Corrigendum: On the calculation of x-ray scattering signals from pairwise radial

Dohn, Asmus Ougaard; Biasin, Elisa; Haldrup, Kristoffer; Nielsen, Martin Meedom; Henriksen, Niels
Engholm; Møller, Klaus Braagaard

Published in:
Journal of Physics B: Atomic, Molecular and Optical Physics

Link to article, DOI:
10.1088/0953-4075/49/5/059501

Publication date:
2016

Document Version
Peer reviewed version

Link back to DTU Orbit

Citation (APA):
https://doi.org/10.1088/0953-4075/49/5/059501

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright
owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately
and investigate your claim.
Corrigendum to: "On the Calculation of X-ray Scattering Signals from Pairwise Radial Distribution Functions"

Asmus O. Dohn *, Elisa Biasin², Kristoffer Haldrup², Martin M. Nielsen², Niels E. Henriksen¹, and Klaus B. Møller ††

¹Department of Chemistry, Technical University of Denmark, Kemitorvet 207, 2800, Kgs. Lyngby
²Department of Physics, Technical University of Denmark, Fysikvej 307, 2800, Kgs. Lyngby

November 12, 2015
When we in Eq. (20) split up the scattering signal into contributions from solvent-solvent terms, solute-solvent (cross) terms, and solute-solute terms, each atom (type) belongs to either the solvent or the solute. Hence, the scattering signal contribution from the solute-solvent (cross) terms, Eq. (20b), should read:

\[
S_c(q) = 2 \sum_i^u \sum_m^v f_i(q) f_m(q) \frac{N_i N_m}{V} 4\pi \int_0^{R_{\text{box}}} r^2 [g_{i,m}(r) - 1] \frac{\sin(qr)}{qr} dr \quad (20b)
\]