THE JOURNAL OF PHYSICAL CHEMISTRY B

ADDITION/CORRECTION

pubs.acs.org/JPCB

What is the Origin of the Prepeak in the X-ray Scattering of Imidazolium-Based Room-Temperature Ionic Liquids? [*The Journal of Physical Chemistry B* **2010**, *114*, 16838–16846 DOI: 10.1021/jp108545z]. Harsha V. R. Annapureddy, Hemant K. Kashyap, Pablo M. De Biase, and Claudio J. Margulis*

This document presents a correction/clarification to Figure 11 in the original article. While the text in section 3.3 of the original article indicates that what is plotted in Figure 11a,b are the form factor weighted atomic subcomponents of $S(q)$, what was actually plotted in that particular figure is

$$\int_0^\infty 4\pi r^2 (g_{ij}(r) - 1)\frac{\sin qr}{qr}\,dr$$

These functions are not weighted by corresponding form factors.

Instead, Figure 1 in the current document shows the properly weighted version of these subcomponents as derived from the following equation:

$$\frac{\rho_o x_i x_j f_i(q) f_j(q) \int_0^\infty 4\pi r^2 (g_{ij}(r) - 1)\frac{\sin qr}{qr}\,dr}{[\sum_i x_i f_i(q)]^2} \quad (1)$$

Figure 1a,b in the current document should be used as a replacement to Figure 11a,b of the original article. All discussions and conclusions of the original article remain correct.

For further clarification, in Figure 2, we show all form factor weighted non-hydrogen contributions to $S(q)$ as derived from eq 1.

Figure 2 shows that, in addition to what is mentioned in the article, at 1.5 $Å^{-1}$ the contribution of C−C, C−N, and C−Cl (or C−F, C−P) subcomponents of $S(q)$ is important. These interactions are either intramolecular or close contact intermolecular.

Figure 2 also shows that C−N and C−C as well as C−F and C−P (or C−Cl) contributions are important to the shoulder peak at 0.9 $Å^{-1}$. As described in the article, cation−cation and anion−anion contributions at this frequency are positive, whereas anion−cation contributions are negative.

Finally, Figure 2 also shows that C−F has a significant negative contribution to the prepeak (i.e., partially cancels the intensity of the prepeak). This overall negative C−F contribution at the prepeak frequency is the result of a positive C_{Head}−F term and a larger negative C_{Tail}−F contribution (results not shown). This is consistent with our

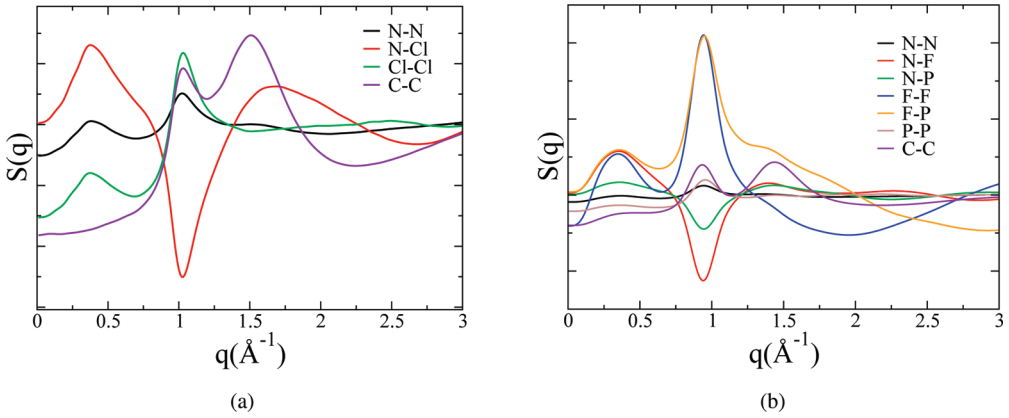

Figure 1. (a) Atomic subcomponents of $S(q)$ in liquid $[C_6MIM][Cl]$ and (b) atomic subcomponents of $S(q)$ in liquid $[C_8MIM][PF_6]$.

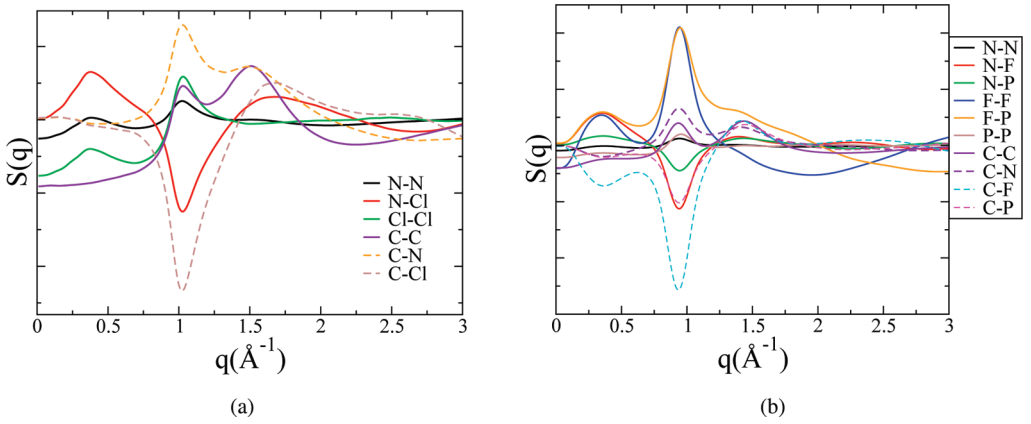

Figure 2. (a) Atomic subcomponents of $S(q)$ in liquid $[C_6MIM][Cl]$ and (b) atomic subcomponents of $S(q)$ in liquid $[C_8MIM][PF_6]$.

explanation in the original article of the prepeak arising from polar groups (anions and cation heads) separated by the longer alkyl tails.

DOI: 10.1021/jp205051t
Published on Web 07/08/2011