Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

The interactions are demonstrated in the **Figure S1 (a) and (b),** anions and water molecules were only demonstrated for a central cationic moiety in order to facilitate the visualization of interactions in [DBMIM][2Br]•[2H_2O].

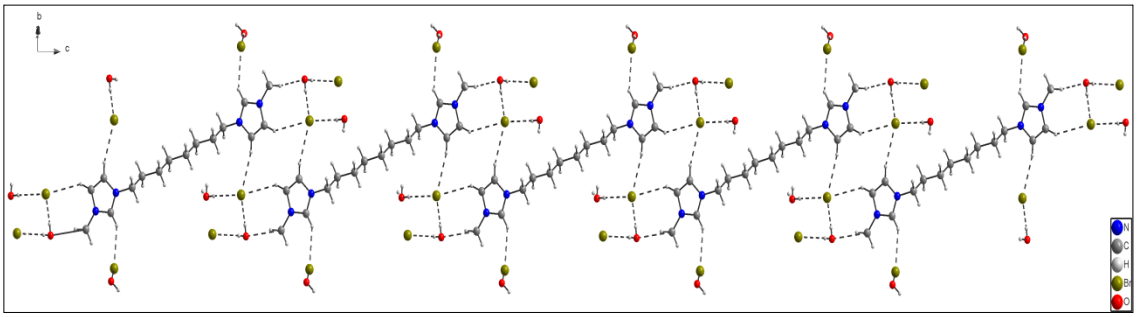
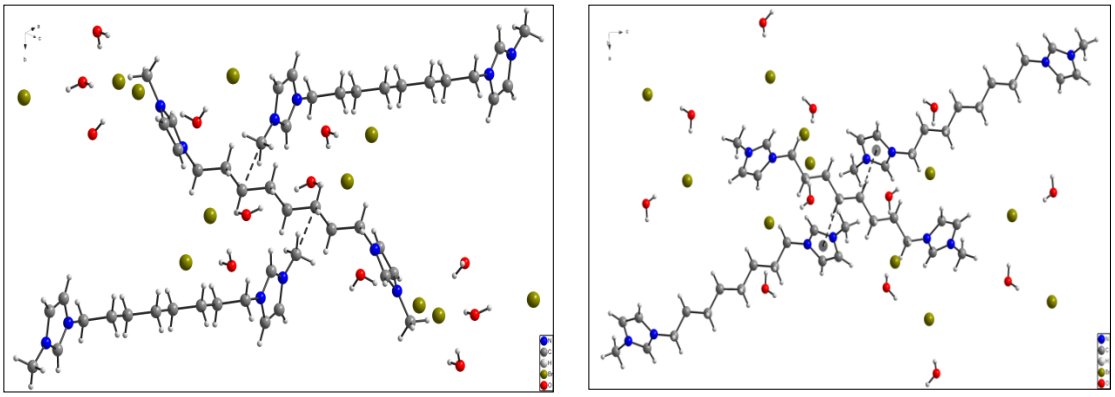


Figure S1. Interactions among water, bromide and imidazolium ring in the crystalline structure of [DBMIM][2Br]•[2H_2O] performed by Diamond Crystal and Molecular Structure visualization. [1]



(a) **(b)**

Figure S2. (a) C-H interactions between two cationic moieties and (**b**) C-H···π interactions between two cationic moieties performed by Diamond Crystal and Molecular Structure visualization. [1]

In the **Figure S3(a)** is showed the PVD of dication and at **Figure S3(b)** is showed the PVD of each anion that are around the dication for [DBMIM][2BF_4]. The **Figure S4** demonstrates the contact surface of dication and a specific anion.

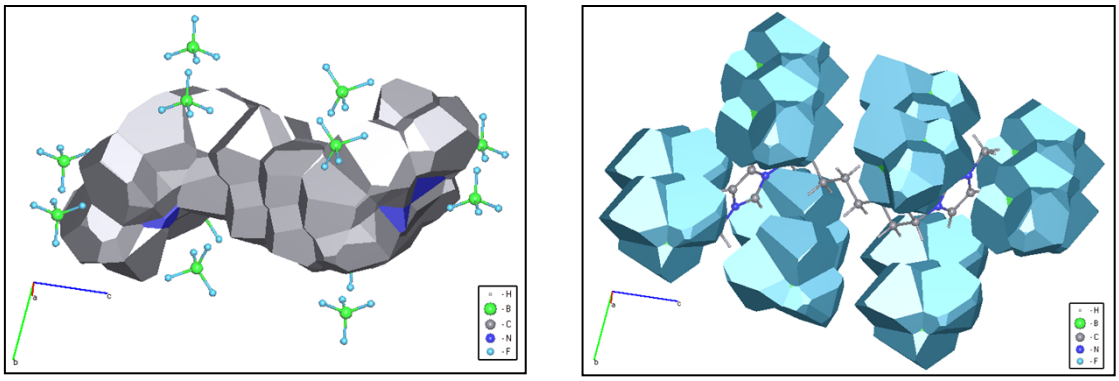


Figura S3. **(a)** VDP for cation of [DBMIM][2BF$_4$]. **(b)** VDP for anions of IL [DBMIM][2BF$_4$] by TOPOS. [2]

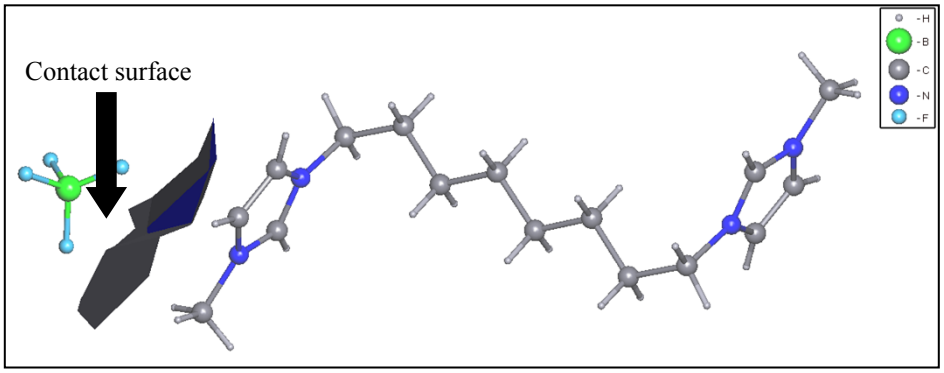


Figure S4. Examples of contact surfaces between dication and anion of IL [DBMIM][2BF$_4$].[2]

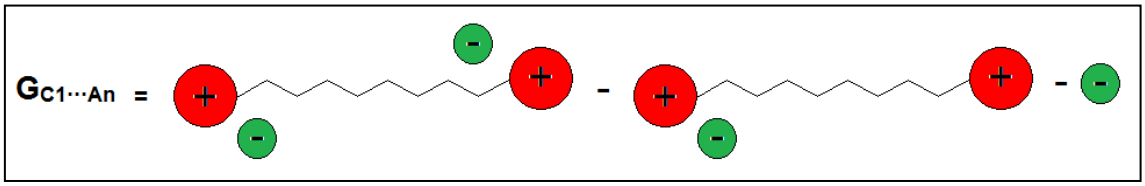


Figure S5 (a) shows schematic representation of calculation to $G_{C1\cdots An}$ for cation/anion interaction in [DBMIM][2BF$_4$] and/or [DBMIM][2Br]•[2H$_2$O].

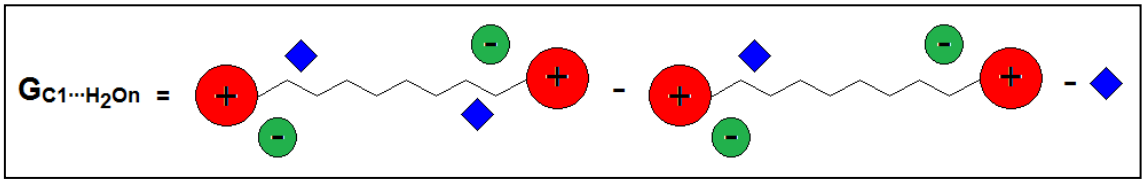


Figure S5. (b) Schematic representation of calculation to energy for water interactions with [DBMIM][2Br]•[2H$_2$O].

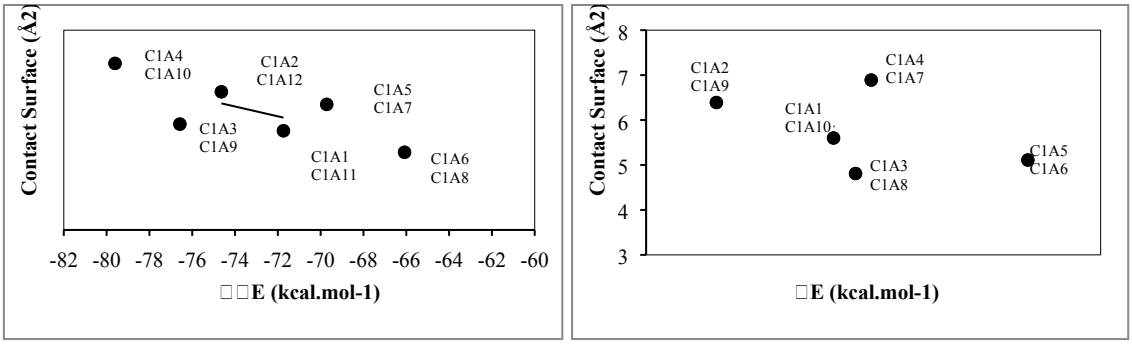


Figure S6. Graphic that demonstrate the interaction energy *versus* surface area in: **(a)** [DBMIM][2BF_4]. Eq. y = -0.6163x – 30.158; r = 0.77. **(b)** [DBMIM][2Br]•[2H_2O]. Eq. y = y = -0.0544x + 1.6314; r = 0.46.

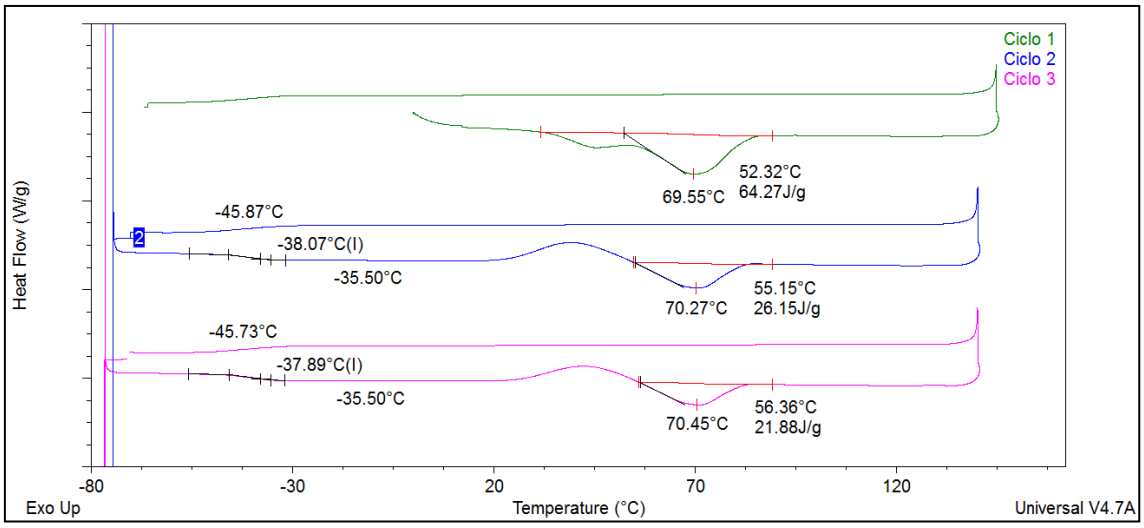


Figure S7. Thermogram of [DBMIM][2BF_4] obtained by DSC.

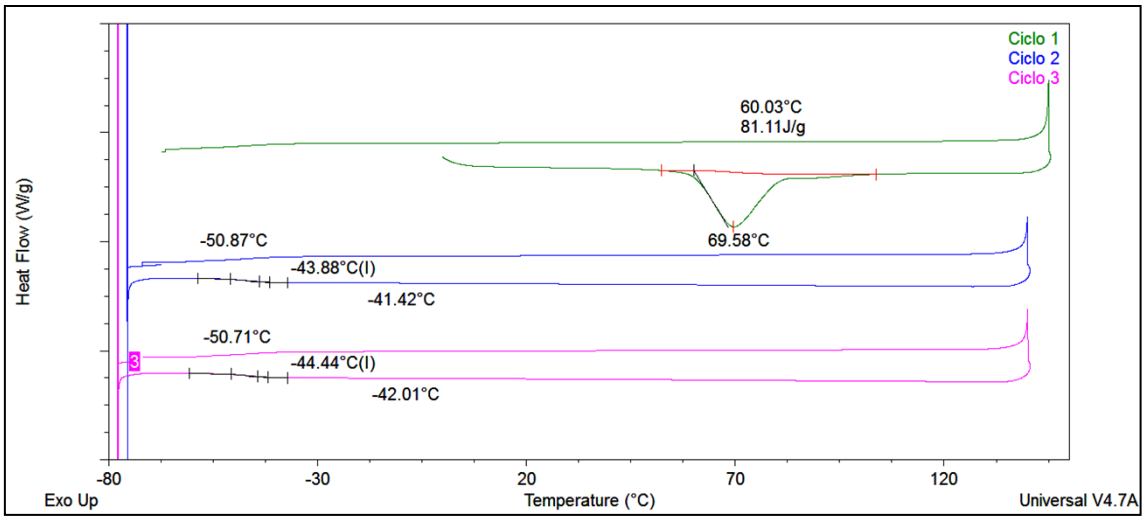


Figure S8. Thermogram of [DBMIM][2Br]•[H_2O] obtained by DSC.

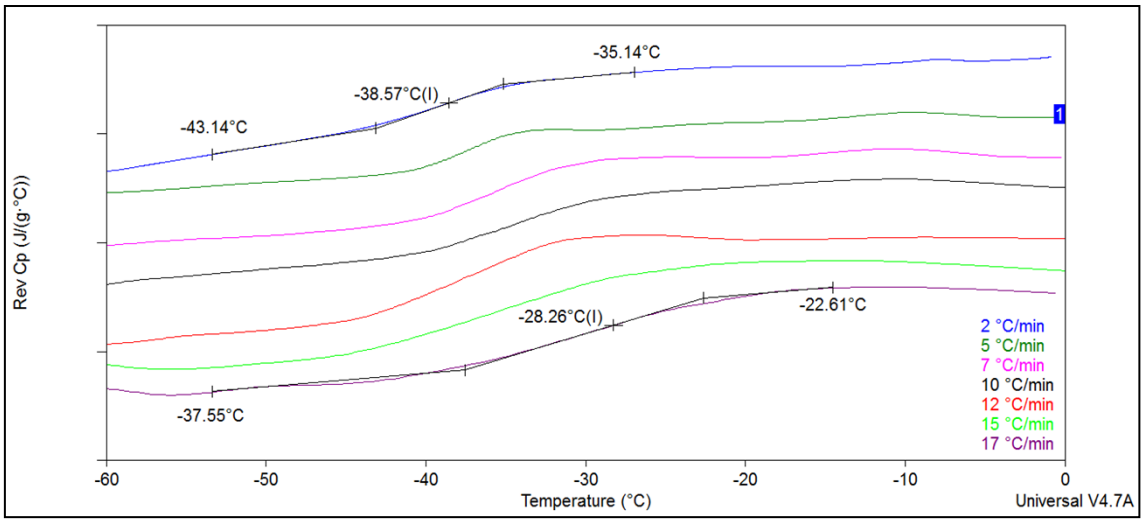


Figure S9. Analysis of amorphous percent by DSC for [DBMIM][2BF_4].

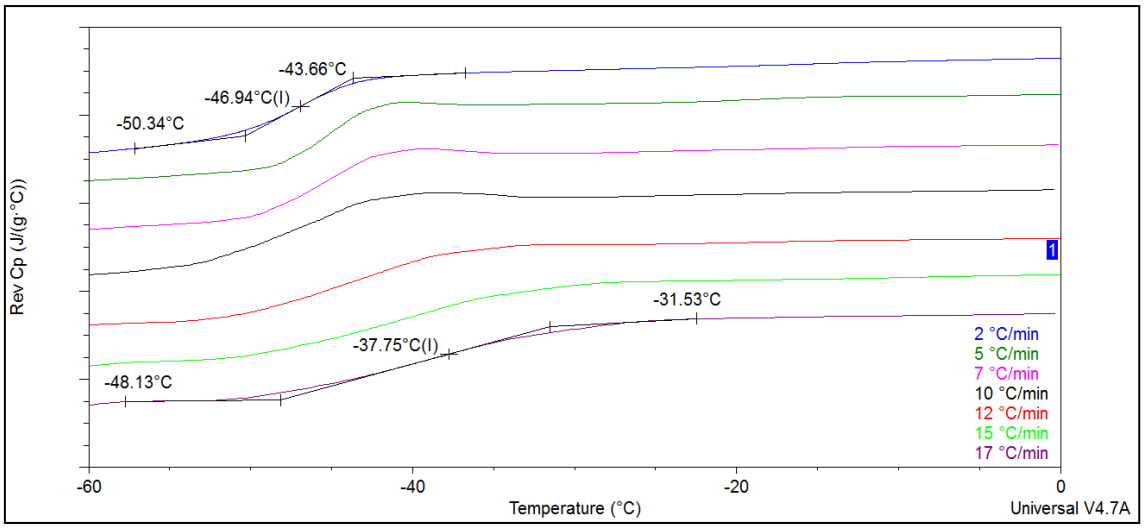


Figure S10. Analysis of amorphous percent by DSC for [DBMIM][2Br]•[H_2O].

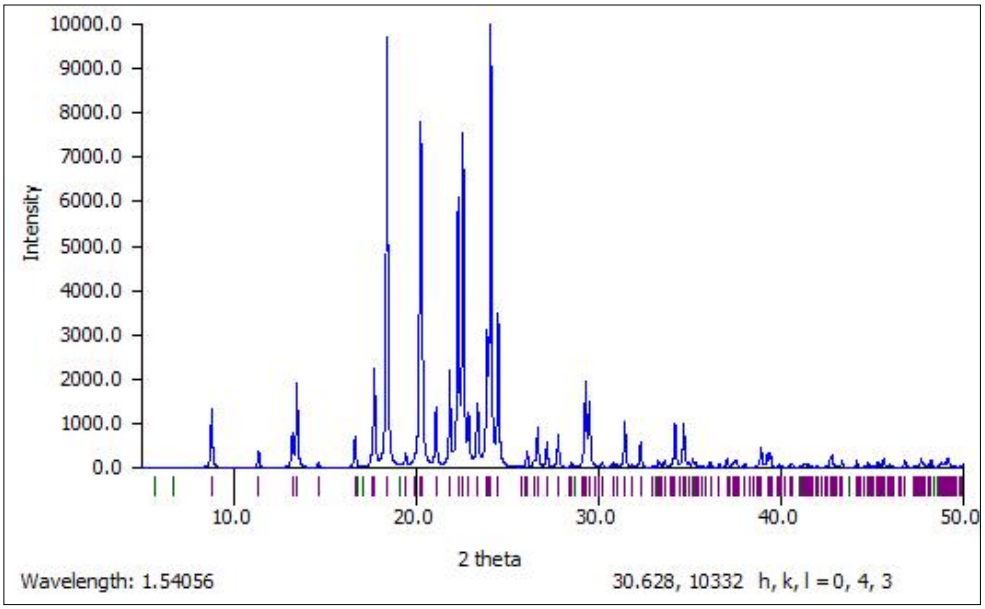


Figure S11. Symulated x-ray powder diffraction of [DBMIM][2BF_4].

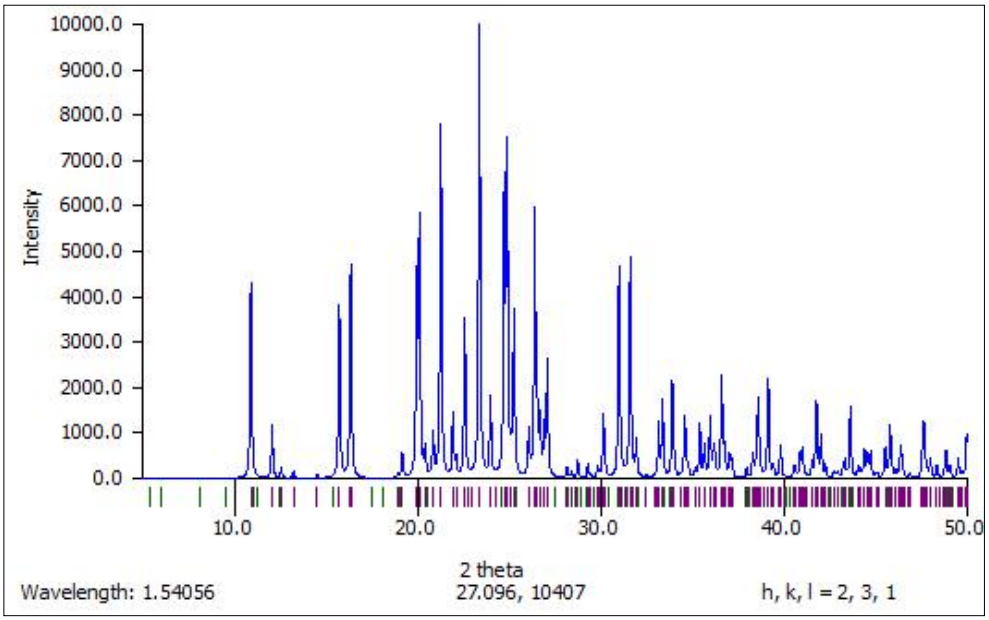


Figure S12. Symulated x-ray powder diffraction of [DBMIM][2Br]•[2H_2O].

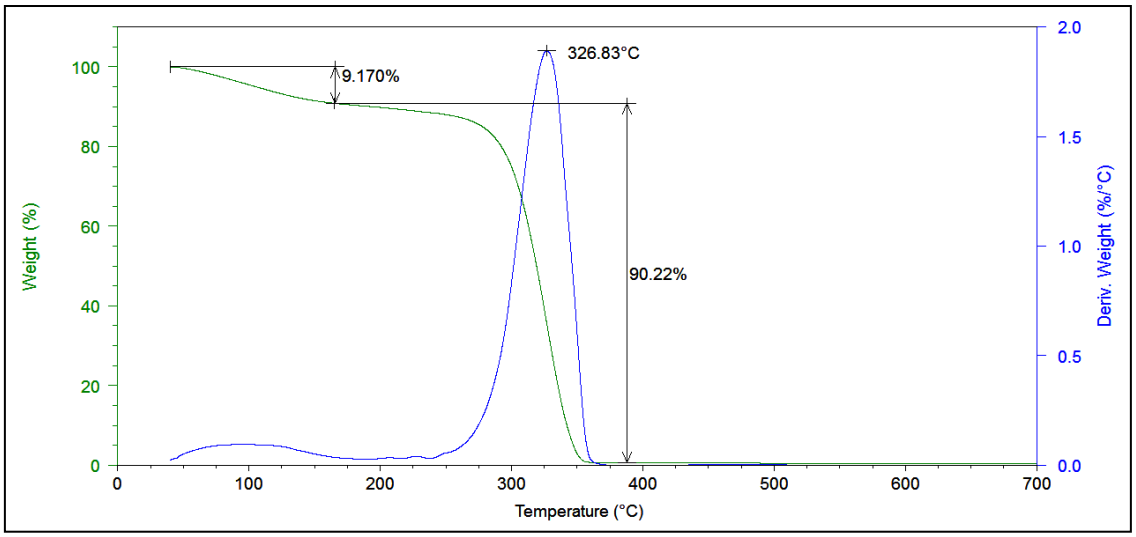


Figure S13. Termogravimetric analysis of [DBMIM][2Br]•[H_2O].

REFERENCES

[1] Dr. Putz, H., Dr. Brandenburg GbR, K., "Diamond - Crystal and Molecular Structure Visualization Crystal Impact." Bonn, Germany, http://www.crystalimpact.com/diamond.

[2] A. P. Blatov, V. A., Shevchenko, "TOPOS® version 4.0 software." Samara State University, Samara, Russia, http://www.topos.ssu.samara.ru.