



Corrigendum: On the calculation of x-ray scattering signals from pairwise radial distribution functions (2015 J. Phys. B: At. Mol. Opt. Phys. 48 244010)

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

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Corrigendum to: "On the Calculation of X-ray Scattering Signals from Pairwise Radial Distribution Functions"

Asmus O. Dohn ^{*1}, Elisa Biasin², Kristoffer Haldrup², Martin M.
Nielsen², Niels E. Henriksen¹, and Klaus B. Møller ^{†1}

¹Department of Chemistry, Technical University of Denmark,
Kemitorvet 207, 2800, Kgs. Lyngby

²Department of Physics, Technical University of Denmark, Fysikvej
307, 2800, Kgs. Lyngby

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* asod@kemi.dtu.dk

† kbmo@kemi.dtu.dk

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:

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