0.2916	940.64	1418.7	209.725	11.07
0.3686	943.44	1426.2	209.099	10.89
0.4333	945.49	1431.5	208.645	10.76
0.5840	949.35	1440.1	207.797	10.55
0.7337	952.91	1447.9	207.021	10.36
1.0917	960.49	1466.0	205.389	9.94
		T = 323.15 K		
0.0752	925.74	1367.1	213.106	12.32
0.1519	927.62	1374.5	212.670	12.13
0.2181	929.34	1377.6	212.275	12.03
0.2916	931.31	1381.4	211.825	11.91
0.3686	934.20	1389.1	211.166	11.71

0.4333	936.28	1394.5	210.696	11.56
0.5840	940.28	1403.5	209.800	11.32
0.7337	943.94	1411.5	208.987	11.11
1.0917	951.76	1430.3	207.272	10.64
		T = 343.15 K		
0.0752	906.43	1291.8	217.642	14.38
0.1519	908.49	1298.6	217.145	14.17
0.2181	910.37	1302.9	216.695	14.01
0.2916	912.51	1308.2	216.185	13.83
0.3686	915.54	1315.4	215.466	13.59
0.4333	917.75	1320.1	214.947	13.43
0.5840	922.02	1329.9	213.952	13.11
0.7337	925.90	1339.7	213.056	12.81
1.0917	934.24	1360.4	211.156	12.20

Standard uncertainties u is $u(\rho) = 0.94$ kg·m^{-3}, $u(u) = 2.9$m·s^{-1}; $u(m) = 0.0007$ mol·kg^{-1}; $u(T) = 0.001$ K, $u(p) = 0.01$ MPa, $u(V_\phi) = 0.009$ cm^3·mol^{-1} and $u(K_\phi) = 0.08$ x10^{-5} cm^3.mol^{-1}.Pa^{-1} (0.68 level of confidence).

Table S2: Total energies in Hartrees and kcal mol^{-1} used to calculate E_{inter}

Structure	**Gas phase**		**DMF**	
	Hartrees	**kcal mol^{-1}**	**Hartrees**	**kcal mol^{-1}**
[Bmim]	-423,284507	-265614,838	-423,377581	-265673,4182
[Bmpym]	-409,644904	-257055,864	-409,736810	-257113,5359
$^{-}$SCN	-491,168763	-308212,819	-491,255428	-308267,2024
$^{-}$Cl	-460,303727	-288844,731	-460,408728	-288910,6205
DMF	-248,587511	-155990,90	-248,599407	-155998,3653
[Bmim][SCN]	-914,593637	-573915,739	-914,641218	-573945,5961
[Bmim][Cl]	-883,737494	-554553,231	-883,792852	-554587,9688
[Bmpym][Cl]	-870,094490	-545992,123	-870,150602	-546027,3341
[Bmim][SCN]-DMF	-1163,20515	-729921,702	-1163,25032	-729950,0419
[Bmim][Cl]-DMF	-1132,349038	-710559,212	-1132,400161	-710591,2926
[Bmpym][Cl]-DMF	-701968,0539	-702000,344	-1118,758875	-702031,2629

NCI and AIM analysis of [Bmim][Cl] + DMF in gas phase

In the [Bmim][Cl]-DMF complex (gas phase) the ionic liquid interacts with the DMF molecule through four specific interactions (Fig. S1a): the first two interactions are where the hydrogen atoms (H34 and H37) of DMF interact with the chloride anion (H34-Cl and H37-Cl); the second two interactions are where two hydrogen atoms (H14 and H20) from the cation of the ionic liquid interact with O38 of DMF via H14-O34 and H20-O38. In the molecular graph (Fig. S1b), the bond critical points (BCPs) of the [Bmim][Cl]-DMF complex are highlighted.

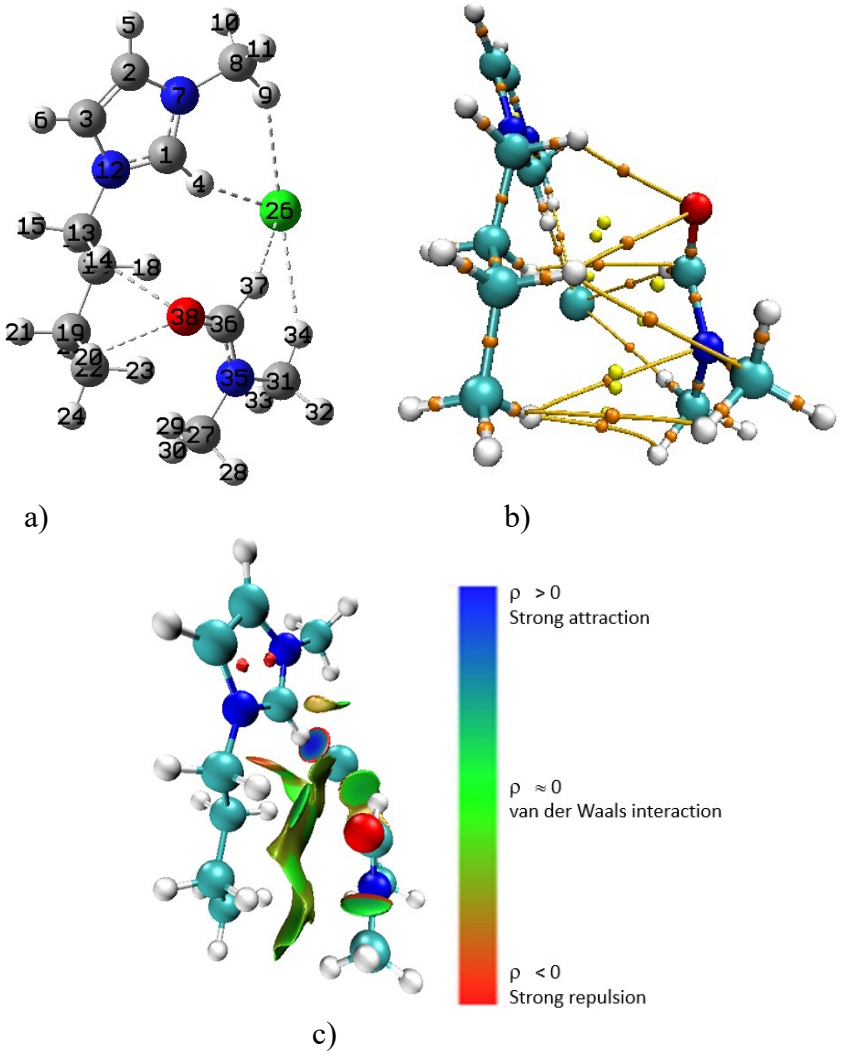


Fig. S1. a) Optimized structure [Bmim][Cl]-DMF in the gas phase b) Molecular graph with BCPs and c) 3D NCI plot.

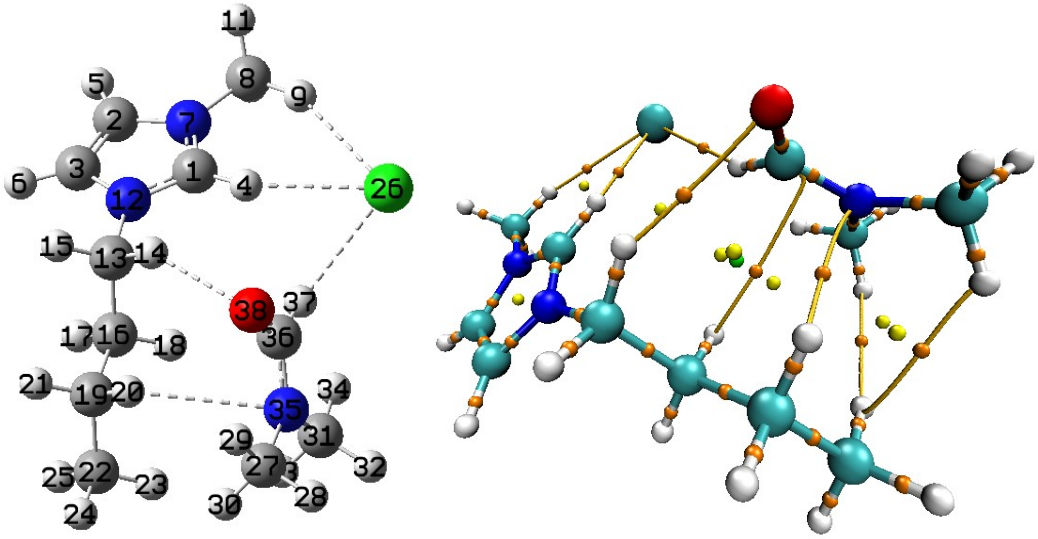
The green isosurface observed between O38-H14, Cl-H37, Cl-H20 as well as Cl-H34, confirm the presence of non-covalent interactions. From the calculated values of $\rho(r)$ and $\nabla^2\rho(r)$ (Table S3), the $\rho(r)$ value is highest for the H14-O38 interaction which indicates that, among the four interactions, this interaction contributes the most to the interaction between the IL and DMF. The NCI plot (Fig. S1c) of [Bmim][Cl]-DMF also reveals a strong non-covalent interaction between the anion of the ionic liquid (Cl26) and H4 of the cation. This is evidenced by the blue isosurface (blue disk) in the 3D NCI plot and the highest electron density value of 0.0327 a.u. at the Cl26-H34 bond critical point (BCP).

Table S3: Bond distances and AIM analysis at selected BCPs for [Bmim][Cl]-DMF in gas phase

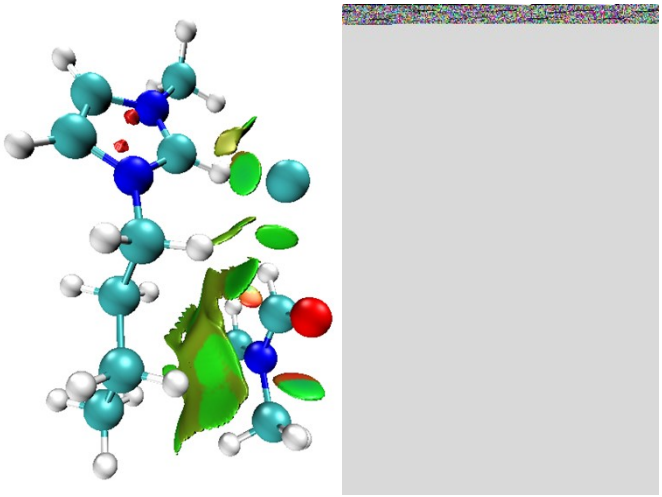
BCP	Distance (Å)	ρ(r) (a.u.)	$\nabla^2\rho(r)$ (a.u.)
H34-Cl	2.72	0.0098	0.0301
H37-Cl	2.68	0.0112	0.0334
H14-O38	2.24	0.0147	0.0538
H20-O38	2.79	0.0057	0.0184

NCI and AIM analysis of [Bmim][Cl] + DMF in solvent

The next part of the calculation was to add the IL complex in DMF solvent. As observed (Fig. S2a and b) there are three possible interactions when the complex is in the solvent environment: H14-O38; H20-N35 and H37-Cl26. Additionally, in solvent, the distance between H34 and Cl26 increases to 3.77 Å as compared to its gas phase value of 2.72 Å (Table S3). The distance between H20 and O38 increases to 2.90 Å in solvent whereas in the gas phase the value was 2.79 Å. The absence of a BCP between H20-O38, and H34-Cl26, in the molecular graph (Fig. S2b) confirm that the binding from the H20-O38 and H34-Cl26 interactions are negligible in this solvent. However, a new interaction between H20-N35 was observed in solvent, which is not present in the gas phase. This suggests that the solvent influences the how the molecule orients itself in solution.



a) b)



c)

Fig. S2. a) Optimized [Bmim][Cl]-DMF in DMF solvent b) Molecular graph with BCPs and c) 3D NCI plot.

All the $\nabla^2\rho(r)$ are positive (Table S4), indicating the interactions are non-covalent. The $\rho(r)$ values calculated at the corresponding BCPs range from 0.0055 to 0.0079 au, suggesting that these interactions are weak van der Waals type in nature. In the gas phase, a strong ion-dipole interaction was observed between the chloride anion (Cl26) and H4 of the cation of the ionic liquid. However, this interaction (H4-Cl26) weakened in solvent, as indicated by the light blue isosurface between these atoms in the NCI plot (Fig. S2c).

Table S4: Bond distances and AIM analysis at selected BCPs for [Bmim][Cl]-DMF in DMF solvent

BCP	**Distance (Å)**	**$\rho(r)$ (a.u.)**	**$\nabla^2\rho(r)$ (a.u.)**
Cl26---H4	2.59	0.0121	0.0388
Cl26---H9	2.83	0.0082	0.0238
H37---Cl26	2.86	0.0078	0.0218
H14---O38	2.57	0.0079	0.0248
H20----N35	2.89	0.0055	0.0182

NCI and AIM analysis of [Bmim][SCN] + DMF in gas phase

Next, we examined the interactions for the [Bmim][SCN]-DMF complex. In the gas phase, there are four bond critical points (BCPs) in the molecular graph (Fig. S3a and b) which are N28-H38, N28-H32, O39-H9 and O39-C2. This suggests that four distinct interactions exist between pairs of atoms in the system. The values of $\nabla^2\rho(r)$ and H(r) for all the BCPs calculated

are positive, suggesting that these interactions are weak in the IL-DMF complex. As already mentioned, NCI plots assist in visualizing nature of interactions with the use of colour to differentiate the interactions. Red denotes steric clashes, green shows weak interactions, and blue indicates strong interactions. The green isosurfaces (Fig.S3c) between the interacting atoms in the [Bmim][SCN]-DMF complex confirms the presence of weak to medium hydrogen bonding. However, the ρ(r) value for O39-H9 for the DMF molecule is largest (0.0133 a.u.) (Table S5), suggesting that this is the strongest interaction in this IL-DMF interaction.

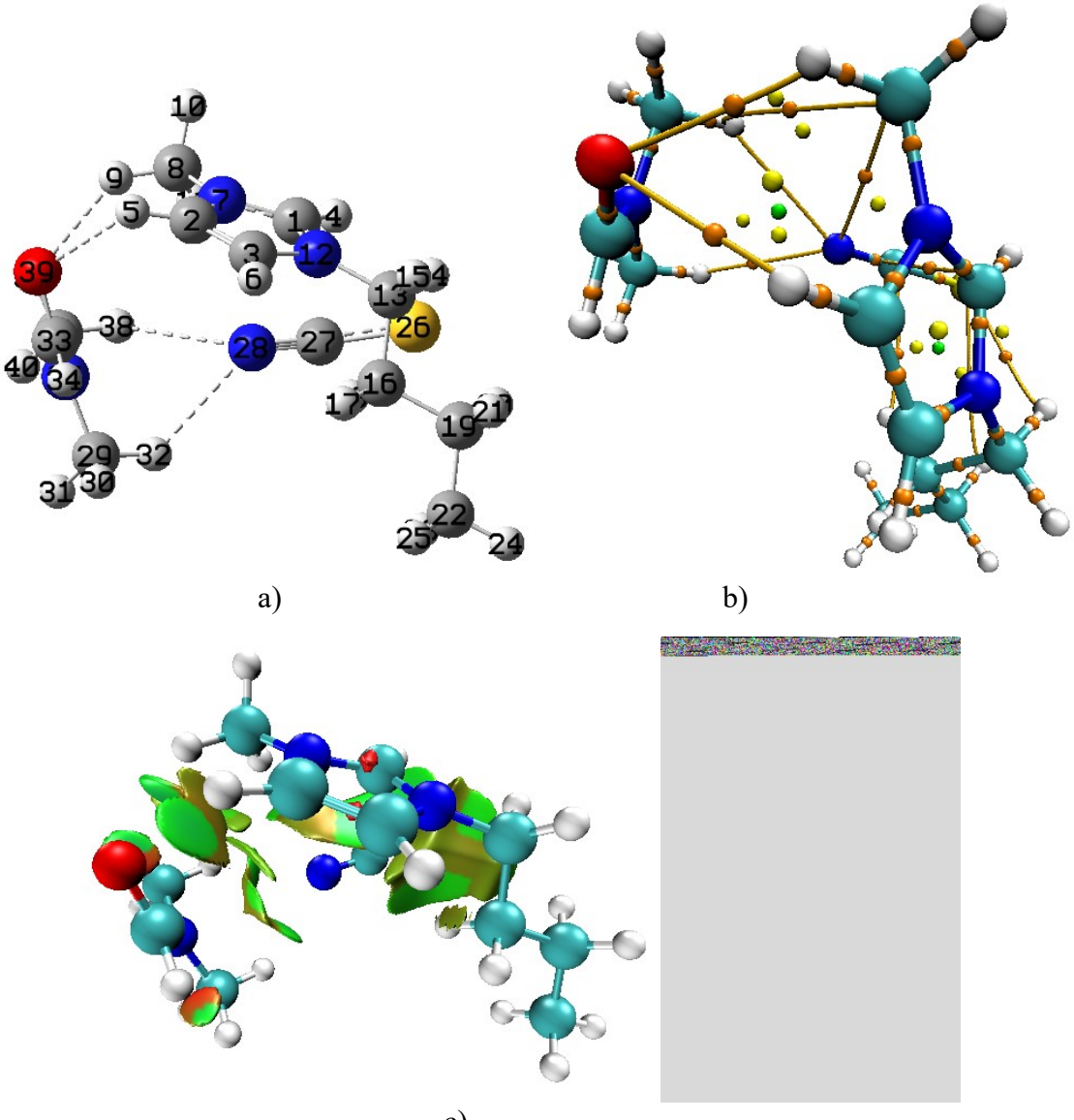


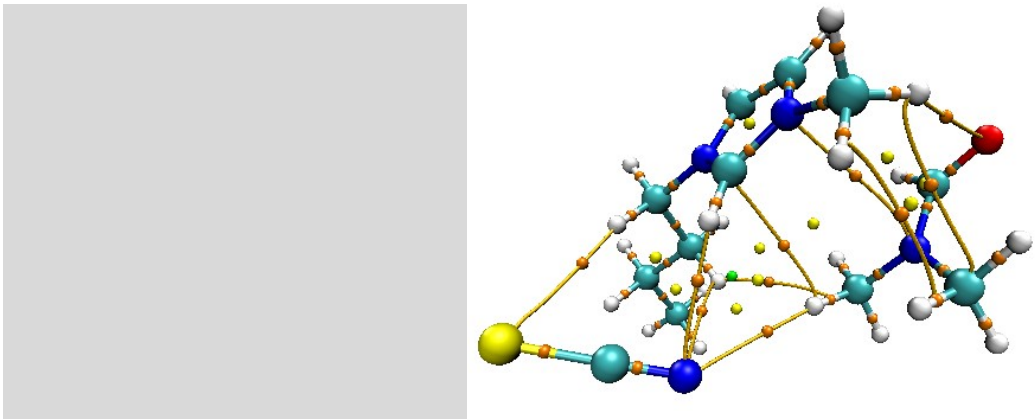
Fig. S3. a) Optimized structure of [Bmim][SCN]-DMF in the gas phase b) Molecular graph with BCPs and c) 3D NCI plot.

Table S5: Bond distances and AIM analysis at selected BCPs for [Bmim][SCN]-DMF in gas phase

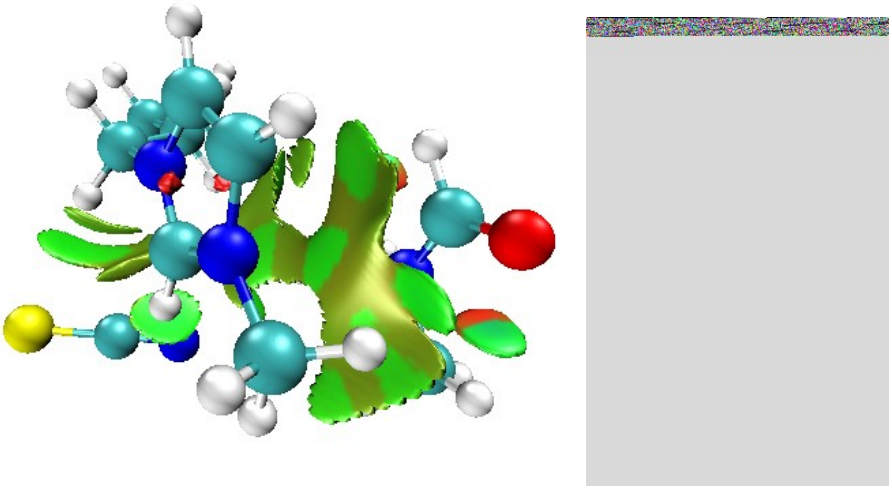
BCP	Distance (Å)	ρ(r) (a.u.)	$\nabla^2\rho(r)$ (a.u.)	H	LOL
N28---H38	2.55	0.00944	0.0304	0.0012	0.1601
N28---H32	2.48	0.0105	0.0344	0.0014	0.1677
O39---H9	2.30	0.0133	0.0465	0.0016	0.1757
O39---H5	2.41	0.0116	0.0416	0.0016	0.1623

NCI and AIM analysis of [Bmim][SCN] + DMF in solvent

When the complex was modelled in DMF solvent, the O39-H5 and N28-H38 interactions were not observed in DMF solvent. The bond distance between N28-H38 increased from 2.55 Å in the gas phase to 3.80 Å (Table S6) in the DMF solvent, which is further proof of the weakened bond in solvent. Similarly, the bond distance between O39-H9 also increased from 2.41 Å in the gas phase to 3.44 Å in DMF, indicating a weak interaction (Fig. S4a and b). Since the bond distances of these interactions are significantly elongated, the bond critical points (BCPs) between these atoms in the molecular graph, do not appear. The bond distance for N28-H32 and O39-H9 also increased in solvent compared to the gas-phase values. The N28-H32 interaction increased from 2.48 Å in the gas phase to 2.76 Å in solvent, while the O39-H9 interaction increased from 2.30 Å (gas) to 2.54 Å (solvent). The electron density ρ(r) at the bond critical point for N28-H32 and O39-H9 are 0.0061 a.u. and 0.0083 a.u., respectively in DMF which highlights the reduced interacting strength in solvent.



a) b)



c)

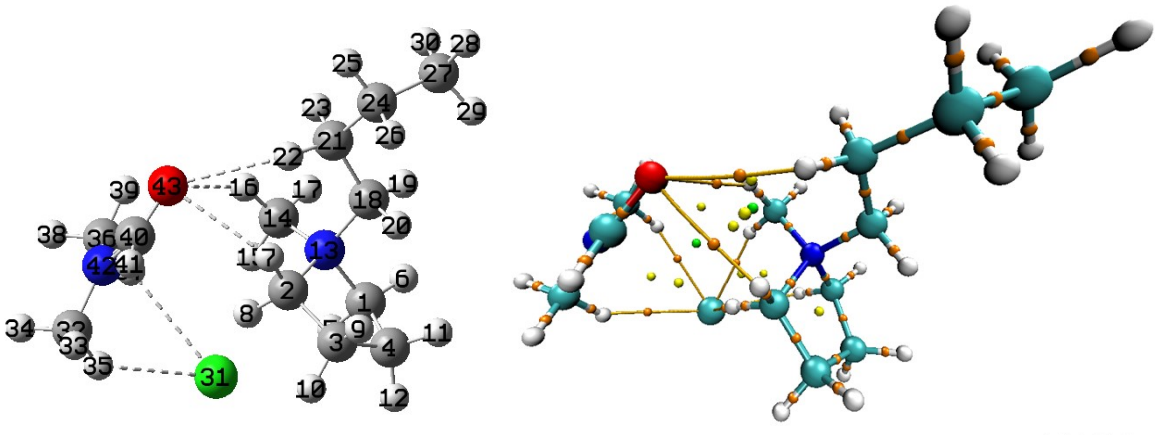
Fig. S4. a) Optimized structure of [Bmim][SCN]-DMF in DMF solvent b) Molecular graph with BCPs and c) 3D NCI plot.

Table S6: Bond distances and AIM analysis at selected BCPs for [Bmim][SCN]-DMF in DMF solvent

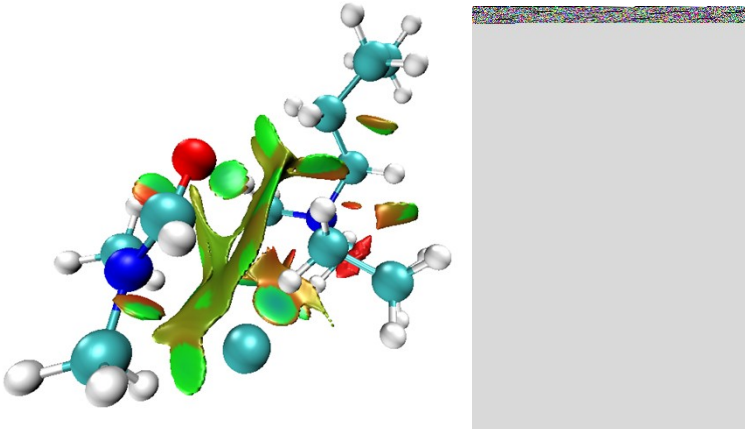
BCP	Distance (Å)	ρ(r) (a.u.)	$\nabla^2\rho(r)$(a.u.)
N28---H32	2.76	0.0061	0.0175
O39---H9	2.54	0.0083	0.0265
N7---N35	3.37	0.0058	0.0179

NCI and AIM analysis of [Bmpym][Cl] + DMF in gas phase

For the Bmpym][Cl]-DMF complex in the gas phase, five non-covalent interactions between DMF and the ionic liquid was observed (Fig. S5a and b). The interactions were between the chloride ion from the ionic liquid with H35 and H37 of the DMF molecule (Fig. S5c). Additionally, the O43 atom of the DMF molecule interacts with H7, H16 and H22 in the cation of the ionic liquid. The calculated $\nabla^2\rho(r)$ values at these BCPs are positive, indicating that these interactions are non-covalent (Table S7). The $\nabla^2\rho(r)$ values show that the O43-H16 interaction is the strongest and should contribute most to the binding of DMF molecule to the ionic liquid.



a) b)



c)

Fig. S5. a) Optimized structure of [Bmpym][Cl]-DMF in the gas phase b) Molecular graph with BCPs and c) 3D NCI plot.

Table S7: Bond distances and AIM analysis at selected BCPs for [Bmpym][Cl]-DMF in gas phase.

BCP	Distance (Å)	ρ(r)	$\nabla^2\rho(r)$
H35---Cl31	2.74	0.0097	0.0291
H37---Cl31	2.78	0.0094	0.0274
O43---H7	2.59	0.0088	0.0289
O43---H16	2.32	0.0129	0.0439
O43---H22	2.58	0.0075	0.025

NCI and AIM analysis of [Bmpym][Cl] + DMF in solvent

The molecular graph of the [Bmpym][Cl]-DMF complex optimized in DMF solvent using the B3LYP-D3 method does not show the interactions: H35-Cl31, O43-H7, and O43-H22. The absence of this interaction can be attributed to the increased bond length between these interacting atoms in the complex. For instance, the O43-H22 distance increased significantly from its gas-phase value of 2.58 Å to 3.31 Å in DMF solvent. The H35-Cl31 bond length increased to 4.08 Å from its gas-phase value of 2.74 Å. However, QTAIM analysis identifies H37-Cl31 and O43-H16 interactions with electron densities (ρ(r)) of 0.0074 and 0.0077 au, respectively. These interactions contribute to binding DMF to the ionic liquid in the DMF solvent. A comparison showed the reduced ρ(r) values, compared to those in the gas phase, indicate that the interactions are weaker and are primarily of van der Waals type in nature.

XYZ Coordinates for the gas phase optimised structures at B3LYP-D3/6-31++G(d,p)

[Bmim][SCN]-DMF

E(B3LYP-D3) = -1163,205153 Hartree

C	-1.03459400	-1.27989300	-0.66481700
C	-0.33033200	0.57450900	-1.63577700
C	-0.00215900	0.63824500	-0.31677200
H	-1.51650000	-2.22744000	-0.47767200
H	-0.22489800	1.28603200	-2.43672700
H	0.49104100	1.40732300	0.25262500
N	-0.97236400	-0.63471700	-1.83123200
C	-1.61334700	-1.09304400	-3.06711500
H	-1.74730100	-0.23071800	-3.71514100
H	-0.99578900	-1.84931700	-3.55280900
H	-2.59058700	-1.49742500	-2.80673300
N	-0.44564900	-0.53512500	0.27185000
C	-0.48941200	-0.82274200	1.71673900
H	-0.74440600	-1.87779300	1.81904100
H	0.51396100	-0.66429000	2.12008600
C	-1.53683600	0.03811400	2.42281100
H	-1.24383300	1.09437200	2.37173200
H	-2.48256600	-0.06160800	1.88432500
C	-1.72635000	-0.38927000	3.87958700
H	-2.02018200	-1.44414000	3.89694900
H	-0.77348400	-0.31490700	4.42012100
C	-2.79281900	0.44592800	4.59002900
H	-3.76014500	0.34565000	4.08979200
H	-2.92128600	0.12673800	5.62770900
H	-2.52941600	1.50886200	4.59994800
S	-3.56309400	-2.89942800	1.21868600

C	-3.86421600	-1.65342100	0.17207500
N	-3.98481600	-0.76590100	-0.59239100
C	-5.14990200	2.22297500	-1.39917700
H	-4.66624500	3.00591600	-0.81291600
H	-6.12286300	2.59316600	-1.73603900
H	-5.28549500	1.34051600	-0.77077800
C	-3.06567700	2.34090900	-2.67219000
H	-2.81136400	3.09066100	-1.90297400
N	-4.32131000	1.88017800	-2.54714900
C	-4.83378200	0.83732300	-3.42550500
H	-4.16056300	0.72133100	-4.27232500
H	-4.90772900	-0.10024800	-2.86983200
O	-2.24550800	2.00859900	-3.52793900
H	-5.82422300	1.12096100	-3.79250100

[Bmim][Cl]-DMF

E(B3LYP) = -1132,34903 Hartree

C	-0.40354300	-1.90475900	-0.73466200
C	-0.75069700	-4.09138600	-0.78121600
C	-0.95922300	-3.65802000	0.49233500
H	-0.15902400	-0.89723400	-1.10237300
H	-0.81248700	-5.07652300	-1.21235800
H	-1.24770100	-4.19298600	1.38140800
N	-0.40456500	-2.98049000	-1.52891300
C	-0.07995100	-2.94128200	-2.95970400
H	0.15098900	-1.90829600	-3.22623000
H	0.78352600	-3.57802200	-3.15361600
H	-0.93762100	-3.29069100	-3.53492100
N	-0.73187300	-2.29289900	0.50101200
C	-0.92940600	-1.38286000	1.65118200
H	-1.95631500	-1.01870300	1.60176900
H	-0.80459500	-1.98864300	2.55174900
C	0.04478800	-0.20834900	1.63849700
H	1.07426100	-0.57578800	1.72129700
H	-0.01569800	0.32047900	0.68314800
C	-0.26641900	0.77860300	2.76732200
H	-1.31624800	1.07869000	2.69032100
H	-0.15484700	0.28357300	3.74045800
C	0.62951500	2.01688800	2.70844100
H	0.51164700	2.53706900	1.75361800
H	0.38833500	2.72178300	3.50899000
H	1.68675400	1.75232500	2.80671400
Cl	0.37230500	0.66527800	-2.42538800
C	-2.65869400	3.32079500	1.30800100
H	-3.25753900	4.20021600	1.04925200
H	-3.28562000	2.60371400	1.83417300

H	-1.84401400	3.64134600	1.96596300
C	-1.32356600	3.52937400	-0.78081700
H	-1.92922900	4.33024700	-1.21928300
H	-0.50346500	3.98673400	-0.21804200
H	-0.88853800	2.91758400	-1.57149900
N	-2.13061900	2.70073500	0.10592500
C	-2.39094200	1.40534200	-0.18964600
H	-1.94187600	1.09141200	-1.14207400
O	-3.02989800	0.62982000	0.52226300

[Bmpym][Cl]-DMF

E(B3LYP) = -1118,709602 Hartree

C	-0.82172000	-2.98577400	-0.60909000
C	-1.44134900	-0.77025500	-0.04996400
C	-1.60462100	-1.58976100	1.23555600
C	-1.12657200	-3.02596100	0.88769200
H	-1.72872300	-3.17284800	-1.18647600
H	-0.01497600	-3.63905800	-0.94253000
H	-1.08097500	0.24513900	0.08109500
H	-2.36988400	-0.77158200	-0.62174800
H	-1.02741400	-1.17142500	2.06331900
H	-2.65472200	-1.58078600	1.52769600
H	-0.24692500	-3.30375600	1.47331200
H	-1.89798400	-3.77086900	1.08253500
N	-0.43964700	-1.54168500	-0.90258700
C	-0.60077000	-1.24251100	-2.36446400
H	-1.60171700	-1.55919200	-2.65604200
H	-0.49025700	-0.17335500	-2.51918500
H	0.16013800	-1.79887200	-2.91347900
C	0.98121200	-1.26810200	-0.45101500
H	1.59514800	-2.05879700	-0.88540700
H	0.99523500	-1.40082800	0.63203500
C	1.52209700	0.11187500	-0.82908400
H	0.75735400	0.87925100	-0.68964400
H	1.77154400	0.13088200	-1.89410500
C	2.77028100	0.47456500	-0.01131800
H	3.06841700	1.49131800	-0.28550000
H	2.50915800	0.51481600	1.05363800
C	3.95511600	-0.47414900	-0.21839000
H	4.84026300	-0.12233000	0.31751700
H	3.74335300	-1.48588500	0.14111500
H	4.21973200	-0.54888800	-1.27824700
Cl	-3.95628200	-2.12962600	-1.86446400
C	-4.84989900	1.39354400	-2.07218000
H	-4.97025200	1.86982400	-1.09780000
H	-5.49579100	1.90502600	-2.79229300

H	-5.13959200	0.34231500	-1.99503400
C	-3.14419400	0.88402800	-3.79069600
H	-3.37300000	-0.18449900	-3.76067900
H	-3.74751600	1.36043000	-4.56921200
H	-2.09075000	1.04239900	-4.01137200
C	-2.49429000	1.93217900	-1.67830600
H	-2.90112100	2.33970200	-0.73604300
N	-3.45784700	1.48312400	-2.49926000
O	-1.28051000	1.91472000	-1.88709700