Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information for

Anion pairs in room temperature ionic liquids predicted by molecular dynamics simulation, verified by spectroscopic characterization

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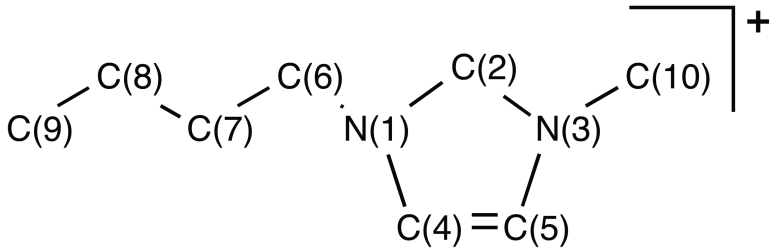

Fig. S1 Chemical structure of $BMIM^+$ with labeled atoms as used throughout the paper.

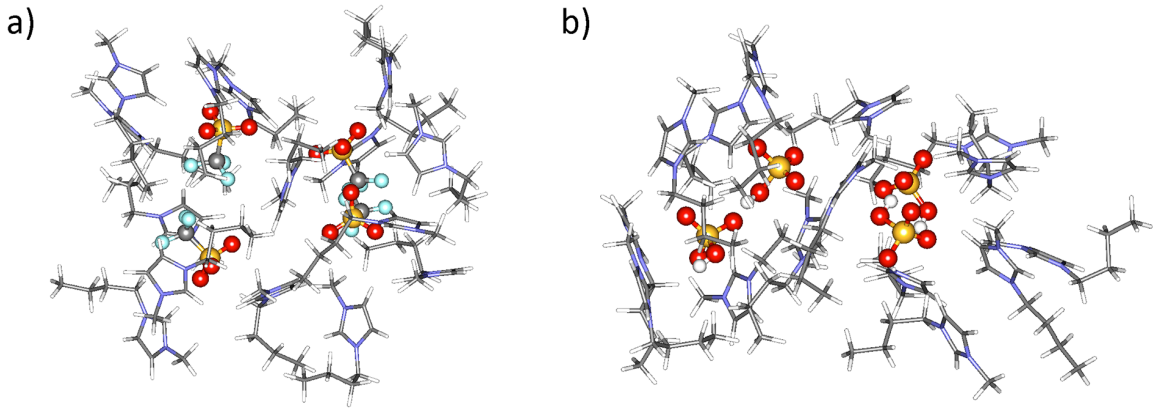

Fig. S2 MD simulation snapshots of a) BMIM OTf and b) BMIM HSO_4. The snapshots show two neighboring anion pairs and their cation cages. Cations are shown with stick model whereas anions are shown with ball and stick model. Carbon atoms are shown in grey, nitrogen atoms in blue, oxygen atoms in red, sulfur atoms in orange, fluorine atoms in light blue, and hydrogen atoms in white.

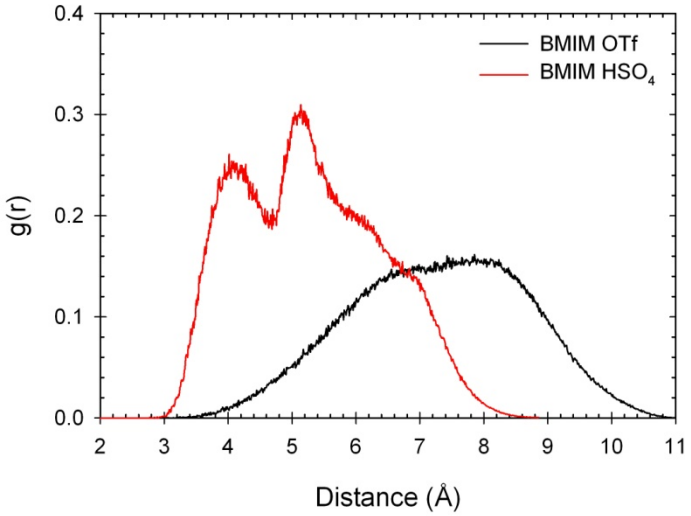

Fig. S3 Radial distribution functions between oxygen atoms of the SO_3 groups of two anions involved in an anion pair. For BMIM OTf, two anions are considered to form a pair if the distance between their C atoms is shorter than the position of the first minimum in the C-C RDF. For BMIM HSO_4, two anions are considered to form a pair if the distance between the H atom of one anion and any of the O atoms of the second anion is shorter than the position of the first minimum in the H-O RDF.

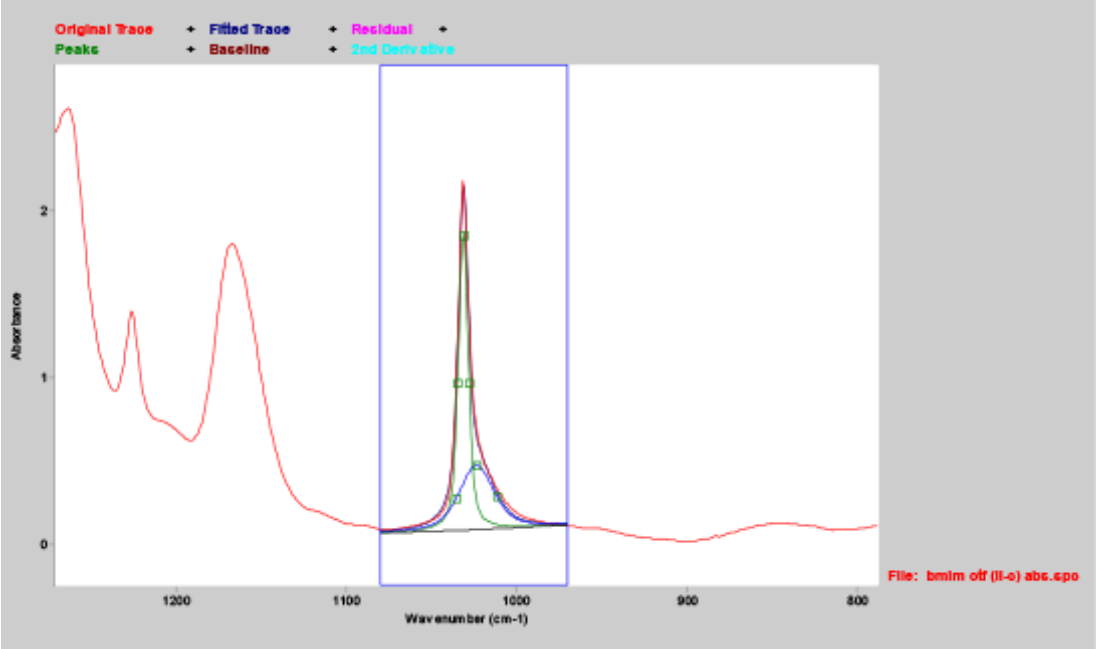

Fig. S4 Deconvolution of the envelop curve at 1028 cm^{-1} in the ATR-FTIR spectrum of BMIM OTf (enlarged region of Fig. 3a in the main manuscript); screenshot from deconvolution using Grams/32 AI.

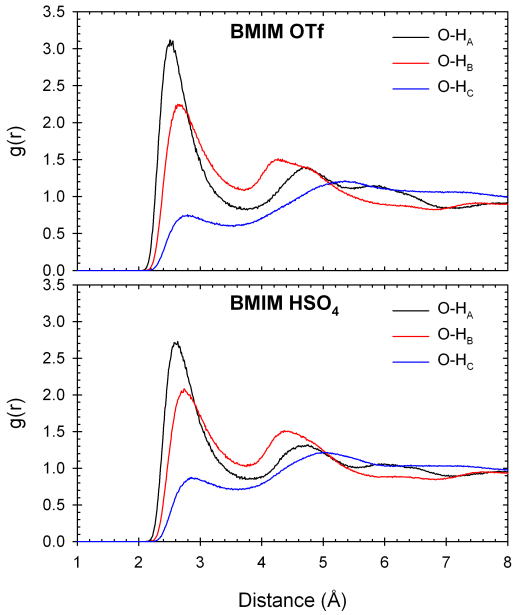

Fig. S5 Cation-anion radial distribution functions between oxygen atoms of the SO_3 group and hydrogen atoms on carbon atoms of the imidazolium ring (H_A), on carbon atoms directly adjacent to the ring (H_B), or on other carbon atoms (H_C) from MD simulations of (top) BMIM OTf and (bottom) BMIM HSO_4.

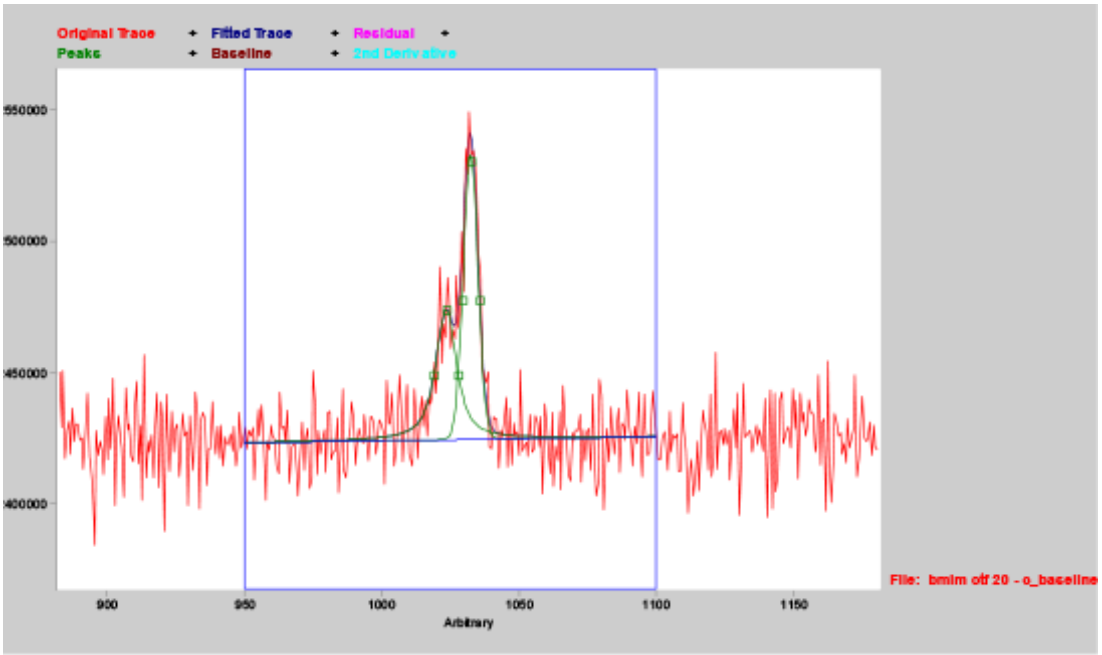

Fig. S6 Deconvolution of the envelop curve at 1032 cm^{-1} in the Raman spectrum of BMIM OTf (enlarged region of Fig. 5a in the main manuscript); screenshot from deconvolution using Grams/32 AI.

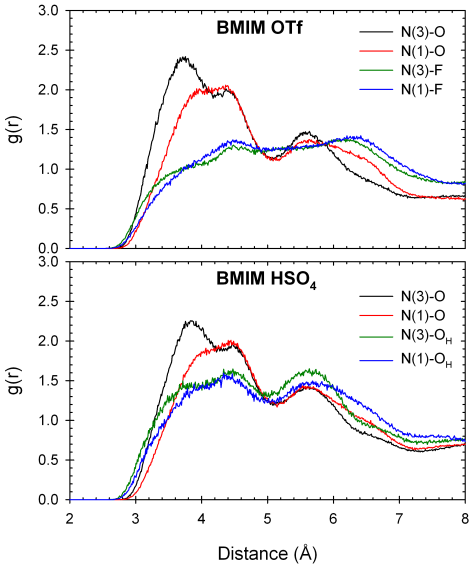

Fig. S7 Cation-anion radial distribution functions from MD simulations of (top) BMIM OTf and (bottom) BMIM HSO_4.

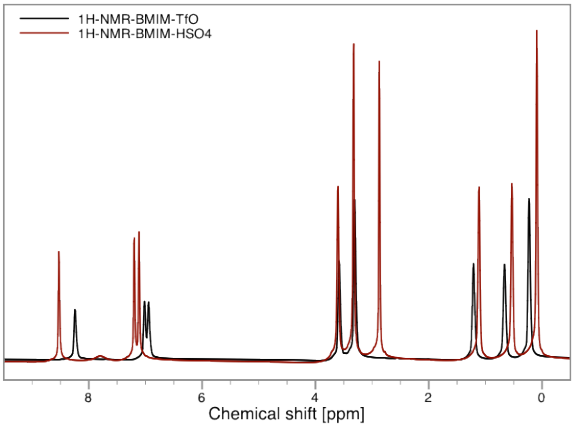

Fig. S8 ^{1}H NMR data of BMIM OTf (black) and BMIM HSO_4 (red).

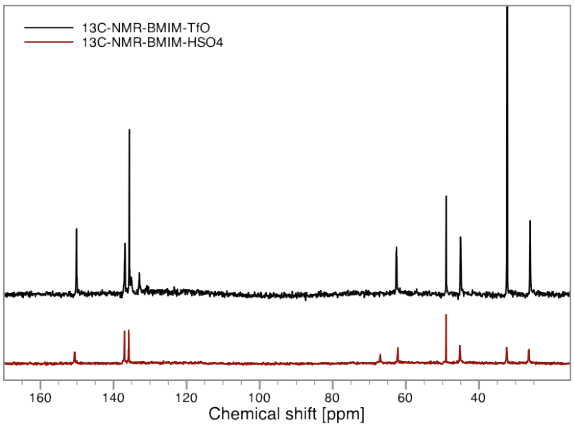

Fig. S9 ^{13}C NMR data of BMIM OTf (black) and BMIM HSO_4 (red).