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Erratum: On improved WKB (uniform asymptotic) quantum conditions, Dunham corrections, the Langer modification, and RKR potentials

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$$\langle i\rangle = S/R + (R-1)^2/4R \quad . \tag{7}$$

Notice that $\langle f\rangle - S = \langle i\rangle - S/R$, so that $\langle f\rangle$ in absorption cannot be found from replacement by $R\langle i\rangle$ for emission. For the linear interaction ($R=1$), $\langle i\rangle = \langle f\rangle = S$, a well known result. For the quadratic interaction ($S=0$), $\langle i\rangle = \langle f\rangle = (R-1)^2/4R$. The expressions for $\langle i\rangle$ and $\langle f\rangle$, [Eqs. (4) and (7)] are in agreement with those expected from moment analysis,[5] namely that

$$M_{\alpha 1} = E_{zp} + \langle f\rangle R\hbar\omega \tag{8a}$$

$$M_{\epsilon 1} = E_{zp} - \langle i\rangle \hbar\omega, \tag{8b}$$

where E_{zp} is the zero-phonon energy (the energy of the $i=0 \rightarrow f=0$ transition): $E_{zp} = E_0 + (1/2)[R(1-2S)-1]\hbar\omega$, and the Ms are the first moments of the band shapes. The Stokes shift (Δ), the difference between the absorption and emission band centroids, is

$$\Delta = (R^2+1)S\hbar\omega R^{-1} + (1/4)(R+1)(R^2-1)\hbar\omega R^{-1} \quad . \tag{9}$$

If one defines $S_\epsilon \equiv S_\alpha/R$ as the "Huang–Rhys factor" appropriate to emission and S_α (equal to S, as used above) as the "Huang–Rhys factor" appropriate to absorption, then Eqs. (4) and (7) assume the symmetrical form

$$\langle f\rangle = S_\alpha + (R-1)^2/4R$$

$$\langle i\rangle = S_\epsilon + (R-1)^2/4R \quad .$$

Equation (3) for $\langle f\rangle$ could, in principle, be calculated as a function of temperature by using the finite temperature forms of $\langle \chi_{at} | \chi_{bf}\rangle$ and B_{ai} and noting that the denominator reduces to $C_{ab}|\langle \phi_a | R | \phi_b\rangle|^2$.

[1]M. D. Sturge, Phys. Rev. B 8, 6 (1973).
[2]M. Lax, J. Chem. Phys. 20, 1752 (1952).
[3]C. S. Kelley, Phys. Rev. B 6, 4112 (1972).
[4]E. Hutchisson, Phys. Rev. 36, 410 (1930).
[5]J. J. Markham, Rev. Mod. Phys. 31, 956 (1959).

ERRATA

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In Eqs. (28) and (29) p should be changed to t.

In the last line of Table I [that for LiH($A\,^1\Sigma^+$)] α_e was miscopied from the reference and should be changed to -0.078305. This decreases Y_{00} and δ on this line to 7.5033 and 0.03201, respectively. The rest of the paper and the conclusions are unchanged.

Also, an erratum by Tietz[1] brings his solution of the Schrödinger equation for his potential into agreement with mine.

I thank John O. Eaves and Kenneth D. Jordan for calling these things to my attention.

[1]T. Tietz, J. Chem. Phys. 43, 1086 (1965).

