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To: Ms. Sunny Sun
Managing Editor, Quantum Beam Science

Date 27th May 2023.

Subject : PDF review manuscript.

Dear Ms. Sunny Sun,

Attached is a revision of our manuscript entitled ***“Review of current software for analyzing total x-ray scattering data from liquids”*** by Leighanne C. Gallington, Stephen K. Wilke, Shinji Kohara and Chris J. Benmore, which we are submitting for consideration for publication in Quantum Beam Science. We thank the reviewers for their recommendation to publish pending minor revisions. The revised manuscript addresses the concern raised by the reviewers as described below. Our changes have been highlighted in red in the marked copy.

We confirm that neither the manuscript nor any parts of its content are currently under consideration for publication in another journal. All authors have approved the manuscript and agree with its submission to Quantum Beam Science.

Regards,

A handwritten signature in black ink that reads 'Chris Benmore'.

Dr. Chris Benmore. Advanced Photon Source, Argonne National Laboratory.

Reviewer 1:

The aim of this review manuscript was to 1) highlight the best practices of the analysis of X-ray scattering data of liquids, and 2) to compare various available software for pair-distribution-function analysis of the X-ray scattering data. The abstract stated clearly these aims and the motivation for the study. The clear motivation for this study is based on the growing number of X-ray scattering data, generated and enabled by the new era of the high-brilliance synchrotron light sources. Thus, the study is very well justified and the aims are highly important and relevant. The results of the study were highly important: the results obtained by the various programs were diverse and showed that there are differences between the analysis programs which the user should be aware of. Thus, this manuscript is highly important for the user community considering the X-ray scattering studies on liquids' structure. So, I recommend publishing of this manuscript with only minor corrections.

We thank reviewer 1 for their feedback and recommendation of publishing this work.

There were some minor issues, that could be checked:

-please include a missing verb/word in the sentence in lines 166-168 ("Hiding errors that could

be due to, for example, severe Q-dependent fluorescence, sample absorption or multiple scattering.")

We have changed this sentence to: "This approach hides errors that could be due to, for example, severe Q-dependent fluorescence, sample absorption or multiple scattering."

-Line 111 and Line 205: the symbols 'c_alfa' (Equation 2) and 'c_beta' (Equation 6) could be explained in the text (or I might have missed the explanation)?

c_α and c_β are the concentrations of atoms of type α and β respectively. We have incorporated this definition into the text as described below.

Line 112 now reads: "where c_α is the concentration of atoms of type α ."

Lines 206-207 now read: "where $n_{\alpha\beta}$ represents the number of atoms of type β that reside between distances r_1 and r_2 from an atom of type α at the origin, c_β is the concentration of atoms of type β , and $g_{\alpha\beta}(r)$ is the Faber-Ziman partial pair distribution function [35] describing α - β pair interactions."

-the use of many terminological words in apostrophes could be perhaps avoided, if possible: these words could be explained better for the reader; including "big-box" (line 219), "small-box" (line 226), "top hat" (line 380)

We have added clarifying text as described below:

Line 220 now reads: "so-called "big-box" (>1000 atoms) atomistic modeling"

Lines 227-229 now read: "'Small-box" (<50 atoms) modelling software, which includes programs such as PDFgui and TOPAS, inherently expect a scaling factor to be applied to $D(r)$ as part of the real-space Rietveld refinement process [42-44]."

Lines 382-383 now read: "*GudrunX* also offers parameters for the so-called "top hat" convolution [60], a Fourier space filtering method used to remove any residual long-wavelength background in $S(Q)$."

-the review is relatively long and the main part of the manuscript is the comparison of the software and their results. So, perhaps the slight shortening of the introductory part (i.e. section 2 of the manuscript) could be considered.

We believe the introductory content in section 2 is crucial to understanding the discussion of software in section 3 and cannot be condensed further without loss of context to the reader. Many reviews are frequently up to 50 pages long. Currently, our review when formatted according to journal guidelines is 21 pages.

Reviewer 2:

Caption of Figure 1:

labels of the left and right panels must be uniformed (always C or always Compton) and defined (mtwf is not defined).

We agree and have updated the right panel of figure 1 to use Compton in lieu of C and MAFF (modified

atomic form factor) in lieu of mtwf (modified total weighting factor).

Line 127:

The maff S(0) value reported in the text is -1.45. the value reported in Figure 2 is -2.0. This unexpected difference should be clarified.

We thank the reviewer for calling our attention to our typo. We have corrected this value to -2.0 in the text.

Lines 166-167:

it seems that the main sentence, supporting the subordinate sentence, is missing.

We have changed this sentence to: "This approach hides errors that could be due to, for example, severe Q-dependent fluorescence, sample absorption or multiple scattering."

Line 410:

Table-1's rows should be better evidenced, because the table is quite confusing.

We have now added borders between the rows of Table 1 to improve readability.

Lines 512-513:

The sentence "The reduced real space resolution for LiquidDiffract and modification function for GudrunX lead to increasing large discrepancies relative to our prior analyses, especially for the 3rd shell" is not immediately clear. Indeed, for GudrunX the nss(3) value is the closest to the original analysis' value.

We thank the reviewer for calling our attention to this error. This sentence has been updated to read: "The reduced real space resolution for LiquidDiffract leads to increasing large discrepancies relative to our prior analyses, especially for the 3rd shell."

The values reported in Table 2 should be expressed with an error, to show quantitatively what are the programs which gives more reliable values, if compared with the original analysis.

We have added the following text to the caption of Table 2: Errors of up to 5% are typical for coordination numbers derived from PDF analyses [2,18].