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1974-11-15

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

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Pack, Russell T., "Erratum: On improved WKB (uniform asymptotic) quantum conditions, Dunham corrections, the Langer modification, and RKR potentials" (1974). *Faculty Publications*. 784.  
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$$\langle i \rangle = S/R + (R-1)^2/4R \quad (7)$$

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,<sup>5</sup> namely that

$$M_{\alpha 1} = E_{sp} + \langle f \rangle R \hbar \omega \quad (8a)$$

$$M_{\alpha 1} = E_{sp} - \langle i \rangle \hbar \omega, \quad (8b)$$

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

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

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

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

$$\langle i \rangle = S_e + (R-1)^2/4R$$

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

<sup>1</sup>M. D. Sturge, Phys. Rev. B 8, 6 (1973).

<sup>2</sup>M. Lax, J. Chem. Phys. 20, 1752 (1952).

<sup>3</sup>C. S. Kelley, Phys. Rev. B 6, 4112 (1972).

<sup>4</sup>E. Hutchisson, Phys. Rev. 36, 410 (1930).

<sup>5</sup>J. J. Markham, Rev. Mod. Phys. 31, 956 (1959).

## ERRATA

### Erratum: On improved WKB (uniform asymptotic) quantum conditions, Dunham corrections, the Langer modification, and RKR potentials [J. Chem. Phys. 57, 4612 (1972)]

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

In the last line of Table I [that for  $\text{LiH}(A^1\Sigma^+)$ ]  $\alpha_e$  was miscopied from the reference and should be changed to  $-0.078305$ . This decreases  $Y_{00}$  and  $\delta$  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<sup>1</sup> 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.

<sup>1</sup>T. Tietz, J. Chem. Phys. 43, 1086 (1965).