MOLECULAR SPECTROSCOPY

An Essential Approach to the Architecture of Diatomic Molecules: 2. How Are Size, Vibrational Period of Time, and Mass Interrelated?¹

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Abstract—In our previous article, we arrived at an essential relationship for T, the classical vibrational period of a given diatomic molecule, at the total electronic energy E; i.e., $T = [4\pi^2/(\sqrt{n_1n_2}h)] \sqrt{gM_0m_e}R^2$, where M_0 is the reduced mass of the nuclei; m_e is the mass of the electron; R is the internuclear distance; g is a dimensionless and relativistically invariant coefficient, roughly around unity; and n_1 and n_2 are the principal quantum numbers of electrons making up the bond(s) of the diatomic molecule, which, because of quantum defects, are not integer numbers. The above relationship holds generally. It essentially yields $T \sim R^2$, for the classical vibrational period versus the square of the internuclear distance in different electronic states of a given molecule, which happens to be an approximate relationship known since 1925 but not understood until now. For similarly configured electronic states, we determine n_1n_2 to be R/R_0 , where R is the internuclear distance in the given electronic state and R_0 is the internuclear distance in the ground state. Furthermore, from the analysis of H₂ spectroscopic data, we found out that the ambiguous states of this molecule are configured like alkali hydrides and Li₂. This suggests that, quantum mechanically, on the basis of an equivalent H₂ excited state, we can describe well, for example, the ground state of Li₂. On the basis of this interesting finding, herein we propose to associate the quantum numbers n_1 and n_2 with the bond electrons of the ground state of any diatomic molecule belonging to a given chemical family in reference to the ground state of a diatomic molecule still belonging to this family but bearing, say, the lowest classical vibrational period, since g, depending only on the electronic configuration, will stay nearly constant throughout. This allows us to draw up a complete systematization of diatomic molecules given that g (appearing to be dependent purely on the electronic structure of the molecule) stays constant for chemically alike molecules and n_1n_2 can be identified to be R_0/R_{00} for diatomic molecules whose bonds are electronically configured in the same way, R_{00} then being the internuclear distance of the ground state of the molecule chosen as the reference molecule within the chemical family under consideration. Our approach discloses the simple architecture of diatomic molecules, otherwise hidden behind a much too cumbersome quantum-mechanical description. This architecture, telling how the vibrational period of time, size, and mass are determined, is Lorentz-invariant and can be considered as the mechanism of the behavior of the quantities in question in interrelation with each other when the molecule is brought into uniform translational motion or transplanted into a gravitational field or, in fact, any field with which it can interact. © 2004 MAIK "Nauka/Interperiodica".

In our previous article [1], we derived the following essential relationship regarding the electronic states of a diatomic molecule:

$$T = \frac{4\pi^2}{h_{\gamma}/n_1 n_2} \sqrt{g \mathcal{M}_0 m_e} R^2$$
(1)

(Eq. (15a) of Part 1), according to the definitions given below. *T* is the classical period of time (in the given electronic state); *R* is the internuclear distance (in this state); \mathcal{M}_0 is the reduced mass; m_e is the electron mass; *g* is a Lorentz-invariant, dimensionless constant depending only on the electronic structure of the molecule, somewhat characterizing how tight the bond is; n_1 and n_2 are the principal quantum numbers of the bond electrons; and *h* is Planck's constant. Herein, we will first of all elaborate on the quantum numbers n_1 and n_2 , chiefly based on Eq. (9a) of Part 1. Note that not much has been reported about the quantum numbers to be associated with the electronic excited states of a complex system [2, 3]. In any case, seemingly nothing similar has been achieved along the line we will present herein.

Below, first we develop a framework that will allow us to handle the problem. Then, we work out the quantum numbers for electronic states configured similarly, as well as for electronic states not configured similarly. Our approach will consequently lead to the proof of an empirical relationship known since 1925 but not understood until now. We provide an application on the basis

¹ This article was submitted by the author in English.

of spectroscopic data of the H_2 molecule. A new systematization of all diatomic molecules will follow.

HOW TO HANDLE THE PROBLEM

The presence of quantum numbers in Eq. (1) is immediately induced by the identification of the righthand side of Eq. (2) of Part 1 as h^2 . This equation is further transformed into Eq. (9b) of Part 1, written for the mere electronic description of the molecule (cf. Eq. (4) of Part 1); i.e.,

$$E_n m_e R_n^2 g_{IN} \sim h^2 \tag{2}$$

(Eq. (9b) of Part 1), according to the definitions given below. E_n is the electronic energy in the *n*th electronic state; R_n is the internuclear distance in the *n*th electronic state; and g_{IN} is a Lorentz-invariant, dimensionless constant (defined in the Appendix of Part 1), also somewhat characterizing how tight the bond is. The excited electronic eigenstates of the molecule should anyway involve quantum numbers.² The simplicity of Eq. (2) clearly leaves no room for quantum numbers to come into play in this equation other than the one right next to h^2 .

Thus, we conclude that a composite quantum number N (i.e., in the case of a diatomic molecule, the product of the two principal quantum numbers to be associated with the bond electrons) should come to multiply h^2 in this equation regarding an excited eigenstate in just the same way that the square of an integer quantum number related to an excited state of a simple wavelike object (such as the hydrogen atom) comes to multiply h^2 . This piece of information means that, when N is somehow known, one can introduce it into the framework of the ground level wavelike description (i.e., the Hamiltonian) of the entity in hand right next to h^2 and, based on Assertion 1 stated in Part 1, as we will detail soon, determine the eigenvalue and the characteristic length delineated by the resulting formulation. However, there is a peculiarity.

Equation (2), in the simple case of the hydrogen atom, shall (with the usual notation) be written as

$$8\pi^2 E_n g_{IN} m_e R_n^2 = n^2 h^2, \quad g_{IN} = 1$$
(3a)

(written for the hydrogen atom); here, E_n is as usual the total energy of the *n*th electronic state of the hydrogen atom, R_n is the corresponding characteristic size, and *n* is the principal quantum number. In the case of the hydrogen atom, g_{IN} is unity regardless of *n*. Thus, in this case, (i) g_{IN} in effect assumes the value of unity in the ground state but also (ii) g_{IN} remains the same at all electronic levels.

Neither property holds for systems of higher complexity, although, as we have shown, an equation similar to Eq. (1) can well be written for any diatomic molecule or, further, any wavelike entity. Nonetheless, we propose to achieve the equality induced by Eq. (2) for a diatomic molecule (following Eqs. (A.3) and (A.4) of the Appendix of Part 1) as framed by Eq. (3a); i.e.,

$$8\pi^{2}E_{n}g_{IN}m_{e}R_{n}^{2} = n_{1}n_{2}h^{2},$$

 $g_{IN} \neq 1$ (3b)

(written for a diatomic molecule). Since g_{IN} appears to be purely related to the electronic structure of the entity in hand, we expect it to remain the same for alike electronic configurations and, thus, for electronic states configured similarly.

However, as one jumps from the ground state of a complex system, such as that of a diatomic molecule, to an excited state of this entity, it is not obvious that the electronic configuration will stay the same; in fact, generally, it will not. Take, for instance, the hydrogen molecule. Its excited electronic states a priori will not bear the same electronic configuration as that of the ground state unless the two electrons are excited in complete symmetry. Even then, the shielding effects may not be the same. This is the peculiarity we wanted to clarify. Thus, as the molecule jumps from its ground state to an excited state, in general, it is not only that h^2 should be multiplied within the framework of the wavelike description by the appropriate composite quantum number but also that we should further represent the change that takes place in the electronic structure. This can, fortunately, be taken care of by a corresponding change in the coefficient g_{IN} of Eq. (3b).

Thereby, we can conceive an excited electronic state as being achieved in two steps:

(1) a switch of the ground state electronic configuration to a new configuration by just a change in g_{IN} ;

(2) a jump from this configuration to a new quantum state bearing the same configuration.

WORKING OUT THE PRODUCT OF QUANTUM NUMBERS FOR SIMILARLY CONFIGURED ELECTRONIC STATES

For electronic states configured like the ground state, we expect that g_{IN} will remain the same. Such an excited state should obey Eq. (3b), along with the quantity $n_1n_2 = N$, made up of the product of the principal quantum numbers of the bond electrons multiplying h^2 . Below, we will call *N* the composite quantum number. This yields the content of the following assertion, related to the formulation of excited electronic states.

Assertion 1. In the case in which the atomic or molecular wavelike object in hand, in a given electronic state, assumes the composite quantum number N, then the eigenvalue and the characteristic length associated with this state become the output of the formulation one

² Any excited eigenstate shall obviously involve quantum numbers. But, here, we are particularly interested in electronic excited eigenstates.

obtains by multiplying h^2 by N in the framework of the ground state description, provided that the two states are configured similarly.

Therefore, the introduction of appropriate quantum numbers into Eq. (3b) in front of h^2 (within the framework of the wavelike description) in order to describe the excited electronic eigenstates of the molecule, as complex as these may be, appears to be the standard procedure for the simplest wavelike objects such as the hydrogen atom (cf. Eq. (3a)), provided that the two states are configured similarly. We can predict the solution of the new setup through Assertion 1 of Part 1; this can indeed be obtained based on a reformulation of this assertion since, evidently, multiplying h^2 by a given number and dividing the masses involved by the Hamiltonian are mathematically identical operations.

Thus, we establish our next assertion, related to the solution of the description of an excited electronic level of the wavelike object in hand.

Assertion 2. In a real wavelike ground description, if, with the aim of expressing an excited eigenstate, h^2 is multiplied by the composite quantum number N, then, concurrently, (i) the magnitude of the total ground energy E_0 associated with the given wavelike object is decreased by as much to become E, the new eigenvalue, and (ii) the corresponding ground state size R_0 stretches by as much to become R, the new size, provided that the two states are configured similarly; in mathematical terms, this is

$$[h^{2} \rightarrow Nh^{2}]$$

$$\Rightarrow \left\{ \left[E_{0} \rightarrow E = \frac{E_{0}}{N} \right], \left[R_{0} \rightarrow R = NR_{0} \right] \right\}.$$
(4)

Note that Assertion 2 holds for any excited eigenstate (rotational, vibrational, electronic, or other). This assertion, for excited states of the molecule configured like the ground state, yields at once

$$N = R/R_0 \tag{5a}$$

(the composite quantum number of the excited eigenstates in the case in which they are configured like the ground state). This assertion, interestingly, holds no matter how complex the molecule may be.

Accordingly, we establish our next assertion.

Assertion 3. The composite quantum number to be associated with an excited eigenstate is merely the ratio of the size the object displays in this excited state to the size the object displays in the ground state provided that the two states are configured similarly.

Assertion 3 can be checked right away for the electronic states of the hydrogen atom. It is amazing that it holds for any object and for any excited eigenstate the object may involve (provided that the eigenstate of concern is configured like the ground state). One can also retrieve the following expected relationship from Eq. (4):

$$N = E_0/E.$$
 (5b)

This yields the following assertion.

Assertion 4. The composite quantum number is the inverse of the eigenvalue related to this eigenstate, where the ground state energy is normalized to unity.

WORKING OUT THE QUANTUM NUMBERS FOR EXCITED STATES NOT CONFIGURED LIKE THE GROUND STATE

What if the electronic structure of the excited state is not the same as that of the ground state? The answer is, promisingly, not complicated. Indeed, since the coefficient g_{IN} in Eq. (2) comes to multiply the mass of the electron, which happens to be the only mass involved in the description of the electronic motion of the diatomic molecule, any change in g_{IN} can evidently be represented by a corresponding hypothetical change in the mass of the electron. If, further, we are concomitantly to consider the change due to the introduction of a composite quantum number N related to the excited eigenstate in question (configured in a different way than the ground state), then, on the basis of Eq. (3b), this state can be described well by merely altering h^2/m_e in the framework of the ground state of the molecule by the coefficient $N(g_{IN})_{initial}/(g_{IN})_{final}$, where the subscripts "initial" and "final" refer, respectively, to the ground state and the excited electronic state under consideration.

The ultimate output can be established right away via Assertions 1 and 2 stated in Part 1, as framed in the following assertion.

Assertion 5. The ratio of the size that a diatomic molecule displays in an excited state to the size it displays in the ground state is equal to $N(g_{IN})_{initial}/(g_{IN})_{final}$, i.e., the composite quantum number to be associated with the excited state multiplied by a coefficient, the inverse of which quantifies how much the ground state electronic configuration is altered overall.

Note that the use of Eq. (5a) along with Eq. (1) requires that the coefficient g not be altered as the molecule passes from its ground level to the given excited electronic state, to allow plotting of T, the classical vibrational period in the given excited electronic state, versus $N^{-1/2}R^2$, where R is the size of the molecule in this eigenstate.

THE DISCLOSURE OF THE EMPIRICAL RELATIONSHIP $\omega r^2 = \text{CONSTANT}$ AND THE COMPLETE SET OF H₂ ELECTRONIC VIBRATIONAL DATA

Recall that the following approximate empirical relationship, evoking very much Eq. (1), was estab-



Fig. 1. T^2 versus r_0r^3 for different electronic states of H₂ (the states corresponding to experimental data off the straight line, denominated by the superscript "*E*," have been identified to be configured as indicated, like the ground states of, respectively, alkali hydrides and Li₂).

lished for a given diatomic molecule back in 1925 yet until now not understood [4–8]:

$$\omega r^2 \approx \text{empirical constant}$$
 (6)

(an approximate relationship written in 1925 for the electronic states of a given molecule), here ω is the classical vibration frequency related to a given electronic state of the molecule and *r* is the corresponding internuclear distance. The empirical constant is then to be determined separately for each diatomic molecule. Equation (6) bears the same meaning as Eq. (1) as far as the dependence of the vibrational period on the internuclear distance is concerned; however, it does not include the quantum numbers.

Equation (1), together with Assertion 3, suggests that we should consider the relationship

$$T = \frac{4\pi^2}{h\sqrt{r/r_0}}\sqrt{g\mathcal{M}_0m_e}r^2 \tag{7}$$

(the relationship written for the classical vibrational period of excited electronic states of a given molecule), where r_0 is the internuclear distance in the very ground state; *T* is the inverse of ω ; and, as usual. r/r_0 in the above relationship, following Assertion 3, is the composite quantum number associated with the electronic state under consideration. However, in order to better display the structure of the interrelation between *T*, \mathcal{M}_0 , and *r*, we will not incorporate $\sqrt{1/r}$ with r^2 and will keep Eq. (7) as it is wherever this is more explanatory.

Equation (7) implies that, for any molecule whose electronic states bear similar configurations for which g

remains about the same, the plot of T^2 versus r^3 should be a straight line.

The approximate empirical constant of Eq. (6) can now be evaluated from Eq. (7) as

empirical approximate constant

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$$=\frac{\sqrt{N}h}{4\pi^2\sqrt{g_0\mathcal{M}_0m_e}}=\omega r^2,$$
(8)

recalling that *N* is the composite quantum number, i.e., r/r_0 (staying indeed roughly the same where *r* is not far from r_0), which means that the constant in question is indeed only approximately a constant, and supposing that the electronic states in question are configured similarly, so that *g* stays practically constant throughout. This entirely discloses the mechanism behind the approximate empirical relationship, Eq. (8), established back in 1925.

Thus, Eq. (8) means that it is not really the quantity ωr^2 that is a constant for electronic states of a given molecule configured similarly but, on the basis of Eq. (7), more likely, it is the quantity

constant =
$$\omega \sqrt{\frac{r_0}{r}} r^2$$
 (9)

(written by the author for electronic states of a given molecule configured similarly); this new constant then is

$$constant = \frac{h}{4\pi^2 \sqrt{g \mathcal{M}_0 m_e}}$$
(10)

(written by the author for electronic states of a given molecule configured similarly). Recall that r_0 dominates the internuclear distance in the ground state. Although r_0 is also a constant for the given molecule, we still choose to keep it on the right-hand side of Eq. (9) to let the dimension of the new constant be the same as that of the classical empirical constant ωr^2 to enable comparison between these two quantities (cf. the right-hand side of Eq. (8)).

As an example, T^2 versus $(r_0/r)r^4$ for the H₂ molecule is sketched in Fig. 1. Thus, some 23 states out of the 29 for which data is available are neatly aligned. Herein, we included H₂⁺, which too seems to display the same g as that of the H₂ ground state; we find $g \approx$ 0.8. The remaining six electronic excited states of H₂ seem to be configured differently. We call these "ambiguous states" (the previous "unambiguous" 23 being seemingly all configured more or less like the ground state of the molecule).

To analyze the remaining six data (out of 29), we note, from Eq. (1), that switching the nuclear reduced mass \mathcal{M}_0 of alkali molecules or alkali hydrides to that of the hydrogen molecule should virtually transpose the corresponding vibrational period into the vibrational



Fig. 2. Period of alkali molecules versus $(1/(r_0/r_{00})^{1/2})(\mathcal{M}_0^{1/2}r_0^2), r_{00}$ is the internuclear distance of H₂.

period of the H_2 electronic state of the same electronic character. Recall that switching the nuclear mass practically does not affect the electronic structure of the molecule, and, accordingly, we should expect that, amongst the H_2 electronic states, there are states configured like the ground electronic states of alkali molecules and alkali hydrides. Therefore, we anticipate that the six ambiguous electronic states of H_2 should be configured just like the corresponding ground electronic states of alkali molecules and alkali hydrides and vice versa [9].

SYSTEMATIZATION OF THE GROUND STATES OF ALL DIATOMIC MOLECULES

In the light of the foregoing discussion, we recall Eq. (15b) of Part 1 (written regarding the ground states of diatomic molecules belonging to a chemical family), which we considered in conjunction with Eq. (15a) (written regarding the electronic states of a given diatomic molecule). Hence, we rewrite Eq. (7) (or the same, Eq. (15a) of Part 1), now, not for the excited levels of a given molecule, but for the ground states of molecules belonging to a given chemical family and, accordingly, being configured alike:

$$T_{0i} = \frac{4\pi^2}{h\sqrt{n_1 n_2}} \sqrt{g \mathcal{M}_{0i}} r_{0i}^2 \text{ (Eq. (15b))},$$

$$n_1 n_2 = \frac{r_{0i}}{r_{00}}$$
(11)

(written by the author for the classical vibrational period of the *i*th member molecule of a given chemical family), where T_{0i} is the ground state largest vibrational period of the *i*th member molecule of the chemical family under consideration; \mathcal{M}_{0i} is the reduced mass; r_{0i} is the ground state internuclear distance of this member;



Fig. 3. Period of (O_2, S_2, Se_2, Te_2) versus $(1/(r_0/r_{00})^{1/2})(\mathcal{M}_0^{1/2}r_0^2), r_{00}$ is the internuclear distance of O₂.

and r_{00} is the internuclear distance of the ground state of the family member chosen as the reference molecule; here, we choose the member bearing the lowest vibrational period. Therefore, T_{0i} versus $\sqrt{\mathcal{M}_{0i}}r_{0i}^2/\sqrt{r_{0i}/r_{00}}$ for chemically alike molecules should display a linear behavior, the slope of which shall furnish g to be associated with the chemical family under consideration.

Thus, we can now write an equation similar to Eq. (9) in regard to the ground states of molecules belonging to a given chemical family:

constant =
$$\frac{\omega_{0i}\sqrt{\mathcal{M}_{0i}}r_{0i}^2}{\sqrt{n_1n_2}} = \frac{\omega_{0i}\sqrt{\mathcal{M}_{0i}}r_{0i}^2}{\sqrt{r_{0i}/r_{00}}}$$
 (12)

(written by the author for the ground states of chemically alike molecules), where ω_{0i} is the inverse of the ground state classical vibrational period of the molecule of concern. Thus, the constant in question shall be expressed as

$$constant = \frac{h}{4\pi^2 \sqrt{gm_e}}.$$
 (13)

However, we still keep the constant r_{00} in the right-hand side of Eq. (12) so as not to have to alter the dimension of the constant in question.

In Figs. 2–8, based on experimental data [10, 11], we present T_{0i} versus $\sqrt{\mathcal{M}_{0i}}r_{0i}^2\sqrt{r_{00}/r_{0i}}$ for eight chemical families for which the coefficient *g* indeed stays neatly constant. The constancy of $\omega_{0i}\sqrt{\mathcal{M}_{0i}}r_{0i}^2\sqrt{r_{00}/r_{0i}}$, in harmony with Eqs. (3) and (4), is quantitatively demonstrated in the fifth columns of Tables 1–7.

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Fig. 4. Period of (N₂, PN, P₂) versus $(1/(r_0/r_{00})^{1/2})(\mathcal{M}_0^{1/2}r_0^2), r_{00}$ is the internuclear distance of N₂.



Fig. 6. Period of different alkali–halogen molecules versus $(1/(r_0/r_{00})^{1/2})(\mathcal{M}_0^{1/2}r_0^2), r_{00}$ is the internuclear distance of KF.

The values g are calculated from Eq. (4) for different chemical families and are presented in Table 8. Note that g vary between 0.4 and 0.01.

Recall that, according to Eqs. (3) and (4), the value of the constancy of $\omega_{0i}\sqrt{\mathcal{M}_{0i}}r_{0i}^2\sqrt{r_{0i}/r_{0i}}$ depends on both *g* and r_{00} (the reference internuclear distance of the family of concern), which makes the constants calculated in the fifth columns of Tables 1–7 differ.

Note further that the standard deviation of the constants in question is roughly 10%. There seem to be two reasons for this. The first one is that chemically alike



Fig. 5. Period of diatomic molecules made of combinations of halogen atoms versus $(1/(r_0/r_{00})^{1/2})(\mathcal{M}_0^{1/2}r_0^2)$, r_{00} is the internuclear distance of F₂.



Fig. 7. Period of diatomic molecules made of atoms belonging to, respectively, the third and seventh columns of the periodic table versus $(1/(r_0/r_{00})^{1/2})(\mathcal{M}_0^{1/2}r_0^2)$, r_{00} is the internuclear distance of BF.

molecules, contrary to our assumption, are not exactly configured similarly, which may indeed mean that g does not remain constant throughout. The second reason is that n_1n_2 (cf. Eq. (2)) for chemically alike molecules (where we choose the molecule with the lowest vibrational period as the reference molecule) may not be considered rigorously equal to r_{0i}/r_{00} .

Along this line, it is of interest to recall that, when we use the principal quantum numbers associated with the bound electrons directly (i.e., with no quantum defects) to compose n_1n_2 instead of using Eq. (2), we come out with the constancy of $\omega_{0i}\sqrt{\mathcal{M}_{0i}}r_{0i}^2\sqrt{n_1n_2}$,

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Fig. 8. Period of diatomic molecules made of atoms belonging to, respectively, the fourth and sixth columns of the periodic table versus $(1/(r_0/r_{00})^{1/2})(\mathcal{M}_0^{1/2}r_0^2)$, r_{00} the is internuclear distance of CO.

which happens not to be any worse than that of $\omega_{0i}\sqrt{\mathcal{M}_{0i}}r_{0i}^2\sqrt{r_{00}/r_{0i}}$ (cf. Eq. (3)) [7, 8].

In the Appendix of Part 1, we predicted that the inverse of g somewhat characterizes the strength of the bond of concern. As one can observe from Table 1, g indeed decreases as the bond becomes stronger. Thus, the higher the number of covalent bonds forming the overall bond of the diatomic molecule, the smaller g will be. Alternatively, the higher the number of free electrons an atom possesses, the looser the bond it will form with say, a halogen, will be and, thus, the higher g, etc. [12].

DISCUSSION

Recall the usual definition of the classical vibrational period, in terms of the reduced mass \mathcal{M}_0 and the force constant k, in the given electronic state:

$$T = 2\pi \sqrt{M_0/k}$$
 (Eq. (8) of Part 1) (14)

(the classical vibrational period in the given electronic state). Equating the right-hand side of this equation with that of Eq. (11) yields

$$k_i = \frac{h^2}{4\pi^2 g m_e r_{0i}^3 r_{00}}$$
(15)

(the force constant written by the author for the ground state of the *i*th member of the given family). The r_{0i}^{-3} dependence of k_i is somewhat trivial if one proposes to relate it to the internuclear distance. This correlation was, in effect, proposed some time ago by Bratoz *et al.*

for alkali hydrides [13, 14].

The proportionality constant Ce^2 , where *e* is the electron charge, was subsequently obtained by Salem and Ohwada [15, 16] on the basis of empirical presumptions, chiefly for molecules containing alkali atoms; more specifically, *C* is approximately determined to be

$$C = \frac{1}{2}(N_i + 1)(N_j + 1), \tag{16}$$

where N_i and N_j are the respective numbers of electrons residing outside of the complete shells of the atoms making up the diatomic molecule.

Recall, however, that, in order to obtain our results above, we followed a totally different path than that empirically inspired by Eq. (8). Moreover, we arrived at our result primarily for electronic states of a given mol-

Molecules	\mathcal{M}_0 , amu	$T_0 (\mathrm{cm}^{-1} \times 10^3 c)$	r ₀ , Å	$\frac{T_0 \sqrt{r_0/r_{00}}}{\sqrt{\mathcal{M}_0} r_0^2}$	Relative error as referred to the average
H ₂	0.50	0.24	0.74	0.62	0.29
Li ₂	3.50	2.89	2.67	0.40	0.15
LiNa	5.33	3.89	2.90	0.40	0.17
Na ₂	11.50	6.34	3.08	0.40	0.15
NaK	14.48	8.06	3.50	0.37	0.22
K ₂	19.49	10.80	3.92	0.37	0.22
KRb	26.83	13.2	4.07	0.36	0.24
Rb	42.47	17.3	4.21	0.36	0.24
RbCs	52.04	20	4.42	0.35	0.27
Cs ₂	66.47	23.8	4.64	0.34	0.29
Average				0.40	0.22

Table 1. Checking the end result for alkali molecules

Note that, here and in Tables 2–8, c is the speed of light in cm/s.

Molecules	\mathcal{M}_0 , amu	$T_0 (\mathrm{cm}^{-1} \times 10^3 c)$	<i>r</i> ₀ , Å	$\frac{T_0 \sqrt{r_0/r_{00}}}{\sqrt{\mathcal{M}_0} r_0^2}$	Relative error as referred to the average
02	8.00	0.64	1.21	0.15	0.17
S ₂	15.99	1.39	1.89	0.12	0.06
Se ₂	39.97	2.56	2.16	0.12	0.06
Te ₂	63.82	4.00	2.59	0.11	0.14
SO	10.67	0.90	1.49	0.14	0.09
Average				0.13	0.10

Table 2. Checking the end result for O_2 -like molecules

Table 3. Checking the end result for N_2 -like molecules

Molecules	\mathcal{M}_0 , amu	$T_0 (\mathrm{cm}^{-1} \times 10^3 c)$	r ₀ , Å	$\frac{T_0 \sqrt{r_0/r_{00}}}{\sqrt{\mathcal{M}_0} r_0^2}$	Relative error as re- ferred to the average
N ₂	7.00	0.43	1.09	0.13	0.08
P ₂	15.49	1.29	1.89	0.11	0.08
PN	9.65	0.76	1.49	0.11	0.00
Average				0.12	0.05

Table 4. Checking the end result for halogens

Molecules	\mathcal{M}_0 , amu	$T_0 (\mathrm{cm}^{-1} \times 10^4 c)$	r ₀ , Å	$\frac{T_0 \sqrt{r_0 / r_{00}}}{\sqrt{\mathcal{M}_0} r_0^2}$	Relative error as re- ferred to the average
F ₂	11.21	9.50	1.44	1.37	0.05
Cl ₂	17.96	17.49	1.99	1.22	0.15
Br ₂	31.15	39.96	2.28	1.70	0.18
I ₂	46.87	63.47	2.67	1.78	0.24
BrF	15.04	15.35	1.76	1.4	0.28
ClF	12.93	12.31	1.63	1.37	0.05
ICl	26.23	27.42	2.32	1.26	0.13
Average				1.44	0.15

Table 5. Checking the end result for CsBr-like molecules

Molecules	\mathcal{M}_0 , amu	$T_0 (\mathrm{cm}^{-1} \times 10^4 c)$	<i>r</i> ₀ , Å	$\frac{T_0 \sqrt{r_0/r_{00}}}{\sqrt{\mathcal{M}_0} r_0^2}$	Relative error as referred to the average
CsBr	52.63	49.92	3.14	1.02	0.52
CsI	71.63	64.94	3.41	1.00	0.5
NaCl	26.46	13.95	2.51	0.56	0.17
NaBr	31.98	17.86	2.64	0.60	0.09
NaI	35.15	19.45	2.90	0.54	0.19
KF	25.64	12.78	2.55	0.51	0.24
KCl	35.95	18.59	2.79	0.55	0.17
KBr	43.55	26.26	2.94	0.65	0.02
KI	47.48	29.89	3.23	0.61	0.09
RbCl	39.53	25.07	2.89	0.66	0.00
Average				0.67	0.20

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Molecules	\mathcal{M}_0 , amu	$T_0 (\mathrm{cm}^{-1} \times 10^4 c)$	r ₀ , Å	$\frac{T_0 \sqrt{r_0 / r_{00}}}{\sqrt{\mathcal{M}_0} r_0^2}$	Relative error as re- ferred to the average
BF	7.26	6.72	1.26	1.44	0.69
BCl	12.06	8.38	1.72	0.88	0.03
BBr	14.77	9.66	1.88	0.80	0.06
AlCl	20.95	15.24	2.13	0.88	0.03
AlBr	26.64	20.11	2.29	0.92	0.08
InCl	31.71	26.82	2.31	1.11	0.3
InI	56.72	60.32	2.86	1.36	0.59
TICI	35.09	29.87	2.55	1.02	0.19
TlBr	52.27	57.98	2.68	1.50	0.76
TlI	66.67	78.31	2.87	1.61	0.89
Average				1.15	0.36

Table 6. Checking the end result, for BF-like molecules

 Table 7. Checking the end result, for CO-like molecules

Molecules	\mathcal{M}_0 , amu	$T_0 (\mathrm{cm}^{-1} \times 10^4 c)$	<i>r</i> ₀ , Å	$\frac{T_0 \sqrt{r_0 / r_{00}}}{\sqrt{\mathcal{M}_0} r_0^2}$	Relative error as re- ferred to the average
СО	4.67	6.86	1.13	2.48	0.46
CS	7.86	8.73	1.53	1.55	0.08
SiO	8.13	10.18	1.51	1.81	0.07
SiS	13.43	14.93	1.93	1.43	0.16
GeO	10.23	13.15	1.65	1.83	0.08
SnO	12.27	14.09	1.84	1.51	0.11
SnS	20.62	25.25	2.06	1.77	0.06
PbO	14.00	14.85	1.92	1.40	0.17
PbS	23.49	27.72	2.39	1.46	0.14
Average				1.69	0.15

Table 8. Bond looseness factors of chemically alike diatomic molecules

Chemical family	$\frac{T_0\sqrt{r_0/r_{00}}}{\sqrt{\mathcal{M}_0}r_0^2} \left(\frac{\mathrm{cm}^{-1} \times 10^4 \ c}{\sqrt{\mathrm{amu}}\mathrm{\AA}^2}\right) = \frac{4\pi^2\sqrt{gm_e}}{h}$	Bond looseness factor (g)
H ₂ , Li ₂ , Na ₂ , K ₂	4.00*	0.34
CO, CS, SiO, SiS, GeO, SnO, SnS, PbO, PbS	1.69	0.06
F ₂ , Cl ₂ , Br ₂ , I ₂ , BrF, ClF, ICl	1.44	0.04
O ₂ , S ₂ , Se ₂ , Te ₂ , OS	1.30	0.04
N ₂ , P ₂ , PN	1.20	0.03
BF, BCl, BBr, AlCl, AlBr, InCl,	1.15	0.03
NBr, InI, TlCl, TlBr, TlI, CsF, CsBr, CsI, NaCl, NaBr, NaI, KF, KCl, KBr, KI, RbCl	0.67	0.01

NaCl, NaBr, Nal, KF, KCl, KBF, Kl, KOCl * Note that this value appears to be ten times greater than the corresponding one present in Table 1 simply because we adjusted T_0 of Table 1, which we multiplied by 10^{-3} , to T_0 , which we multiplied by 10^{-4} , through Tables 4–7; the same holds for the corresponding values we picked from Tables 2 and 3. ecule. The literature we reviewed does not deal at all with this aspect.

Note further that recent trials on the problem of transferable spectroscopic constants, despite satisfactory results they may furnish, are far from displaying how the fundamental quantities of mass, space, and time (i.e., clock mass, clock size, and period of time of the clock motion) are structured in interrelation with each other in the architecture of molecules [17]—in fact, just the way our Eqs. (1) and (2) reveal.

CONCLUSIONS

It was an original idea of the author that, owing to the end results of the special theory of relativity, as well as those of the general theory of relativity, the space size, the clock mass, and the period of time to be associated with any real wavelike object ought to be organized in exactly a given manner; i.e., (period of time) ~ (clock mass)(space size)²; we call this occurrence the universal matter architecture relation or, in short, the UMA relation.

In this work, we were able to demonstrate the occurrence in question concerning the vibrational structure of a diatomic molecule in regard to either the electronic states of a given molecule configured alike or the ground states of molecules belonging to a given chemical family (and, thus, practically configured similarly).

Our approach led us to the derivation of an empirical relationship known since 1925 but not understood until now, as well as to a new systematization of diatomic molecules. Thus, our approach reveals the simple architecture of diatomic molecules, otherwise hidden behind a much too cumbersome quantum-mechanical description. This architecture, displaying how the vibrational period of time, size, and mass are determined, is Lorentz-invariant and can conversely be considered as the mechanism of the behavior of the quantities in question in interrelation with each other when the molecule is brought into uniform translational motion or transplanted into a gravitational field or, in fact, any field with which it can interact [18, 19].

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