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Errata: Relativistic Ab-Initio Calculations of the Properties of Ionic Solids

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Relativistic ab-initio calculations of the properties of ionic solids

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Section 2*c*(iii), on the calculation of the functions $\chi_n^{ab}(r)$ damping the inter-ionic dispersive attractions, needs three types of correction, two being of notation.

(1) In all the formulae (2.27)–(2.39), the distance R is that between the pair of interacting ions and should thus be $x_{ab}R$.

(2) Equation (2.34*c*) contained the two errors that $\tilde{P}_5(x)$ on the right-hand side should be $\tilde{P}_6(x)$ and that the denominator in the last term should be 691 200 and not 69120, so that (2.34*c*) should read

$$P_9(x) = \tilde{P}_6(x) + \tfrac{1}{5120}x^7 + \tfrac{1}{46080}x^8 + \tfrac{1}{691\,200}x^9.$$

Equation (2.35) needs to be corrected by replacing both occurrences of $\exp(-d_{a2}R)$

by $\exp(-d_{b1}R)$ so that after replacing R by r, the distance between the interacting pair of ions, this becomes

$$\begin{aligned}\chi_6^{ab}(r) = \{1 + d_{a1}d_{b1}[(d_{a1}/d_{b1}) - (d_{b1}/d_{a1})]^{-5} \\ \times[Q_1(d_{a1}, d_{b1}, r)\exp(-d_{a1}r) - Q_1(d_{b1}, d_{a1}, r)\exp(-d_{b1}r)]\}^2 \\ + \tfrac{2}{9}d_{a1}^2 d_{b1}^2 r^4[(d_{a1}/d_{b1}) - (d_{b1}/d_{a1})]^{-10} \\ \times[Q_2(d_{a1}, d_{b1}, r)\exp(-d_{a1}r) - Q_2(d_{b1}, d_{a1}, r)\exp(-d_{b1}r)]^2.\end{aligned}$$

(3) In equation (2.37), $\chi_8^{ab}(R)$ has been used in two different ways. Retaining its correct definition in equation (2.21) and replacing R by r, (2.37) should read

$$\chi_8^{ab}(r) = [C_8^{DQ}(ab)\chi_8^{DQab}(r) + C_8^{QD}(ab)\chi_8^{QDab}(r)]/C_8(ab)],$$

which differs in that the quantities on the right-hand side previously designated $\chi_8^{ab}(r)$ and $\chi_8^{ba}(r)$ have been replaced by $\chi_8^{DQab}(r)$ and $\chi_8^{QDab}(r)$. The left-hand side of (2.38) should read $\chi_8^{DQab}(r) =$ and not $\chi_8^{ab}(r) =$ so that (2.38) yields the damping function for just that part of the dipole–quadrupole interaction which arises from the interaction of a dipole instantaneously present on ion a with the quadrupole it induces on ion b. Also the two occurrences of both d_{a1} and d_{b1} should be replaced by d_{a2} and d_{b2}, respectively, so that (2.38) should read

$$\begin{aligned}\chi_8^{QDab}(r) = \{1 + [(d_{b2}/d_{a2}) - (d_{a2}/d_{b2})]^{-6} \\ \times[Q_3(d_{a2}, d_{b2}, r)\exp(-d_{a2}r) + Q_4(d_{a2}, d_{b2}, r)\exp(-d_{b2}r)]\}^2 \\ + \tfrac{8}{675}(d_{b2}r)^4[(d_{b2}/d_{a2}) - (d_{a2}/d_{b2})]^{-12} \\ \times[Q_5(d_{a2}, d_{b2}, r)\exp(-d_{a2}r) - Q_6(d_{a2}, d_{b2}, r)\exp(-d_{b2}r)]^2.\end{aligned}$$

The damping function $\chi_8^{QDab}(r)$ is given by interchanging the labels a and b so that $\chi_8^{QDab}(r) = \chi_8^{DQba}(r)$. These typographical errors do not affect the numerical results because the latter were obtained from a computer program which correctly evaluated all the damping functions.

The results for MgO calculated with the damping of the dispersion energy contained slight inaccuracies because there was an error in the data input in the computation of the O^{2-} $2p^5$ 3s state needed to evaluate the O^{2-} dispersion damping parameter d_{a1}. The value of 1.820 in table 3 should be replaced by 1.696. This slightly changes the computed values of D_e, R_e and B in the column headed (6) in table 6 which should be 3014 kJ mol^{-1}, 4.098 au and 18.0×10^{10} N m^{-2}.

I thank Dr A H Harker of AEA Industrial Technology for drawing to my attention some of the inaccuracies in the reported formulae for the dispersion damping functions.