UNEXPECTED PROPERTIES OF THE MORSE OSCILLATOR

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Analytical solutions for the Morse oscillator are used to evaluate $\langle V \rangle_n$ and $\langle T \rangle_n$. For all bound states $\langle V \rangle_n = \frac{\hbar\omega_e}{2}\left(n+\frac{1}{2}\right)$. This result is identical to the result that is obtained for the harmonic oscillator with the same quadratic force constant. Consequently, all of the anharmonicity in the energy of the quantum states of a Morse oscillator is incorporated in $\langle T \rangle_n$. This finding is tested for realistic diatomic potential functions for Ar-Xe, Be_2 and the $E-$state of Li_2. Analysis of $\langle V \rangle_n / \left(n+\frac{1}{2}\right)$ for these systems shows that this quantity is well approximated by $\omega_e/2$ over large ranges of n. Implications of this result to polyatomic systems and for vibration to translation collisional energy transfer are discussed.[a]

[a] A. B. McCoy, *Chem. Phys. Lett.*, **501**, 603-607 (2011).