Erratum: Jahn–Teller effect in tetrahedral d 1 metal complexes [J. Chem. Phys. 81, 1861 (1984)]

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collide essentially only with solid surfaces. Let $p(l_s)$ be the probability that Knudsen limit trajectories exceed l_s from random starting positions in the pore space. The probability for no Knudsen limit surface collisions occuring between distances l_s and $l_s + dl_s$ is $1 - K dl_s$, where K is a positive constant. Since averaging for $P(l_s)$ is taken over a macroscopically homogeneous and isotropic volume, the probability $P(l_s + dl_s)$ is equal to the product of the independent probabilities $P(l_s)$ and $P(dl_s)$. This gives

$$\frac{d}{dl_s} P(l_s) = -KP(l_s) \tag{5}$$

which upon integration results in $P(l_s) = \exp(-Kl_s)$. The distribution of interest is

$$p(l_s) = \frac{-d}{dl_s} P(l_s) = \frac{1}{r_0} e^{-l_s/r_0}, \tag{6}$$

where r_0, equal to the mean value of l_s, replaces $1/K$.

The porous media mean free path l_e results from the integration of the product of Eqs. (4b) and (6) over all possible l_s,

$$l_e = \frac{l_0}{r_0} \int_0^\infty \left\{ \exp\left(\frac{-l_s}{r_0}\right) - \exp\left[-l_s\left(\frac{l_0 + r_0}{l_0 r_0}\right)\right]\right\} dl_s \tag{7a}$$

$$= \frac{l_0 r_0}{l_0 + r_0}. \tag{7b}$$

rearranging Eq. (7b) shows $l_e^{-1} = l_0^{-1} + r_0^{-1}$. This form of l_e^{-1} is analogous to those of free path models for electron and phonon diffusion in solids.[8] In each case additivity of the inverses of interparticle effects and particle-medium effects result.

Combining Eqs. (1) and (7b) provide the final expressions

$$D_e = \tfrac{1}{3} f(\epsilon)\bar{v} \frac{l_0 r_0}{l_0 + r_0} = \frac{f(\epsilon) D_0}{1 + \mathrm{Kn}} \tag{8a}$$

and

$$D_e^{-1} = [f(\epsilon)D_0]^{-1} + [\tfrac{1}{3} f(\epsilon)\bar{v} r_0]^{-1}. \tag{8b}$$

The Knudsen number Kn in Eq. (8a) is the ratio l_0/r_0. By equating the last term in Eq. (8b) to D_K^{-1}, the inverse of the Knudsen diffusivity, the Bosanquet result is obtained. The Bosanquet formula, $D_e^{-1} = [f(\epsilon)D_0]^{-1} + D_K^{-1}$, is applicable in the Knudsen limit ($\mathrm{Kn} \gg 1$), the continuum limit ($\mathrm{Kn} \ll 1$), as well as intermediate ranges of Kn. The derivation presented here demonstrates that the Bosanquet result arises through the influence of pore surface collisions on the free path distribution.

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The relationships (10) were erroneously evaluated. The right expressions are

$$A_2 = \frac{1}{R^2}(e_\sigma - e_\pi), \tag{10a}$$

$$b_{\epsilon\epsilon} = -\frac{\sqrt{3}}{R^2}\left(e_\sigma - \frac{5}{3} e_\pi\right), \tag{10b}$$

$$b_{\tau\tau} = \frac{3}{2R^2}\left(e_\sigma - \frac{5}{3} e_\pi\right), \tag{10c}$$

$$c_{\tau\tau} = \frac{7}{6R^2}\left(e_\sigma - \frac{1}{3} e_\pi\right). \tag{10d}$$

Accordingly column I of Table I should read

$e_\sigma = 6655\ \mathrm{cm}^{-1}$,
$e_\pi = 520\ \mathrm{cm}^{-1}$,
$A_1 = 458\ \mathrm{cm}^{-1}/\text{Å}$,
$A_2 = 1340\ \mathrm{cm}^{-1}/\text{Å}^2$,
$E_{JT} = 37\ \mathrm{cm}^{-1}$,
$b = -4946\ \mathrm{cm}^{-1}/\text{Å}$,
$c = -2397\ \mathrm{cm}^{-1}/\text{Å}$,
$c_1 = -4814\ \mathrm{cm}^{-1}/\text{Å}$.

All conclusions of the paper remain still valid.