Kratzer Potential for Vibrational Levels in Molecular Hydrogen

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The vibrational part of the dihydrogen Hamiltonian obeys a quantized Sommerfeld-Kratzer potential, which takes into account internal H_2 symmetries. All constants ω_e, k_e, and r_e needed for the H_2 vibrational system derive from hydrogen mass. Ionic Kratzer bond theory gives covalent bond energy within 0.08% and all levels within 0.02%, which is 30 times better than with a Dunham oscillator and as accurate as early ab initio quantum mechanics.

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1. Introduction

Physicists focus on the simple line spectrum of atom H with fine and hyperfine structure and less on the more complex band spectrum of molecule H_2 [1]. Since Bohr's simple, fairly accurate atom theory made H prototypical for atomic spectroscopy, a simple bond theory should make H_2 prototypical for molecular spectroscopy [2]. However, only a complex quantum mechanics (QM) theory can account accurately for H_2 levels and its potential energy curve (PEC) [3, 4]. During the last decades, the rigour of ab initio QM has been abandoned in favour of density functional theory (DFT) while simpler Bohr-type bond theories remain of interest [5]. Since for both H and H_2, the role of internal symmetries is still uncertain, we expand on these symmetries for H_2.

By its complexity, QM also fails on a simple analytical function for PECs, i. e. a low parameter universal function (UF) [2, 6, 7], needed to unify shape-invariant, asymmetric PECs [2]. This justifies many attempts to find a UF, usually dealt with using Dunham theory [8]. If H_2 is supposed to be the best starting point to get at universal behaviour, its vibrational levels must be understood with a simple low-order oscillator like Dunham's or Kratzer's, a thesis we develop here [2, 6].

Since anharmonicity flaws the harmonic oscillator (HO), which is important for physics [9], we confront it with the H_2 spectrum in Section 2. Dunham and Kratzer oscillators are in Section 3. In Section 4, the three H_2 parameters r_0, ω_e, and k_e are derived solely from mass m_H. In Section 5, effects of P and C for H_2 are quantified and old quantum theory leads to a quantized Kratzer bond theory. The accuracy of Dunham and Kratzer oscillators in Section 6 not only shows that Kratzer's is superior to Dunham's but also that a Kratzer theory is as accurate as earlier ab initio QM [10]. Internal H_2 symmetries are discussed in Section 7. Implications for the theory of the chemical bond are in Section 8. Section 9 concludes.

2. Quantum Harmonic Oscillator and Anharmonicity in Bond H_2

H_2 rotator-vibrator levels $E_{v,J}$ vary with vibrational and rotational quantum numbers v and J. For vibrational levels v ($J = 0$), Schrödinger's quantum harmonic oscillator (HO) [11] gives equally spaced levels with

$$E_{v+1/2} = \omega_e(v + 1/2) \quad \text{or} \quad E_{v+1/2}/\omega_e = v + 1/2, \tag{1}$$

where ω_e is the fundamental vibrational frequency. Nevertheless, (1) disagrees with the observed H_2 anharmonicity. A series expansion in half integer v

$$\begin{aligned} E_{v+1/2} = {} & \omega_e(v + 1/2) - \omega_e x_e(v + 1/2)^2 \\ & + \omega_e y_e(v + 1/2)^3 - \dots \end{aligned} \tag{2}$$

gives a better agreement but this is equivalent with an expansion in integer v

$$E_v = A + Bv + Cv^2 + Dv^3 - \dots. \tag{3}$$

Table 1. Observed vibrational data for the $X^1\Sigma_g{}^1$ state of H_2 [12] (in cm^{-1}).

v	Vibrational differences (quanta) ($\Delta G(v+\frac{1}{2})$ in [12])	Vibrational energies or levels $E(v,0)$ ($G_0(v)$ in [12])
0	4402.93	0.00
1	4161.14	4161.14
2	3925.79	8086.93
3	3695.43	11782.36
4	3467.95	15250.31
5	3241.61	18491.92
6	3013.86	21505.78
7	2782.13	24287.91
8	2543.25	26831.16
9	2292.93	29124.09
10	2026.38	31150.47
11	1736.66	32887.13
12	1415.07	34302.20
13	1049.16	35351.36
14	622.02	35973.38

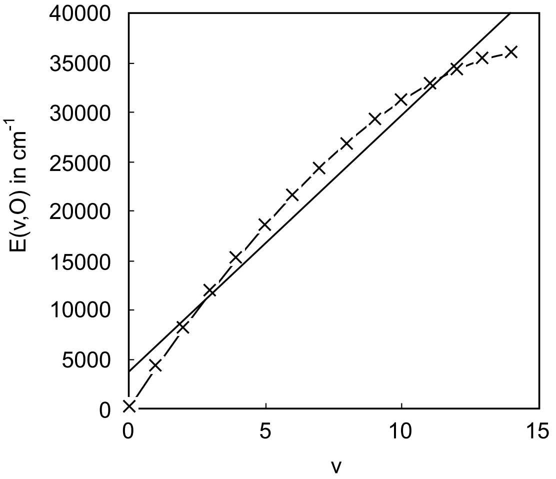

Fig. 1. Plot of 14 vibrational levels $E(v,0)$ [12] versus v. Linear fit (straight line); second-, fourth-, and sixth-order fits coalesce to a single broad curve (–×–).

Coefficients A, B, C, ... derive from those in (2), e. g. $A=\frac{1}{2}\omega_e(1-x_e+y_e-\ldots)\ldots$. Figure 1 gives the $E_v(v)$ plot for all 14 observed H_2-levels in Table 1 [12]. The first-, second-, fourth-, and sixth-order fits give errors of respectively 1839.93, 111.84, 7.15, and 0.24 cm^{-1}. In second-order fit, $E_v=[-161.11+4397.26v-128.19v^2]\ \mathrm{cm}^{-1}$, suggested by Morse [13,14], gives errors of 112 cm^{-1}. Even a sixth-order fit is not of spectroscopic accuracy. With errors of 3.2 cm^{-1}, earlier ab initio QM [10] ranks between fourth- and sixth-order fits. With errors of 1840 cm^{-1}, (1) obviously fails for the simplest and stable vibrator in nature, H_2.

Using reduced mass, equilibrium separation r_0, and kinetic energy $T=\frac{1}{2}\mu v_0{}^2=\frac{1}{2}\mu\omega_e{}^2r_0{}^2$, the vibrator energy $E_0=T_0+V_0$ depends on V_0, according to $-\frac{1}{2}k_er_0{}^2$ (Hooke, Dunham) or $-\frac{1}{2}e^2/r_0$ (Coulomb). For $E_0=0$, the fundamental frequency ω_e is available with the equations

Hooke, Dunham:

$$E_0=\tfrac{1}{2}\mu_H\omega_e{}^2r_0{}^2-\tfrac{1}{2}k_er_0{}^2=0; \quad\quad (4)$$
$$\mu_H\omega_e{}^2=k_e \text{ or } \omega_e=\sqrt{(k_e/\mu_H)},$$

Coulomb:

$$E_0=\tfrac{1}{2}\mu_H\omega_e{}^2r_0{}^2-\tfrac{1}{2}e^2/r_0=0;$$
$$k_e=e^2/r_0{}^3; \quad\quad (5)$$
$$\mu_H\omega_e{}^2=e^2/r_0{}^3 \text{ or } \omega_e=\sqrt{[e^2/(\mu_Hr_0{}^3)]}.$$

Hooke's equation (4) gives a standard HO relation but fails to identify k_e. Coulomb's equation (5) identifies k_e as

$$k_e=e^2/r_0{}^3, \quad\quad (6)$$

giving $\omega_e=4390\ \mathrm{cm}^{-1}$ as observed (see below). With Dunham's coefficient $a_0=\frac{1}{2}k_er_0{}^2$ [2,7,8], all asymptotes converge to ionic bond energy D_{ion}:

$$V(r_0)=a_0=\tfrac{1}{2}k_er_0{}^2=\tfrac{1}{2}e^2/r_0=\tfrac{1}{2}D_{\mathrm{ion}} \approx 79000\ \mathrm{cm}^{-1}. \quad\quad (7)$$

The only asymptote missing in (7) is the covalent bond energy $D_e=36118.3\ \mathrm{cm}^{-1}$ (see Section 6.3), which is much smaller than (7), but the standard for scaling the spectroscopic constants [2,7]. With (5)–(6), it is evident that, if r_0 for H_2 is available classically, ω_e or k_e are available too (Section 6).

3. Revisiting the HO: Dunham and Kratzer Potentials

Sinusoidal solutions for HO (1) derive from Hooke's force $F=-k_er$ and Newton's second law $F=ma$ [11]. With $V(r)=\frac{1}{2}k_er^2$, a Hooke-Dunham HO potential behind (4)

$$V_{HO}=\tfrac{1}{2}k_e(r-r_0)^2=\tfrac{1}{2}k_er_0{}^2(r/r_0-1)^2=a_0d_D{}^2 \quad (8)$$

is so firmly entrenched that alternatives are rarely employed, although it is wrong [2,15]. Variable

$$d_D=(r/r_0-1) \text{ or } r/r_0=1+d_D \quad\quad (9)$$

transforms (8) in $V_{\mathrm{HO}} = a_0 d_{\mathrm{D}}^2$, where $a_0 = {}^1\!/_2 k_{\mathrm{e}} r_0^2$. $V_{\mathrm{HO}}/a_0 = d_{\mathrm{D}}^2$ has the solutions $\pm d_{\mathrm{D}}$ for the r-dependence in non-convergent, symmetric PECs. Even Dunham's more flexible series expansion

$$V_{\mathrm{HO}} = a_0 d_{\mathrm{D}}^2 (1 + a_1 d_{\mathrm{D}} + a_2 d_{\mathrm{D}}^2 + \ldots) \tag{10}$$

faces convergence problems [7]. Asymmetric PECs, convergent without expansions, use alternatives:

$$\begin{aligned} d_{\mathrm{SK}} &= (1 - r_0/r) = [1 - 1/(1 + d_{\mathrm{D}})] \\ &= d_{\mathrm{D}}/(1 + d_{\mathrm{D}}), \end{aligned} \tag{11}$$

$$\begin{aligned} V_{\mathrm{SK}} &= {}^1\!/_2 k_{\mathrm{e}} r_0^2 (1 - r_0/r)^2 = a_0 (1 - r_0/r)^2 \\ &= {}^1\!/_2 (e^2/r_0)(1 - r_0/r)^2, \end{aligned} \tag{12}$$

respectively, which is the dimensionless Sommerfeld[1]-Kratzer variable (11) and potential (12) [2, 15]. Reduced V_{SK}/a_0 gives the solutions $\pm d_{\mathrm{SK}}$ for asymmetric, convergent PECs [2, 7, 15] but is ionic (see further below). For a classical approach to H_2 based on (12), r_0 must be available with classical physics.

4. Classical Equilibrium Separation r_0 in H_2

An independent classical calculus of r_0 will lead to a classical ω_{e} using

$$\omega_{\mathrm{e}} = \sqrt{(k_{\mathrm{e}}/\mu)}/(2\pi c) = \sqrt{[e^2/(\mu r_0^3)]}/(2\pi c). \tag{13}$$

The only classical formula available for spherical point-like particles with mass m_x is

$$m_x = (4\pi/3)\gamma_x r_x^3 \tag{14}$$

with γ_x, the density (g/cm^3) and $4\pi/3$, the spherical form factor, applicable for two spheres in a H_2 dumbbell. Questions emerge for micro-systems: (a) Is (14) adequate for H_2 concerning form factor and density; (b) Is $2m_{\mathrm{H}}$ or reduced mass ${}^1\!/_2 m_{\mathrm{H}}$ needed?; (c) Do results apply for r_0 in $D_{\mathrm{ion}} = e^2/r_0$ or for $2r_0$ in $a_0 = {}^1\!/_2 k_{\mathrm{e}} r_0^2 = {}^1\!/_2 e^2/r_0$, all appearing in (7)?

The sum of electron and proton mass [21] is $m_{\mathrm{H}} = 1/(5.97538.10^{23})$ g. With $\gamma_{\mathrm{H}} = 1$ g/cm^3, (14) gives

$$\begin{aligned} r_{\mathrm{H}} &= [(3m_{\mathrm{H}})/(4\pi\gamma_{\mathrm{H}})]^{1/3} = 7.36516 \cdot 10^{-9}\ \mathrm{cm} \\ &= 0.736516\ \mathrm{\AA} \end{aligned} \tag{15}$$

as classical radius r_{H}, whereas $r_{\mathrm{B}} = 0.529177$ Å. Since $r_{\mathrm{HH}} = 2r_{\mathrm{H}}$, r_0 is $r_{\mathrm{HH}} = 1.473032$ Å, which is typical for a virial rather than a Coulomb energy (observed $r_0 = r_{\mathrm{HH}} = 0.740144$ Å [22]), if γ_x=1 g/cm^3 makes sense[2].

The classical result r_0 (15) immediately gives (i) with (13), the fundamental H_2 vibrational frequency[3], equal to

$$\omega_{\mathrm{e}} = 4410.1722\ \mathrm{cm}^{-1}, \tag{16}$$

where 4402.93 cm^{-1} [12] or 4401.213 cm^{-1} [22] are observed; (ii) with (7), a virial energy for H_2, equal to half the ionic bond energy D_{ion} or

$$-V_0 = e^2/(2r_{\mathrm{H}}) = a_0 = 78844.9125\ \mathrm{cm}^{-1} \tag{17}$$

(observed $a_0 = {}^1\!/_2 k_{\mathrm{e}} r_0^2 \approx 79000$ cm^{-1} [24]); (iii) with the same dimension for (16) – (17), a quantum hypothesis emerges. The small ratio of step $\omega_{\mathrm{e}} \sim 4400$ cm^{-1} (16) and total gap $a_0 \sim 79000$ cm^{-1} (17) shows that a number steps v as in (1) – (3) is needed to cover this gap. This ratio is the number

$$\begin{aligned} q = \omega_{\mathrm{e}}/a_0 &= 4410.1722/78844.9125 \\ &= 0.05593477, \end{aligned} \tag{18}$$

which can bring in quantization following step δ_{v}, function of v. Hence, bond quantum hypothesis

$$r/r_0 - 1 = \Delta/r_0 = d_{\mathrm{HO}} = \delta_{\mathrm{v}} = qv \tag{19}$$

must be plugged in variable d_{HO} and d_{SK} for potentials V_{HO} and V_{SK} (see Section 6). With (15), mass m_{H} indeed provides with three fundamental parameters ω_{e}, r_0, and k_{e} for bond H_2.

5. Kratzer Bond Theory. Connection with C, P, and CP in H_2

5.1. Vibrational H_2 Energy and CP Symmetries

The Hamiltonian **H** (or energy E) for four-particle system H_2 (with pairs of charge-conjugated leptons a, b

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[1] Sommerfeld first used (11) for H [16, 17]. His pupil Kratzer used it for a general bond theory [18] and their colleague Kossel [19] for an ionic bond theory. Fues [20] solved the wave equation for (12).

[2] For systems with constant m_x/γ_x, all r_x are (nearly) equal, as observed for isotopomers H_2, D_2, and T_2 [23].

[3] The same formula for an electron ($m_{\mathrm{e}} = m_{\mathrm{H}}/1837.15267$ and radius r_{B}) gives $\omega_{\mathrm{e}} = 219474.65$ cm^{-1} $= 2 \cdot 109737.31$ cm^{-1}, or twice the Rydberg e^2/r_{B} [21]. This shows how the internal mechanics of H and H_2 are intimately connected.

and nucleons A, B) consists of four kinetic and six potential energy terms [24]:

$$\begin{aligned}\mathbf{H} = {}&{}^1\!/\!_2 p_a{}^2/m_a + {}^1\!/\!_2 p_b{}^2/m_b + {}^1\!/\!_2 p_A{}^2/m_A \\ &+ {}^1\!/\!_2 p_B{}^2/m_B - e^2/r_{aA} - e^2/r_{bB} - e^2/r_{bA} \\ &- e^2/r_{aB} + e^2/r_{ab} + e^2/r_{AB}.\end{aligned} \quad (20)$$

With n, v, and J for electronic E_{elec}, vibrational E_{vib}, and rotational energies E_{rot}, total energy obeys $E = E_{\text{elec}} + E_{\text{vib}} + E_{\text{rot}} = E_n + E_v + E_J$. Subtracting[4] $E_0 = E_n = {}^1\!/\!_2 m_a v_a{}^2 + {}^1\!/\!_2 m_b v_b{}^2 - e^2/r_{aA} - e^2/r_{bB}$ and neglecting $E_{\text{rot}} = E_J$, (20) becomes $E_{\text{vib}} = E - E_0 \approx {}^1\!/\!_2 m_A v_A{}^2 + {}^1\!/\!_2 m_B v_B{}^2 - e^2/r_{bA} - e^2/r_{aB} + e^2/r_{ab} + e^2/r_{AB}$. Notations $r = r_{bA} = r_{Ba}$ and $mv^2 = m_A v_A^2 = m_B v_B^2$ ($m = 1836.15 m_e$ close to $m_H = 1837.15 m_e$) lead to $\Delta E = \Delta T + \Delta V$ or

$$\begin{aligned}\Delta E &= E - E_0 \\ &\approx 2({}^1\!/\!_2 mv^2) - 2e^2/r + (e^2/r_{AB})(1 + r_{AB}/r_{ab}) \\ &= mv^2 + (e^2/r_{AB})[(1 + r_{AB}/r_{ab} - 2r_{AB}/r)] \\ &\equiv mv^2 + (e^2/r_{ab})[(1 + r_{ab}/r_{AB} - 2r_{ab}/r)] \\ &\equiv mv^2 + (e^2/r)[(r/r_{AB} + r/r_{ab} - 2)],\end{aligned} \quad (21)$$

where all three composite Coulomb terms ΔV are equal. For large r_{AB}, $r_{AB} \approx r_{ab}$ gives $\Delta E = E - E_0 \approx mv^2 + 2e^2(1/r_{AB} - 1/r)$. With r_0 and $r_{AB} = r_1 = a_1 r_0$, $r = r_2 = a_2 r_0$ and factor ${}^1\!/\!_2$, we get

$$\begin{aligned}{}^1\!/\!_2 \Delta E &\approx {}^1\!/\!_2 mv^2 + (e^2/r_0)(r_0/r_{AB} - r_0/r) \\ &= {}^1\!/\!_2 mv^2 + (e^2/r_0)(r_0/r_1 - r_0/r_2) \\ &= {}^1\!/\!_2 mv^2 + (e^2/r_0)(1/a_1 - 1/a_2),\end{aligned} \quad (22)$$

a simple result for E_{vib} (see also Section 6.1). To proceed with all equivalent variants in (21), the most appropriate scaling aid must be found. Since nucleons have the greater inertia, we prefer scaling by r_{AB}, which appears in ionic bonding, is important in BO (Born-Oppenheimer) approximations and is the common variable for PECs [24].

Magnitude and sign of Coulomb terms in (21) depend on the configuration (geometry) of H_2, which is subject to internal symmetries [25]. The ionic solution $-e^2/r_{AB}$ for (21) would require either that coefficient $(1 + r_{AB}/r_{ab} - 2r_{AB}/r)$ for e^2/r_{AB} in (21) is not only constant but also negative. Its final sign depends on geometry related operator parity $\mathbf{P}^2 = 1$ or geometry independent charge operator $\mathbf{C}^2 = 1$ [25]. To accommodate for this algebra, we use a form factor $\pm A_r$, defined as

$$\pm A_r = \pm(1 + r_{AB}/r_{ab} - 2r_{AB}/r). \quad (23)$$

Its subscript r refers to scaling by r_{AB}, its magnitude to the H_2 geometry, and its sign ± to the discrete values allowed by internal symmetry C. Energy (21) rewritten as

$$\begin{aligned}E_{\text{vib}} &= \Delta E (= \Delta\mathbf{H}' = p^2/m \pm A_r e^2/r_{AB}) \\ &= +mv^2 \pm A_r e^2/r_{AB}\end{aligned} \quad (24)$$

has positive kinetic energy T and positive or negative potential energy V, but this algebra must be in line with classical physics. Only attractive $-A_r e^2/r_{AB}$ can give a stable bond, repulsive $+A_r e^2/r_{AB}$ cannot[5] [25, 26].

Proceeding with (24) and its periodic motion (for vibration and rotation, see Section 4.2), angular velocity ω, velocity $v = \omega r$, and angular momentum $p = m_H v = m_H \omega r$ lead to the classical equation:

$$\Delta E = +m_H \omega^2 r_{AB}{}^2 \pm A_r e^2/r_{AB}. \quad (25)$$

This cannot only be interpreted by vibrations $\omega^2 = A_r e^2/(\mu_H r^3)$ like (7) but also by rotations obeying Kepler's third law $\omega^2 r_0{}^3 = A_r e^2/\mu_H = C$. For rotations coupled to vibrations, old quantum theory gives

$$p_1 = f\hbar/r_1, \quad p_2 = f\hbar/r_2, \quad \text{and} \quad p_{HH} = f\hbar/r_{HH}, \quad (26)$$

where f is a field factor. With Bohr's theory as guideline, all relations and identities easily follow:

$$\begin{aligned}&\text{(a)} \quad 2m_H \omega^2 r^3 = 2m_H v^2 r = A_r e^2 \quad \text{or} \\ &\qquad v^2 = {}^1\!/\!_2 A_r e^2/(m_H r), \\ &\text{(b)} \quad 2m_H \omega r^2 = 2m_H v r = 2p_H r = f\hbar \quad \text{or} \\ &\qquad v = {}^1\!/\!_2 f\hbar/(m_H r), \\ &\text{(c)} \quad v = A_r e^2/(f\hbar) \quad \text{and} \\ &\qquad r = {}^1\!/\!_2 (f^2/A_r)(\hbar^2/(m_H e^2)).\end{aligned} \quad (27)$$

For $A_r = 1$, the field scale factor f in (27) can be identified by using the classical r_0 (15):

$$\begin{aligned}&r_0 = {}^1\!/\!_2 f^2\hbar^2/(m_H e^2) \sim [(3m_H/(4\pi\gamma_H))]^{1/3} \quad \text{and} \\ &f \sim m_H{}^{2/3}(\hbar/e)[3/(4\pi\gamma)]^{1/6} \sim 1/q\end{aligned} \quad (28)$$

in agreement with (18), pending corrections for reduced mass and the virial.

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[4] The use of v for vibrational quantum number as well as for velocity must be clear from the context given.

[5] Ionic $-e^2/r_{AB}$ is only suspicious for two neutral atoms when $r_{AB} \gg r_{\text{crit}}$, with r_{crit} the critical distance, where ionic and non-ionic PECs cross [25]. At closer range, particle transfers can occur. Generically, ionic $-A_r e^2/r_{AB}$ is also obtained, independent of geometry or without particle transfer, by charge inversion symmetry C in one atom [25].

With (26), kinetic energy $T = p_{\mathrm{H}}{}^2/m_{\mathrm{H}} = (f^2\hbar^2/m_{\mathrm{H}})/r^2$ can now be plugged in (24). The result is

$$\begin{aligned}\Delta\mathbf{H}' &= \pm A_{\mathrm{r}} e^2/r + m_{\mathrm{H}}\omega^2 r^2\\ &= \pm A_{\mathrm{r}} e^2/r + (f^2\hbar^2/m_{\mathrm{H}})/r^2 \\ &= \pm A_{\mathrm{r}} e^2/r + [f^2\hbar^2/(m_{\mathrm{H}} e^2)](e^2/r^2).\end{aligned} \tag{29}$$

Using constants $A = A_{\mathrm{r}} e^2$ and $B = e^2 f^2\hbar^2/(m_{\mathrm{H}} e^2)$, this is of general Kratzer form:

$$V(r) = A/r + B/r^2. \tag{30}$$

The equilibrium $\mathrm{d}V/\mathrm{d}r$ at r_0, gives $B = -{}^1\!/\!_2 A r_0$ for the stable solution $\mathrm{V}_{\mathrm{SK}}(r_0) < 0$, since $B/r^2 > 0$. We get

$$\begin{aligned}&\Delta\mathbf{H}' = -A_{\mathrm{r}} e^2/r + {}^1\!/\!_2 A_{\mathrm{r}} e^2/r^2 \quad \text{or}\\ &\Delta''\mathbf{H} = \Delta\mathbf{H}' + {}^1\!/\!_2 A_{\mathrm{r}} e^2/r_0 \\ &\quad = +({}^1\!/\!_2 A_{\mathrm{r}} e^2/r_0)(1 - r_0/r)^2 = V_{\mathrm{SK}},\end{aligned} \tag{31}$$

the Sommerfeld-Kratzer Coulomb potential (12) for $-A_{\mathrm{r}} = -1$. Quantum theory gives solution (31) or (12) for vibrational H_2 levels obeying a Kratzer, not a Dunham oscillator [2, 25].

The second derivative d^2/dr^2 of (29) for the force constant equations leads to

$$\omega_{\mathrm{e}}{}^2 = A_{\mathrm{r}} e^2/(m_{\mathrm{H}} r_0{}^3); \quad k_{\mathrm{e}} = A_{\mathrm{r}} e^2/r_0{}^3, \tag{32}$$

which is impossible with Hooke's law for Schrödinger's HO (1), see Section 2. The reduced mass μ for H_2,

$$\begin{aligned}\mu &= m_{\mathrm{H}} m_{\mathrm{H}}/(m_{\mathrm{H}} + m_{\mathrm{H}})\\ &= m_{\mathrm{H}}/(1 + m_{\mathrm{H}}/m_{\mathrm{H}}) = {}^1\!/\!_2 m_{\mathrm{H}},\end{aligned} \tag{33}$$

gives the scale factor $s = {}^1\!/\!_2$ for dimer $H_2 = H_{\mathrm{a}} H_{\mathrm{B}}$. The dimensionless recoil correction in $AB(m_{\mathrm{A}}, m_{\mathrm{B}})$ is

$$s = 1/(1 + m_{\mathrm{a}}/m_{\mathrm{B}}). \tag{34}$$

Following Section 2, $A_{\mathrm{r}} e^2$ simplified to e^2 means that the inter-atomic field is ionic [27]. At r_0

$$k_{\mathrm{e}} = A_{\mathrm{r}} e^2/r_0{}^3 \equiv e^2/r_0{}^3 \tag{35}$$

implies that the Coulomb attraction $-e^2/r_0$, i. e. ionic bond energy D_{ion}, appears for covalent H_2 [2, 27]. We found [27] that plugging observed $r_0 = 0.74$ Å [22] in (35) returns observed $k_{\mathrm{e}} = 5.7.10^5$ dyne/cm and $\omega_{\mathrm{e}} \approx 4400\ \mathrm{cm}^{-1}$ for H_2 [12, 22], see Section 2.

5.2. Quantum Hypothesis for H_2 Vibrations and Connection with Intra-Molecular Rotations

Like (25) – (27), the angular velocity v_{e} for a rotating electron m_{e} in H derives from the ratio of radial equilibrium condition $m_{\mathrm{e}} v_{\mathrm{e}}^2/r = e^2/r^2$ and quantum rule for angular momentum $m v_{\mathrm{e}} r = pr = n\hbar$, or

$$v_{\mathrm{e}} = m_{\mathrm{e}} v_{\mathrm{e}}^2 r/m_{\mathrm{e}} v_{\mathrm{e}} r = e^2/(n\hbar) = \alpha c/n \tag{36}$$

without recoil. Using Bohr radius r_{B} and H-size differences Δ_{H}

$$\begin{aligned}&r = e^2/m_{\mathrm{e}} v_{\mathrm{e}}^2 = n^2\hbar^2/(m_{\mathrm{e}} e^2) = n^2 r_{\mathrm{B}},\\ &\Delta_{\mathrm{H}} = r - r_{\mathrm{B}} = r_{\mathrm{B}}(n^2 - 1)\end{aligned} \tag{37}$$

are incompatible with the linear rule (26). Quantization of the field by $1/n$ instead of the angular momentum by n, gives the same rotational energies for H, $E_{\mathrm{n}} = -R_{\mathrm{H}}/n^2$, since

$$v_{\mathrm{e}} = m_{\mathrm{e}} v_{\mathrm{e}}^2 r/m_{\mathrm{e}} v_{\mathrm{e}} r = (e^2/n)/\hbar \tag{38}$$

is identical with (36). Unlike (37), field quantization $1/n$ brings in a linear n-dependence

$$r = \hbar/(m_{\mathrm{e}} v_{\mathrm{e}}) = n\hbar^2/(m_{\mathrm{e}} e^2) = n r_{\mathrm{B}} \tag{39}$$

instead of a quadratic n^2-dependence in (37). Linearly quantized r-differences

$$\Delta_{\mathrm{r}} = r - r_{\mathrm{B}} = (n-1) r_{\mathrm{B}} = \ell r_{\mathrm{B}} \tag{40}$$

bring in Sommerfeld's secondary quantum number $\ell = n - 1$. With (40), H_2 quantization needs $\Delta_{\mathrm{r}} = r - r_0 = (n-1) r_0$, a linear, instead of a quadratic integer quantum number. Reduced equivalent

$$\Delta_{\mathrm{r}}/r_0 = r/r_0 - 1 = (n-1) = \ell \tag{41}$$

validates quantum hypothesis for vibrations in bonds (19), if ℓ is denoted by the number v in (1). With this information, we can apply rule (19) for any separation r.

6. Quantization of Symmetric Linear and Asymmetric Inverse Field Shifts

Quantum hypothesis (19) for inverse[6] and linear Kratzer and Dunham variables gives:

Kratzer:

$$r_0/r = r_0/(r_0 \pm \Delta) = 1/(1 \pm \Delta/r_0) = 1/(1 \pm \delta_{\mathrm{r}}), \tag{42a}$$

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[6] $\mathrm{H_a}$ and $\mathrm{H_b}$ in $\mathrm{H_2} = \mathrm{H_a H_b}$ can be distinguished by mass m_{a} and m_{b} and sizes r_{a} and r_{b}. As in a balance, this gives $m_{\mathrm{a}} r_{\mathrm{a}} = m_{\mathrm{b}} r_{\mathrm{b}} (= C)$,

Dunham:

$$r/r_0 = (r_0 \pm \Delta)/r_0 = (1 \pm \Delta/r_0) = (1 \pm \delta_\mathrm{r}), \quad (42\mathrm{b})$$

where δ_r or δ_v is the numerical equivalent of a step (25) – (27). Difference Δ

$$r - r_0 = +\Delta = +{}^1\!/\!{}_2\Delta - (-{}^1\!/\!{}_2\Delta) \quad (43)$$

is distributed in an anti-symmetric way, i. e. left and right to the center of mass, placed at the origin, but equal in absolute magnitude and based on the arithmetic average. In terms of symmetries, (43) gives symmetric H_2. However, symmetric (43) is different in Dunham and Kratzer variables (42).

6.1. The v-Dependence: Different Analytical Form for Quantized Dunham and Kratzer Oscillators

(i) The symmetric distribution (43), applied to Dunham's procedure for $r = r_0 \pm \Delta$, gives

$$r/r_0 = 1 \pm \Delta/r_0 = (1 \pm \delta_\mathrm{r}) = (1 \pm \delta_\mathrm{v}), \quad (44)$$

where left and right are avoided by virtue of (43). Dunham potential (8) away from r_0 becomes ${}^1\!/\!{}_2 k_\mathrm{e} r_0^2 (r/r_0)^2 = a_0 (r/r_0)^2 = a_0 (1 \pm \delta_\mathrm{r})^2$. With (19), reduced Dunham potential differences are

$$\begin{aligned} V'_\mathrm{Du} - V'_0 = \Delta V'_\mathrm{Du} &= -{}^1\!/\!{}_2 (1 - qv)^2 + {}^1\!/\!{}_2 \\ &= +qv - {}^1\!/\!{}_2 q^2 v^2. \end{aligned} \quad (45)$$

Using a_0 (24) and q (25), the numerical result of Dunham H_2 theory in cm^{-1} is:

$$\Delta V_\mathrm{Du} = \Delta E_\mathrm{v} = 4410.17v - 123.34v^2\ \mathrm{cm}^{-1}. \quad (46)$$

This is close to the observed second-order fit in Section 2 but with a large error of 111 cm^{-1}. The improvement over HO (1) is considerable but a parameter for qv cannot reduce these errors.

(ii) Quantization for a Kratzer potential gives a problem with the anti-symmetric or left-right symmetric distribution (43). Inverse $r_0/r = r_0/(1 \pm \Delta)$ does not account for positions of H_a and H_b with respect to their common center, i. e. $\pm{}^1\!/\!{}_2\Delta$ in (43). Equivalent rearrangements of the four inter-atomic Coulomb terms in (20) led to (22), where the composite the Coulomb sum $(e^2/r_0)(r_0/r_\mathrm{a} - r_0/r_\mathrm{B})$ gives similar inverse separations $1/r_\mathrm{A} = 1/(r_0 - {}^1\!/\!{}_2\Delta)$ and $1/r_\mathrm{B} = 1/(r_0 + {}^1\!/\!{}_2\Delta)$.

Applying these formally to a Kratzer variable gives

$$\begin{aligned} r_0/r_\mathrm{A} - r_0/r_\mathrm{B} &= r_0(r_\mathrm{B} - r_\mathrm{A})/r_\mathrm{A} r_\mathrm{B} \\ &= 1/(1 - {}^1\!/\!{}_2\delta_\mathrm{r}) - 1/(1 + {}^1\!/\!{}_2\delta_\mathrm{r}) \\ &= \delta_\mathrm{r}/(1 - {}^1\!/\!{}_4\delta_\mathrm{r}^2). \end{aligned} \quad (47)$$

Using (19), a more complex quantized v-dependence appears for a Kratzer theory,

$$1/(1 - {}^1\!/\!{}_2 qv) - 1/(1 + {}^1\!/\!{}_2 qv) = qv/(1 - {}^1\!/\!{}_4 q^2 v^2), \quad (48)$$

instead of the simpler linear qv-dependence in Dunham's (45). The reduced Kratzer oscillator difference is

$$\begin{aligned} \Delta V'_\mathrm{Kr} &= -{}^1\!/\!{}_2 [1 - qv/(1 - {}^1\!/\!{}_4 q^2 v^2)]^2 + {}^1\!/\!{}_2 = \\ &+qv/(1 - {}^1\!/\!{}_4 q^2 v^2) - {}^1\!/\!{}_2 q^2 v^2/(1 - {}^1\!/\!{}_4 q^2 v^2)^2 \end{aligned} \quad (49)$$

to be compared with Dunham's (45). In cm^{-1}, the numerical Kratzer result is

$$\begin{aligned} \Delta V_\mathrm{Kr} = (&+4410.17v - 123.34v^2 - 3.49v^3) \\ &/(1 - 0.00078v^2)^2\ \mathrm{cm}^{-1}. \end{aligned} \quad (50)$$

Its accuracy is discussed in Section 6.2. Relation (50) gives higher-order terms in v as in (2) – (3), to accommodate for anharmonicity. A parameter for qv in (48) can affect goodness of fits.

Maximum v_0 for variable qv gives v/v_0. For Dunham, $(1 - x)^2 = (1 - v/v_0)^2$ and $x = v/v_0 = 0$ returns the well depth; $x = 1$ or $v = v_0$ gives zero. For Kratzer $(1 - y)^2$, $y = (v/v_0)/[1 - {}^1\!/\!{}_4 (v/v_0)^2] = qv/[1 - {}^1\!/\!{}_4 (qv)^2]$, $y = 1$ implies that $qv = 1 - {}^1\!/\!{}_4 (qv)^2$ or $v^2 + 4v/q - 4/q^2 = 0$. Solving for v_0 gives

$$\begin{aligned} v_{0(\mathrm{Kr})} &= v_{0(\mathrm{Du})}/[{}^1\!/\!{}_2 (1 + \sqrt{2})] \\ &= 17.877967/1.207107 = 14.811, \end{aligned} \quad (51)$$

i. e. 14 levels as observed (see Table 1). The fact that band 15 is missing is in line with Kratzer theory (51) and is confirmed by the greater number of levels, observed for D_2 and T_2 [22, 23].

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where C is a constant, with dimensions $(\mathrm{e/v})^2$, leading to recoil (34) using $m_\mathrm{a}/m_\mathrm{b} = r_\mathrm{b}/r_\mathrm{a}$. Hence, relations between m_x and r_x obey $m_x = C/r_x$ or $r_x/C = 1/m_x$. If r_HH required addition, reduced mass μ appears naturally

$$r_\mathrm{HH} = (r_\mathrm{a} + r_\mathrm{b}) = C(1/m_\mathrm{a} + 1/m_\mathrm{b}) = C(m_\mathrm{a} + m_\mathrm{b})/(m_\mathrm{a} m_\mathrm{b}) = C/\mu.$$

If mass m_HH required addition, reduced separation $\rho = r_\mathrm{a} r_\mathrm{b}/(r_\mathrm{a} + r_\mathrm{b})$ appears naturally, too:

$$m_\mathrm{HH} = m_\mathrm{a} + m_\mathrm{b} = C(1/r_\mathrm{a} + 1/r_\mathrm{b}) = C(r_\mathrm{a} + r_\mathrm{b})/(r_\mathrm{a} r_\mathrm{b}) = C/\rho.$$

This explains (47) below since, if reduced separation is ρ_+ by sum, reduced separation ρ_- by difference obeys

$$1/\rho_- = 1/r_\mathrm{a} - 1/r_\mathrm{b} = (r_\mathrm{b} - r_\mathrm{a})/r_\mathrm{a} r_\mathrm{b}.$$

Table 2. Errors for H_2 levels $E(v,0)$ with Dunham (second- and fourth-order) and Kratzer (second-order) functions (in cm^{-1}).

v	Observed $E(v,0)$	Dunham second-order	Dunham fourth-order	Kratzer second-order
0	0.00	161.11	8.08	3.57
1	4161.14	53.18	−8.34	−3.91
2	8086.93	−33.74	−8.43	−3.94
3	11782.36	−94.63	−1.67	−0.77
4	15250.31	−126.64	5.20	2.45
5	18491.92	−128.61	8.56	4.15
6	21505.78	−101.96	7.09	3.59
7	24287.91	−50.66	1.75	1.13
8	26831.16	18.13	−4.81	−2.02
9	29124.09	92.98	−9.39	−4.48
10	31150.47	157.65	−8.71	−4.51
11	32887.13	188.98	−1.59	−1.37
12	34302.20	155.08	9.30	4.04
13	35351.36	11.66	13.69	6.80
14	35973.38	−302.54	−10.72	−4.73
	absolute error	**111.84**	**7.15**	**3.43**
	% error	**0.536**	**0.044**	**0.021**

6.2. Normalization of Quantized Dunham and Kratzer Oscillators. Formal Results

Dunham variable δ_{Du} and normalized Kratzer variable δ_{Kr}/p, respectively, equal to

$$\delta_{\mathrm{Du}} = qv, \tag{52}$$

$$\begin{aligned}\delta_{\mathrm{Kr}}/p &= (1/p)[1/(1-{}^{1}\!/\!{}_{2}pqv) - 1/(1+{}^{1}\!/\!{}_{2}pqv)] \\ &= qv/(1-{}^{1}\!/\!{}_{4}p^2q^2v^2),\end{aligned} \tag{53}$$

imply normalizing factor 1 for qv in Dunham's (52) but $1/(1-{}^{1}\!/\!{}_{4}p^2q^2v^2)$ in Kratzer's (53). A Kratzer oscillator needs harmonic mean $[(1-{}^{1}\!/\!{}_{2}pqv)(1+{}^{1}\!/\!{}_{2}pqv)] = (1-{}^{1}\!/\!{}_{4}p^2q^2v^2)$, in line with a harmonic oscillator. A normalization is needed for a parabola $(a-x)^2 = a^2(1-x/a)^2$, where x can be adapted by factor $1/a$ to restore (52) or (53). The accuracy of a second-order fit in (53) for H_2 is at maximum for $p = 0.83795$.

The second-order fits for plots of levels versus δ_{Du} (52) and $\delta_{\mathrm{Kr}}/0.83795$ (53) in Figure 2 are

$$\begin{aligned}E_{\delta(Du)} = {}& -40971.3574\delta_{\mathrm{Du}}^2 + 78614.1312\delta_{\mathrm{Du}} \\ & - 161.1126\,\mathrm{cm}^{-1},\end{aligned} \tag{54}$$

$$\begin{aligned}E_{\delta(Kr)} = {}& -40754.1814\delta_{\mathrm{Kr}}^2 + 76766.2419\delta_{\mathrm{Kr}} \\ & - 3.56576\,\mathrm{cm}^{-1},\end{aligned} \tag{55}$$

with respective goodness of fit of $R^2 = 0.9998627$ for (54) and $R^2 = 0.9999999$ for (55). Although all coefficients are as theoretically expected, they do not give a normalized parabola (see also Section 6.3). Errors for (54) and (55) show great differences, as shown in Table 2 and Figure 3. Errors of 0.021% for (55) almost vanish when compared with Dunham's: they are 30 times smaller than 0.54% for (54) and 530 times smaller for HO (1), with errors of 1840 cm^{-1} (see Section 2). Kratzer's second-order fit is even better than Dunham's fourth-order fit, with errors of 7 cm^{-1} (see Table 2). Errors of 3.5 cm^{-1} in Kratzer's theory compare with those of 3.2 cm^{-1} in early QM [10].

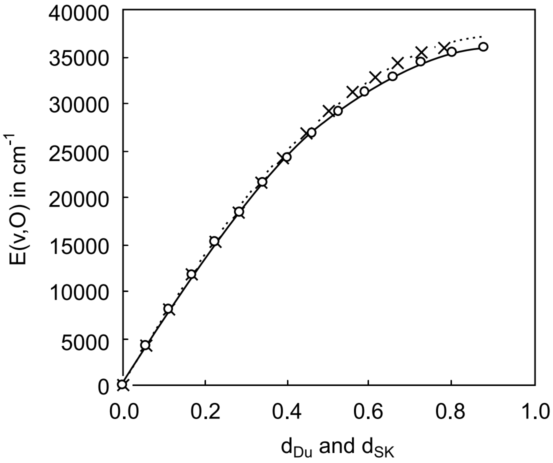

Fig. 2. Plot of $E(v,0)$ versus Dunham d_{DU} (curve ×) and Kratzer d_{SK} (curve ∘) variables with second-order fits.

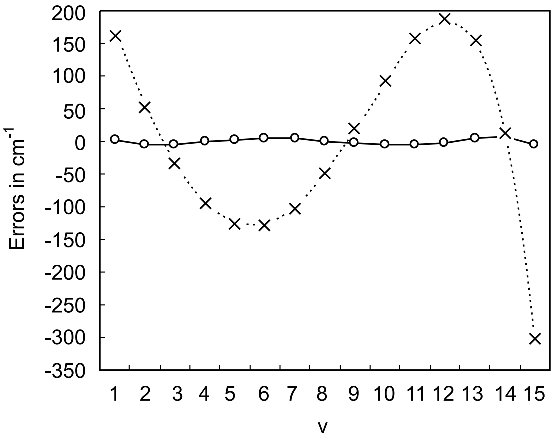

Fig. 3. Errors for $E(v,0)$ for H_2 (in cm^{-1}) with second-order fits for Dunham (×) and Kratzer (∘) oscillators.

6.3. Parabolic Behaviour: Covalent H_2 Bond Energy D_e from Ionic Energy D_{ion}

Covalent H_2 bond energy D_e is obtained directly from ionic bond energy D_{ion} by making (54) and (55)

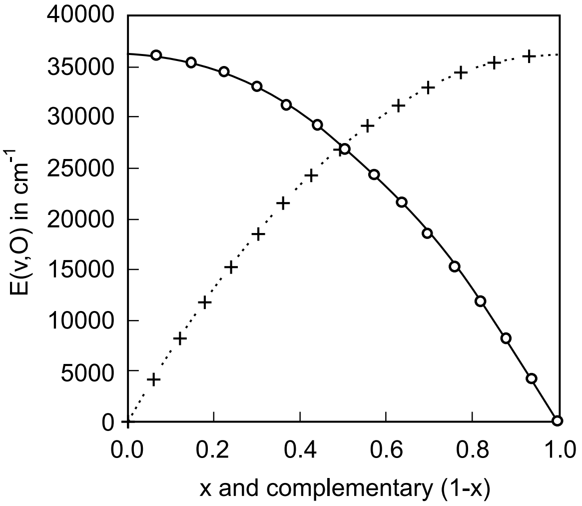

Fig. 4. Energy levels $E(v,0)$ for H_2 (in cm^{-1}) with Kratzer parabola (59) versus x (curve +) and with (57) versus complementary $1-x$ (curve *circ*), giving D_e as intercept (see text).

a perfect parabola $(1-\delta')^2 = (1-2\delta'+\delta'^2)$. Coefficient ratio $40754 \cdot 1814/(1/2 \cdot 76766 \cdot 2419)$ in (55) gives $\delta'_{Kr} = 1.061774\delta_{Kr}$ and $\delta'_{Du} = 1.042341\delta_{Du}$ for (54). Plotting energies versus variables x and $1-x$ as in Figure 4 gives well depth or covalent bond energy D_e as intercept in

$$E_{x(Du)} = [-37710.3788x^2 - 0.0000x + 37549.2663]\ cm^{-1}, \quad (56)$$

$$E_{x(Kr)} = [-36150.0077x^2 + 0.0000x + 36146.4419]\ cm^{-1}. \quad (57)$$

The covalent bond energy D_e of H_2, is 37549.27 cm^{-1} for Dunham's theory (error 3.96%) but

$$D_e = 36146.442\ cm^{-1} \quad (58)$$

for Kratzer's theory (error 0.078%). Result (57) is illustrative for the behaviour of a linear Coulomb term, made invisible by complementarity. In fact,

$$E_{\delta'} = [-36150.0077\delta'^2 + 72300.0154\delta' - 3.5658]\ cm^{-1} \quad (59)$$

gives $72300.0154 \equiv 2,36150.0077$ as required. This ionic term in (59) gives covalent D_e (58) within 0.078% of observed $D_e = 36118.3\ cm^{-1}$, better than early QM[7] [24].

7. Internal H_2 Symmetries

Since bisecting H_2, allowed by stoichiometry or mass conservation, gives two hydrogen atoms, we must verify whether one is either an exact copy (*P* even) or a mirror image (*P* odd) of the other. CP-effects in H_2 are available by the differences between them or the ratios of ±1 and the form factor $\pm A_r$ (23), related to the errors in Table 2. *C* is a discrete symmetry ±1, whereas *P* is a geometry dependent (continuous) symmetry $\pm x$, where x may vary with the H_2 structure, on which the form factor A_r gives evidence. Errors for bands T_v are those for levels in Table 2, multiplied by $E_v/(T_{0.0}+E_v)$, where $T_{0.0}$ is 90203.52 cm^{-1} or 90206.1 cm^{-1} [12]. This gives an average error for T_v of only 0.005%. Whatever and however complicated the 3D H_2 structure, its geometry remains constant (within 0.005%) according to the Kratzer bond theory. The second-order fit for observed terms,

$$T_v = [36150.0077\delta'^2 - 72300.0154\delta' + 90207.0858]\ cm^{-1}, \quad (60)$$

reveals why, after all, a negative ionic attractive Coulomb term $-e^2/r_{AB}$ shows for covalent H_2.

The discrete symmetry behind $-A_r$, i. e. attractive $-e^2/r$, can only derive from two atom centers in a H_2 dumbbell, occupied by $+e$ and $-e$. Classically, this is achieved with an ion pair but this requires unlikely[8] particle transfers at long range. Yet, $-e^2/r$ is also obtained with charge inversion *C* but this transforms an atom in an antiatom, i. e. antihydrogen $\underline{H}$ [25]. Although *C*-based solutions are the more generic, they are usually not allowed by the prospect of $H\underline{H}$ annihilation [25].

Whatever the reason for attractive $-e^2/r$ (by virtue of *C* or by the creation of an ion pair), odd or inversion symmetry *P* always leads to atom centers with a positive +1 and a negative mark −1, independent of the sign of charges on these marks. Although *P* in H_2 is reasonably well obeyed (within 0.005%) for a fixed H_2 geometry (one atom being the mirror image of the other by inversion symmetry), it is still uncertain whether internal symmetry *P* in H_2 is violated or not. To get more certainty about *P*, the origin of the small errors (< 0.005%) must be retraced. In [26], we show

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[7] In 1927, Heitler and London obtained $r_0 = 0.80$ Å, $\omega_e = 4800\ cm^{-1}$, and $D_e = 3.14$ eV or 25300 cm^{-1} [24].

[8] Attractive ionic bonding $-e^2/r$ needs a particle transfer between atoms X. Large energy gap $IE_X - EA_X$ (IE_X and EA_X are ionization energy and electron affinity), makes particle transfers in ionic bonding, improbable at long range $r \gg r_0$.

that this origin resides in an extra H_2 symmetry, not yet discussed.

8. Discussion

(i) A connection between D_{ion} and D_{e} affects the theory of the chemical bond: ionic bonding rationalizes covalent bonding in H_2. Reduced $\mu_{\text{ion}} = 1/2m_{\text{H}}[1-(m_{\text{e}}/m_{\text{H}})^2]$ differs from $\mu_{\text{cov}} = 1/2m_{\text{H}}$ by only $3 \cdot 10^{-5}\%$. Resonance between ions $[H^+H^-;\ H^-H^+]$ avoids a permanent dipole moment [25].

(ii) Magnitude and sign of the term in A_{r} show that only attractive $V = -e^2/r_{\text{AB}}$, not mutually exclusive repulsive $+e^2/r_{\text{AB}}$ can lead to stable H_2. Hence, the H_2 dumbbell is anti-symmetrical $\odot\otimes$ or $\otimes\odot$, instead of symmetrical $\odot\odot$ or $\otimes\otimes$. Nevertheless, symmetry based solutions for bonds generate problems with C for neutral H (formation of antihydrogen $\underline{\text{H}}$ [25]). We discuss some of these issues more in depth in [26].

(iii) Kratzer Coulomb energy $-e^2/r_0$ is important for universal behaviour and a UF [2,27]. Only scaling by ionic D_{ion} [7,27] unifies constants of ionic and covalent bonds between all monovalent atoms in the Periodic Table [2,27–29]. Why D_{ion} is a better scaling aid than D_{e} [2,27] is understood with (60), since D_{ion}, related to -72300.0154δ', is the first scaling aid [2,27,28], whereas D_{e} only appears in second instance, see (57) and (59). Difficulties for scaling without D_{e} [29] are in line with shortcomings of Dunham theory, as reported here.

(iv) Universal behaviour is usually connected with the smooth $G(F)$-plot of Varshni functions F for α_{e} and G for $\omega_{\text{e}}x_{\text{e}}$, whereby F and G are relate to the Dunham coefficients a_1 and a_2 in (3) and r/r_0 [2,6,7]. With Kratzer, higher-order terms in r seem superfluous, whereas higher-order terms in v are generated by the link between v and r_0/r. The quadratic term $1/2(e^2/r_0)(\omega_{\text{e}}/a_0)^2 = [0.5\cdot 4410.17^2/78844.91 = 123.34]\ \text{cm}^{-1}$ agrees with the observed H_2 levels. This second-order Kratzer term is close to H_2 anharmonicity $\omega_{\text{e}}x_{\text{e}}$ of $123.07\ \text{cm}^{-1}$ [6,12,22]. In Dunham's (10) it is related to the fourth-order term and the coefficient a_2 [2,7].

(v) For chemistry, Morse and Dunham potentials are used more widely than Kratzer's [2] but the interest in this function [30] remains justified, as it connects rotations (rolling [31]) with vibrations.

(vi) Recent double photoionization experiments on H_2 [32] led to non-Heitler-London ionic states for the H_2 ground state, which is in line with the present ionic Kratzer bond theory [33].

(vii) For isotopomers HD, D_2... the results must be as accurate as for H_2, since with the approximation $m_{\text{D}} = 2m_{\text{H}}$, similar r_0 values are obtained for D_2. This suffices to extend ionic bonding to covalent isotopomers [22,23], without giving details here.

(viii) Why H_2 only shows 14 bands is understood with maximum $v = 14.81$ (51), deriving from m_{H}.

(ix) Despite the good performances of an ionic model for covalent H_2, it fails, just like early ab initio QM [10], on spectroscopic accuracy. However, errors of $3.5\ \text{cm}^{-1}$ with simple Kratzer theory are almost the same as errors of $3.2\ \text{cm}^{-1}$ with the more complicated and elaborate QM methods [10]. In both cases, errors are larger than with the recent QM [3]. To remove small errors of Kratzer theory for H_2, it suffices to adapt symmetries by going over from an achiral to a chiral bond model [26].

9. Conclusion

A first-principles Sommerfeld-Kratzer potential accounts quite accurately for H_2 vibrations. A simple bond theory exists, which is in line with the existence of a UF. Ionic Kratzer bond theory for covalent H_2 differs from the conventional Dunham oscillator and the QM theories. This theory only needs hydrogen mass m_{H} as input to assess the full H_2 vibrational spectrum and links the ionic with the covalent bond energy. A symmetry-adapted Kratzer theory gives spectroscopic accuracy (errors of order 0.00002%) for prototypical chiral bond H_2, as we will show in [26].

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