

**THE INVESTIGATION OF THE RELATIONSHIP ELECTRONIC ENERGY ~
[VIBRATIONAL FREQUENCY] X [INTERNUCLEAR DISTANCE]², REGARDING
THE VIBRATIONAL ELECTRONIC STATES OF HYDROGEN MOLECULE**

Tolga Yarman (Isik University, Maslak, Istanbul, Turkey), Faruk Yarman (Turkish Defence Industry and Manufacturer Association), Fatih Ozaydin (Isik University, Maslak, Istanbul, Turkey)

The first author has previously established the following relationship between the *minimum electronic energy* E_{\min} , and the *lowest vibrational frequency* ω_{\min} at this energy level, in regards to various *vibrational electronic states* of a given diatomic molecule:^{1,2}

$$E_{\min} = 4\pi^2 M_0 g_k \omega_{\min}^2 r_{\min}^2 ; \quad (1)$$

here M_0 is the *reduced mass* of the molecule, r_{\min} the *internuclear distance* associated with ω_{\min} , and g_k a *coefficient* usually around *unity*, insuring the equality; for electronic states configured alike, we expect the coefficient g_k , to remain practically the same.

Let $E(r)$ be the *electronic energy of the molecule*, at a given state, with respect to the *internuclear distance* r .

$E(r)$ can indeed be as usual, fairly expressed in terms of the *force constant* k_{\min} , associated with ω_{\min} as³

$$E(r) = E_{\min} + \frac{1}{2} k_{\min} (r - r_{\min})^2 . \quad (2)$$

It should be emphasized that this relationship, does not display *characteristics* such as “*anharmonicity*” and “*dissociation*”; but throughout this work we are dealing with only the *lowest vibrational level of the states* of concern. Thus, even when we look at an *exited electronic state*, Eq.(2) is quite valid, around the *lowest vibrational level* of it.

$E(r)$ vanishes at the *abscissa* r_{00} , which we can define with respect to r_{\min} , as

$$r_{00} = p r_{\min} \text{ [value which makes } E(r), \text{ vanish] ;} \quad (3)$$

p is an *unknown parameter* at this stage, though it appears to be roughly around 2.

Eqs.(2) and (3), provides us with the possibility of expressing E_{\min} , as

$$E_{\min} = \frac{1}{2} k_{\min} (p - 1)^2 r_{\min}^2 . \quad (4)$$

Let us define g_k as

$$g_k = \frac{(p-1)^2}{2} . \quad (5)$$

Using the familiar expression

$$\omega_{\min} = \frac{1}{2\pi} \sqrt{\frac{k}{M_0}} , \quad (6)$$

we can *finally* arrive at Eq.(1).

Note that Eq.(5) depicts two value for p , and in fact, there are two roots r_{00} , fulfilling Eq.(3).

E_{\min} is normally given as

$$E_{\min} = E_{0\min} - T_e , \quad (7)$$

where $E_{0\min}$ is the *magnitude of the ground state electronic energy of the molecule*, and T_e a tabulated quantity.³

Eq.(1) then becomes

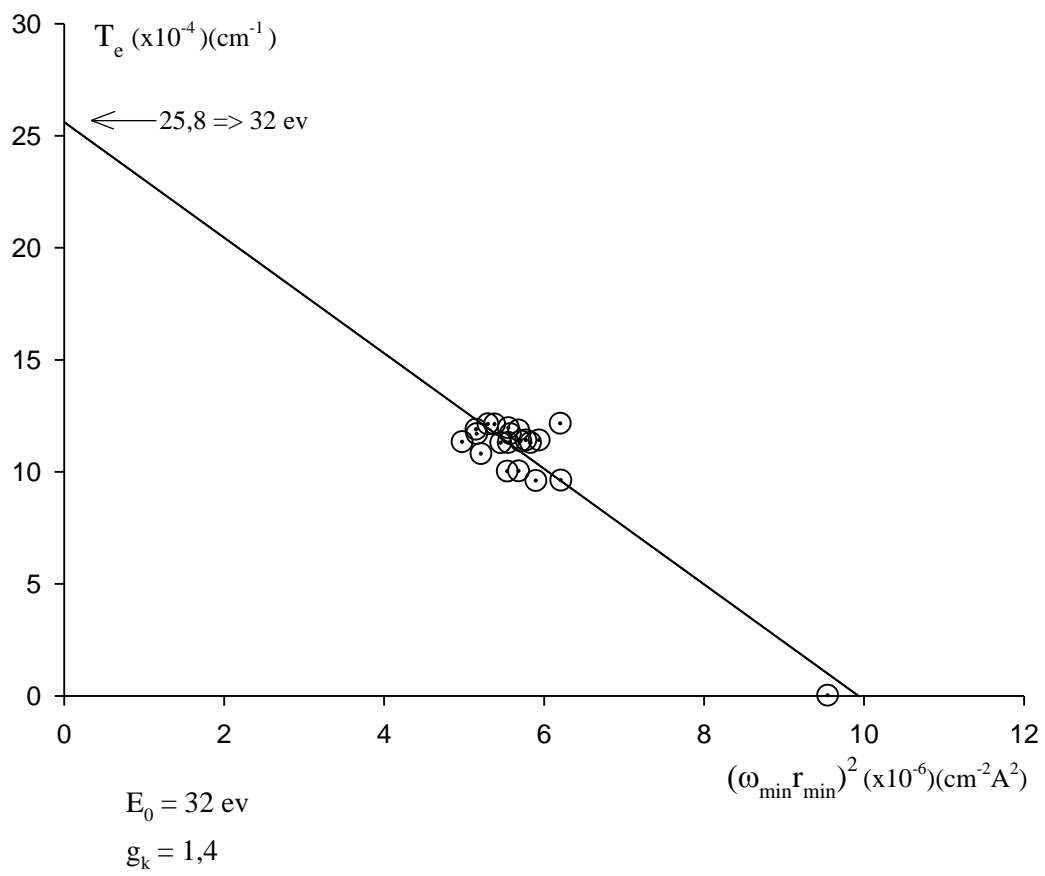
$$T_e = E_{0\min} - 4\pi^2 M_0 g_k \omega_{\min}^2 r_{\min}^2 . \quad (8)$$

Thence the plot of T_e for the electronic states bearing the same g_k , versus $\omega_{\min}^2 r_{\min}^2$, should come out as a decreasing straight line; it indeed does. The intersection of this straight line with the T_e axis, furnishes $E_{0\min}$, the *ground state electronic energy*, and the slope of it furnishes the coefficient g_k .

Note that Eq.(8) is valid for any diatomic molecule. We check this equation, on the basis of H_2 , the only molecule providing us with abundant data. Thus, out of some twenty pairs of electronic data, for which g_k is *practically the same as that of the ground state*, we have drawn T_e versus the $\omega_{\min}^2 r_{\min}^2$, to obtain a nicely decreasing straight line, whose intersection with the axis of T_e , satisfactorily furnishes $E_{0\min} \approx 32$ ev (instead of ≈ 31.5 ev).

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