Finding a universal function valid for 200 bonds, Xie and Hsu [1] stated that (i), contrary to [2], the Sutherland parameter is a valid scaling factor, and (ii) ‘Based on the scaling analysis of 300 diatomic molecules, [1] pointed out [2] that the Sutherland parameter $\Delta$ can never be a universal scaling factor’, which are two inaccurate representations of [2]. Contrary to [1], I showed 25 years ago [3] that a \textit{covalent} Sutherland parameter $\Delta$ is not universal because its ionic equivalent is superior [2,3]. This incorrect assessment of my work by Xie and Hsu [1] might be due to omission of refs. 2 and 3 from [4], as Xie acknowledged [5] (see also [6]). Xie’s 200-bond study [4] cited a 150-bond study [7] but not my work involving 400 bonds [2]. Xie and Hsu [1] failed to distinguish between \textit{covalent} and ionic Sutherland parameters [3], an important distinction according to [8]. Ref. [1] refers to 3 parameters $\alpha$, $\beta$ and $\gamma$ [4], needed to improve the poor QM PEC (potential-energy curve) for H$_2$; to align the theoretical and observed PEC, 3 parameters are known [2,3,7,8] to suffice. For scaling, a Dunham expansion [1] requires the \textit{covalent} Sutherland parameter, $\Delta_{\text{cov}}=\frac{1}{2} k_2 r_0^2 / D_{\text{cov}}$, in which appear $L_0=(\frac{41 D_{\text{cov}}/f_0)^{1/2}}{1}$ and the $n$th force constant $f_n=dV/dr^n$, but Xie and Hsu [1] did not even mention the better ionic alternative [2]. From first principles one can explain why scaling with the \textit{covalent} Sutherland parameter $\Delta_{\text{cov}}=\frac{1}{2} k_2 r_0^2 / D_{\text{cov}}$ (for A+B→AB), used in [1,4], is less efficient than with the ionic $\Delta_{\text{ion}}=\frac{1}{2} k_2 r_0^2 / D_{\text{ion}}$ (for A$^+$+B→AB) [2,3].

The solution of wave equations for bonds has encountered difficulty since 1930. Fixing the asymptotes as $D_{\text{cov}}$ leaves potentials uncertain (Morse, Pekeris, Dunham…), whereas fixing the potentials (Coulomb, Kratzer) gives asymptote problems. This dilemma can be rationalized with \textit{covalent} and ionic Sutherland parameters. The two are algebraically distinguished with Hooke-type Dunham $U_0(r)$ and Coulomb-type Kratzer $U_k(r)$ oscillators having asymptotes $a_0$ and $a$, respectively:

$$U_0(r) = a_0(1-r/n_0)^2 = a_0(1-N)^2 = \frac{1}{2}k_2r_0^2(1-r/n_0)^2 \quad (1)$$

$$U_k(r) = \frac{A}{1-n_0/r_0^2} = \frac{A}{1-N/N(N-1)^2} \quad (2)$$

Although both forms are zero at $N=1$, as Dunham’s oscillator (1) can never converge to its own asymptote $a_0$, expansions are needed [9], whereas Kratzer’s form (2) invariably converges to $A$, even without expansions [9]. Force constants $k_2=2D_{\text{cov}}/r_0^2$ for (1) and $k_2=2A/r_0^2$ for (2) determine PEC-shapes at the energy minimum. Dunham’s primary coefficient $a_0=\frac{1}{2}k_2r_0^2$ cannot be calculated simply from first principles and typically differs (strongly) from $D_{\text{cov}}$ [2]. For Dunham’s (1) to be used for scaling (with a \textit{covalent} Sutherland parameter $\Delta_{\text{cov}}=a_0/D_{\text{cov}}$), severe adaptations are needed on either side of $r_0$. With a Kratzer Coulomb law $-e^2/r$ in (2) for ionic bonding (consistent with nuclear repulsion in a B-O approximation), the force constant is obtainable algebraically from first principles: $k_2=\frac{e^2}{r_0^3}$ gives $A=\frac{1}{2}e^2/r_0^2$ which ensures that $\Delta_{\text{ion}}=\frac{1}{2}(e^2/r_0^2) / D_{\text{ion}}$, readily understood with classical physics. $U(n_0)=-e^2/r_0^2$ the ionic bond energy [2,3,9], gives $\Delta_{\text{ion}}=\frac{1}{2}$. Despite its simplicity, this mechanism yields, for so-called \textit{covalently} bound H$_2$ ($n_0=0.7414$ Å), $A=2e^2/r_0=78300$ cm$^{-1}$ and $k_2=\frac{e^2}{r_0^3}=5.7 \times 10^8$ dyne/cm, consistent with observation, even for H$_2$ for which the Dunham asymptote $a_0=79500$ cm$^{-1}$ in (1) and $k_2=a_0/4B_0=5.7 \times 10^8$ dyne/cm. For H$_2$, \textit{ab initio} ionic theory gives vibrational frequency $\omega_0=4390$ cm$^{-1}$, near the observed 4400 cm$^{-1}$. This nearly exact result from first principles for H$_2$, possible only with Kratzer’s (2), makes a physically reliable ionic Sutherland parameter more suitable than a \textit{covalent} one. As this direct connection with chemical bonding is absent from [1,4], Xie and Hsu incorrectly assessed some essentials of molecular scaling related to (1) and (2), as exposed in [2,3,9].

Kratzer’s form (2) appears not only in a symmetry-reduced Hamiltonian for H$_2$ [9] but also in Sommerfeld’s famous double square-root equation for the H fine structure [10], later recovered by Dirac in QED [11]. Sommerfeld-Kratzer’s Coulomb-based universal potential $U_k(N)=\frac{1}{2}(e^2/r_0)(1-N)^2$ for H$_2$ in (2) demonstrates exactly why the prototypical molecule H$_2$ is for molecular spectroscopy what the prototypical atom H and Bohr’s $U_0(n)=\frac{1}{2}(e^2/r_0^2)(1-n^2)$ are for atomic spectroscopy [2]. Kratzer-type scaling with an ionic Sutherland parameter [2,3,9] then becomes essential, contrary to published conclusions [1,4].

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