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Erratum: The structure of liquid 1,2 dichloroethane by neutron diffraction. I. Molecular structure, full pair correlation function, and temperature effects [J. Chem. Phys. 87, 7171 (1987)]

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Due to an error in the data corrections and subsequent extrapolation to $Q \rightarrow 0$ of the measured differential cross section ($0.3 \leqslant Q \leqslant 23$), the (extrapolated) small-angle region was incorrectly treated. The low-Q data region was recorrected using a cadmium-rod dataset taken for the same geometrical arrangement as well as an experimental value for the isothermal compressibility (at 298 K) of 1.119×10^{-19} $m^2\,N^{-1}$.[1]

A reanalysis of the structure factors affected by this correction was performed and the corrected estimates [total Fourier transforms and full pair correlation functions $g(r)$] are shown in Figs. 1 and 2.

The abovementioned errors introduced a phase distortion in Figs. 7 of the paper which should be replaced by the two figures given here.

The predictions for the intramolecular structure and temperature-difference effects are not affected by the error in the small-angle data.

Most of the conclusions of the paper pertaining to intermolecular structure are still valid since they were taken on qualitative grounds and compared with a previously reported Monte Carlo simulation. The main effect of the mentioned correction is to shift the most prominent $g(r)$ peak from 8 to ~ 6 Å, with a second maximum ~ 10 Å.

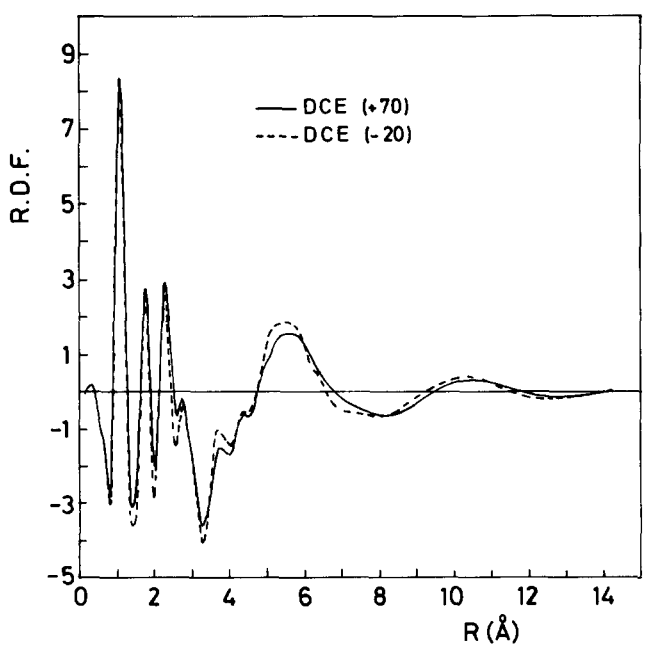

FIG. 1. Total Fourier transforms of the $S_m(Q)$ structure factors at two extreme temperatures.

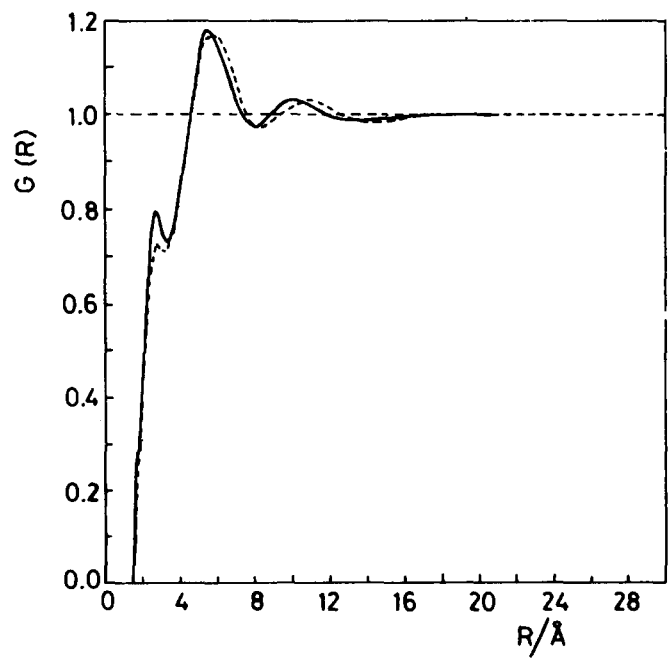

FIG. 2. Full pair correlation functions for $-20\,^{\circ}C$ (full curve) and $+70\,^{\circ}C$ (dashed curve).

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Further work on decomposition of the total $g(r)$ into its pair contributions using chlorine isotopes is, at present, in progress as well as the analysis of the measured correlation function by means of new simulation data.

[1]D. M. Newit and K. W. Weale, J. Chem. Soc. **1951**, 3092.

Erratum: Accurate theoretical modeling of NaCl [J. Chem. Phys. 84, 867 (1986)]

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Misprints have been uncovered in recent papers[1-3] reporting the interaction potentials between halogen anions and alkaline cations. Concerning Ref. 1, Table IV has a misprint: the F coefficient for the $+\ -$ interaction has a wrong sign and should read $+3.994\,29$. Concerning Ref. 2, the potential function, Eq. (10) on page 500, should read

$$V(r) = Z_i Z_j e^2/(4\pi\epsilon_0 r) + (A_{ij} r^{B_{ij}} + C_{ij} r) e^{-D_{ij} r} + E_{ij} r^{-F_{ij}}.$$

Concerning Ref. 3 the correct analytical expression for the $+\ +$ interaction is the one given above. Finally, the potential for the $F^- F^-$ interaction is also incorrectly reported in Ref. 3. Using the analytical expression given above, the following parameters (in a.u.) should be used:

$$A = -28.010\,22,\ B = -4.515\,42,\ C = -0.054\,46,$$
$$D = 0.637\,66,\ E = 23.872\,59,\ F = 5.552\,92.$$

An alternative set is $A = 1.037\,33$, $B = 0.010\,24$, $C = 0.324\,10$, $D = 0.798\,16$, $E = 0.0$, and $F = 0.0$.

We thank Dr. F. Jenc (Philipps-Marburg University) and Dr. V. K. W. Cheng (University of Hong Kong) for having called our attention to problems in Refs. 1, 2, and 3.

[1]P. K. Swaminathan, A. Laaksonen, G. Corongiu, and E. Clementi, J. Chem. Phys. **84**, 495 (1986).
[2]A. Laaksonen and E. Clementi, Mol. Phys. **56**, 495 (1986).
[3]P. K. Swaminathan and E. Clementi, J. Phys. Chem. **91**, 1020 (1987).

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