Electronic Supplementary Information

Effect of protonation on the solvation structure of solute *N*-butylamine in an aprotic ionic liquid

Kei Hashimoto,[a] Kenta Fujii,[b,] Koji Ohara,[c] and Mitsuhiro Shibayama,[d,]**

[a.]Yokohama National University, 79-5 Tokiwadai Hodogaya-ku Yokohama, Kanagawa 240-8501, Japan

[b.]Graduate School of Sciences and Technology for Innovation, Yamaguchi University, 2-16-1 Tokiwadai, Ube, Yamaguchi 755-8611, Japan. E-mail: k-fujii@yamaguchi-u.ac.jp

[c.]Japan Synchrotron Radiation Research Institute (JASRI), 1-1-1 Koto, Sayogun Sayocho, Hyogo, 679-5198, Japan

[d.]Institute for Solid State Physics, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan. E-mail: sibayama@issp.u-tokyo.ac.jp

Table S1. Compositions and densities of the systems for the MD simulations.

Solute species (concentration)[a]	Density / g cm^{-3}		Solute	Cation	Anion
	MD[b]	Exp[c]			
$BuNH_2$ (15 mol%)	1.537	1.475	45	256	256
$BuNH_2$ (30 mol%)	1.496	1.414	110	256	256
$BuNH_3^+$ (30 mol%)	1.607	1.501	110	256	366

[a] Mol fraction of solute in IL, $[C_2mIm][TFSA]$

[b] Densities obtained from MD simulations.

[c] Densities obtained from experiments.

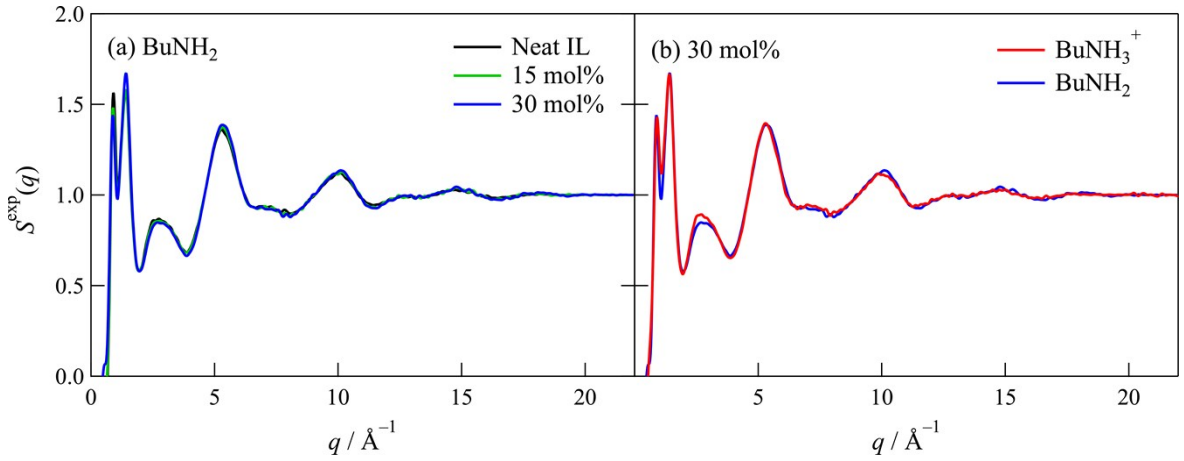

Fig. S1. $S^{exp}(q)$'s for the (a) 0–30 mol% $BuNH_2$ and (b) 30 mol% $BuNH_3^+$ in $[C_2mIm][TFSA]$ solutions in the whole q-range examined in this work.

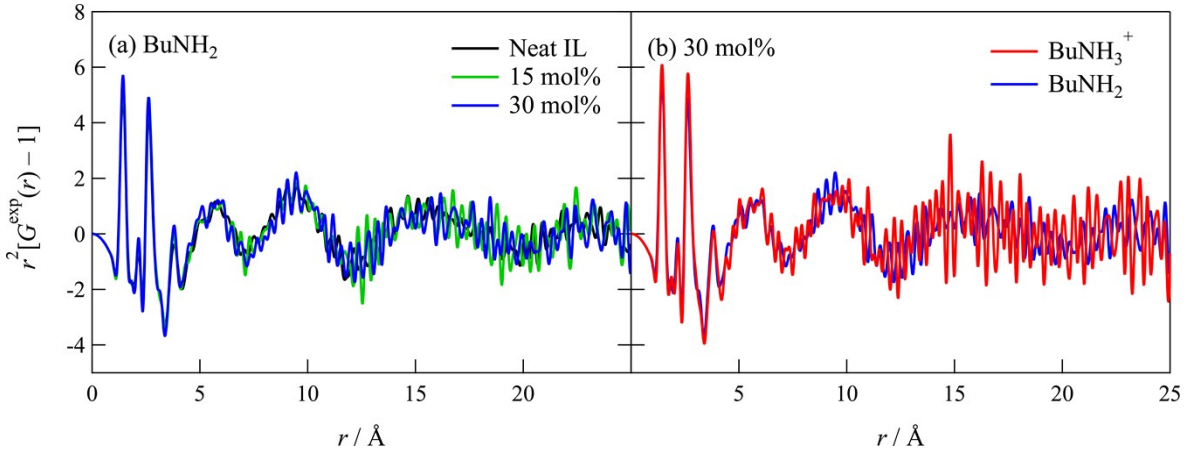

Figure S2. $r^2[G(r) - 1]$'s for the (a) 0–30 mol% $BuNH_2$ and (b) 30 mol% $BuNH_3^+$ in $[C_2mIm][TFSA]$ solutions in the whole r-range examined in this work.

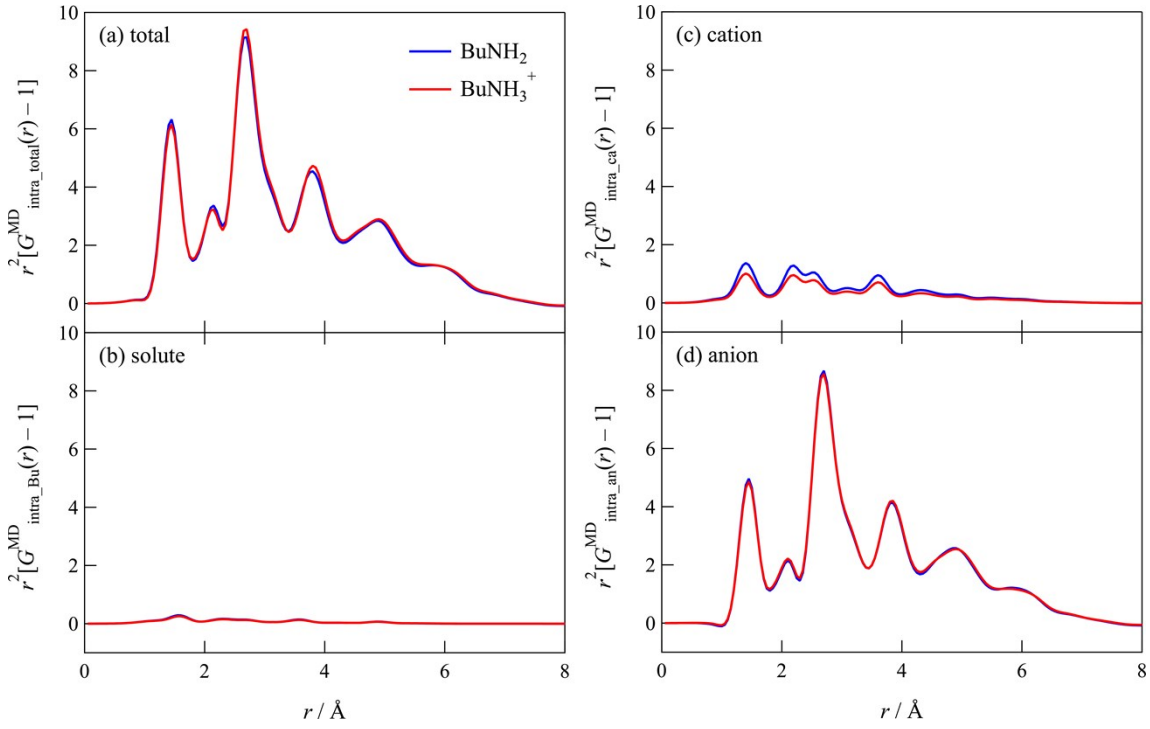

Figure S3. X-ray weighted (a) $G^{MD}_{intra\_total}(r)$, as a form of $r^2[G(r) - 1]$ obtained from MD simulations for 30 mol% $BuNH_2$ and $BuNH_3^+$ in $[C_2mIm][TFSA]$ solutions, together with the partial $G^{MD}_{intra}(r)$'s for (b) solutes ($BuNH_2$ and $BuNH_3^+$): $r^2[G^{MD}_{intra\_Bu}(r) - 1]$, (c) C_2mIm^+ cation: $r^2[G^{MD}_{intra\_ca}(r) - 1]$, and (d) $TFSA^-$ anion: $r^2[G^{MD}_{intra\_an}(r) - 1]$ interactions.

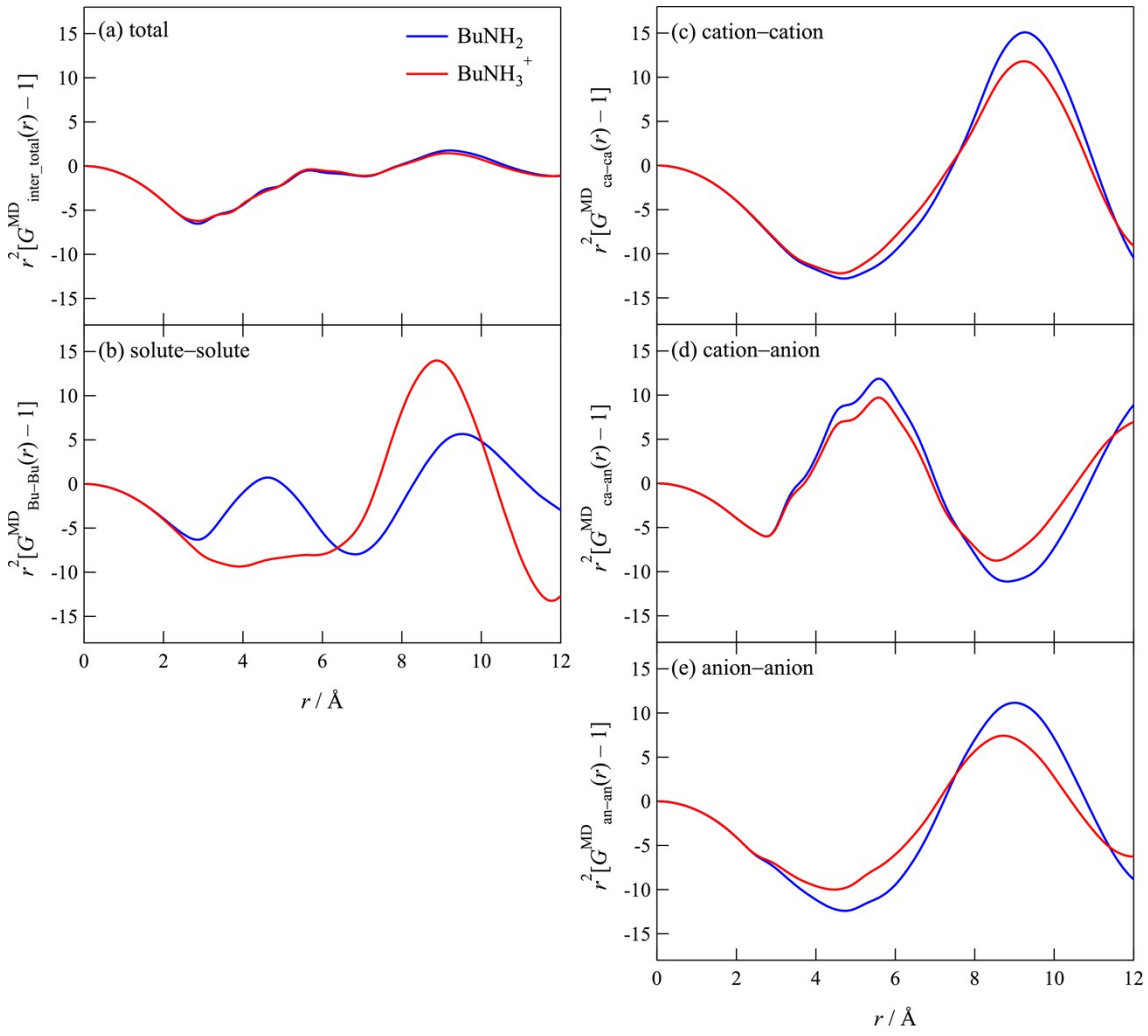

Figure S4. X-ray weighted (a) $G^{MD}_{inter\_total}(r)$, as a form of $r^2[G(r) - 1]$ obtained from MD simulations for 30 mol% $BuNH_2$ and $BuNH_3^+$ in $[C_2mIm^+][TFSA^-]$ solutions, together with the partial $G^{MD}_{inter}(r)$'s for (b) solute−solute: $r^2[G^{MD}_{Bu-Bu}(r) - 1]$, (c) cation−cation: $r^2[G^{MD}_{ca-ca}(r) - 1]$, (d) cation−anion: $r^2[G^{MD}_{ca-an}(r) - 1]$, and (e) anion−anion: $r^2[G^{MD}_{an-an}(r) - 1]$ interactions.