

DIATOMIC MOLECULES' ENIGMATIC CONSTANCY AS THE PRODUCT OF THEIR DISSOCIATION ENERGY AND INTERATOMIC DISTANCE

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ABSTRACT

In this contribution, we show that the product *dissociation energy* (\mathcal{D}) \times *interatomic distance* (\mathcal{R}) with regards to a straightforward taxonomy of diatomic molecules comes to assume a relatively high and virtually constant value; it is so much so that the heavier the diatomic molecules at hand, the closer $\mathcal{D}\mathcal{R}$ approaches e^2 (where e is the elementary charge in esu). This occurrence is studied herein separately under families arranged from chemically-alike diatomic molecules. Each family (such as the set made of “pairs of strictly alkali atoms” or “pairs of strictly halogen atoms” or “pairs of alkali-halogen atoms”, etc...) is thus composed of diatomic molecules formed of atoms bearing similar electronic configurations; whereby we initially ended up dealing with 18 families in total. In addition to those, we brought together 10 more families of diatomic molecules each composed of *heavy metal atoms* belonging respectively to each of the ten columns drawn from the three rows of heavy metals under the Periodic Table, and observed an even better conformance. $[\text{Sc}_2, \text{Y}_2, \text{La}_2]$ is the first family in question. $[\text{Ti}_2, \text{Zr}_2, \text{Hf}_2]$ and $[\text{Va}_2, \text{No}_2, \text{Ta}_2]$ are the next two families. $[\text{Zn}_2, \text{Cd}_2, \text{Hg}_2]$ delineates the last family of heavy metal diatomic molecules of concern. Let us stress that *each of these sets* embodies diatomic molecules made of heavy metal atoms belonging to the *given column of the Periodic Table*; thusly bearing alike electronic configurations. We further coined 5 more families made of heavy metal hydrides, oxides, chlorides, and alkalines. We were motivated to undertake the present research in the light of our insight with regards to i) the *general non-opacity character of neutral bodies* vis-à-vis electrical field transmission, and thusly ii) the *attractional electric property of neutral bodies* – which underlines the disclosed constancy where, particularly for diatomic molecules comprising heavy atoms, the increase in $\mathcal{D}\mathcal{R}$ happens to get aligned with the increase in atomic weight 1 (A_1) \times atomic weight 2 (A_2).

Keywords: Diatomic molecules, dissociation energy, interatomic distance, electronic configuration

1. Introduction

In the present study, we analyze the entire set of diatomic molecules starting with their simplest representative, the hydrogen molecule H_2 . The non-relativistic quantum mechanical description of this molecule is well-known.¹ It embodies 2 Laplacian operators for the 2 constituent protons, and 2 Laplacian operators for the 2 bonded electrons, along with $2+2=4$ sets of coordinates for each of the 4 particles of concern – with all of them being incorporated into the same wave function; thus bearing $4\times 3=12$ space coordinates altogether. The potential energy \mathcal{V} to be inputted to said description is composed of the summation of 4 terms expressing, respectively, i) the interaction between the protons, ii) the interaction between the electrons, iii) the interaction between one of the two protons and the electron neighboring the other proton, and iv) the interaction of the other proton with the electron of the former proton. The complete description amounts to an eigenvalue-eigenfunction (\mathcal{E} -) Schrödinger Equation.

Such a complicated equation is to be handled approximately, but still satisfactorily – separating, on the one hand, the description of the electronic configuration around the fixed nuclei (which are then situated at a variable distance r from each other) and, on the other hand, the description of the nuclei vibrating under the scrutinized electronic configuration, as well as in the face of the force of repulsion that they exert onto each other. The original eigenfunction is

thence written as the product $\psi_e \psi_N$, where ψ_e is the eigenfunction of the first description and ψ_N that of the second. Each of these eigenfunctions bears 6 space coordinates.²

The first description we mentioned pertaining to the electrons coupled to the fixed nuclei is made of 2 Laplacian operators representative, respectively, of the 2 electrons of the H₂ molecule; the potential energy V_e it embodies is the original potential energy \mathcal{V} , but decreased by the repulsion energy V_n of the nuclei e^2/r – with e being the elementary charge in *esu*, while the magnitude of the eigenvalue E_e of this equation is, in effect, the dissociation energy $D(r)$ of the molecule at the given distance r of the nuclei were E_e negative at the given r .

The second description we mentioned above, obtained via the decomposition of the original Schrödinger Equation written for the H₂ molecule and appertaining to the motion of the nuclei under the electronic configuration of concern, is also made of 2 Laplacian operators, each representing respectively the 2 protons. The potential energy V_N of this equation is made of the summation of the eigenvalue E_e (to be pinned down via solving the former description) and the repulsive potential energy $V_n=e^2/r$ of the nuclei – *with the eigenvalue E_N of this equation constituting the vibrational total energy of the molecule, where the nuclei are separated by the distance r .*

The difference of the eigenvalue \mathcal{E} (to be associated with the wavefunction ψ through the solution of the original Schrödinger Equation) and the potential energy $\mathcal{E}-\mathcal{V}$ inputted to this latter equation amounts to the summation of $[E_e - (\mathcal{V}-V_n)]$ (*associated with the first description*) and $[E_N - (E_e - V_n)]$ (*associated with the second description*), so that \mathcal{E} comes to be practically equal to E_N .

In this undertaking, we focus on $|E_e|$, which is tapped from the *first description* we just summarized – and pertaining to the electronic configuration of the molecule with its protons fixed at the distance r – and which is drawn out of the original Schrödinger Equation describing the H₂ molecule in its entirety. We call it $|E_e|=D(r)$. More precisely, we are interested in the value of $|E_e|=D(r)$ at the ground state of the molecule, with the corresponding separation distance of the nuclei becoming r_{min} . We will call $D(r_{min})$, in short, \mathcal{D} , and r_{min} , in short, \mathcal{R} .

Everything becomes much more complicated for diatomic molecules heavier than H₂. At the same time, one can recall the fact that dissociation energy decreases with weight – thusly with increasing interatomic distance. No matter what the general case may be, there are exceptions with regards to this premise (*as shall be exemplified by some results we will present below*); still, it looks appealing and, a posteriori, very interesting to examine the product $\mathcal{D} \times \mathcal{R}$.

For this purpose, we will visit basically Herzberg (1964),³ together with Huber & Herzberg (1979),⁴ where, practically all existing diatomic molecules' measured *dissociation energy* \mathcal{D} , and *internuclear distance* \mathcal{R} , had been earlier presented, thusly as *older data (1964)* and *more recent data (1979)*. We will accordingly take the opportunity to compare the *older data*, with the *more recently adopted ones*. It is interesting to notice that, this will help us to rectify *deviating plots, drawn on older data*.

Furthermore, chiefly, with regards to *heavy metals*, data reported only more recently,^{5,6,7,8,9,10} will be used. We will certainly indicate, for all data we will make usage of, throughout, *specifically* the reference, it is borrowed from. It is moreover primordial to point out *that computed values* for \mathcal{D} and \mathcal{R} , in many cases, are available in the literature.¹¹ We take this advantage to check out the measured data we use, also to complete our analysis, as much as we can, via adding to our scope, diatomic molecules recently tapped, where yet only *computed data* are provided. In any circumstance, relevant references, for all computed data (*in effect for all data*), will be indicated wherever usage of, is made.

We thus tabulate below the product $\mathcal{D} \times \mathcal{R}$ with respect to the entire body of diatomic molecules to show that it turns out to be *virtually a constant value* for chemically-alike diatomic molecules composed of atoms bearing similar electronic configurations. The constant value of

concern is shaped already for moderately light molecules of the given kind, and approximately holds the same for moderately heavy molecules. Strikingly, it can further delineate an ascending trend, despite the fact that the complexity increases even further with increasing weight, just as we had anticipated beforehand (see section 2).

Further on, we present plots of $\mathcal{D} \times \mathcal{R}$ versus the product of the atomic masses (section 3). Then we analyze the dissociation energy $D(r)$ – upon which, we anticipate that, in the zone near the ground state, it can be satisfactorily represented by the tractable form $k^2 e^2/r$; where k is a constant associated with the electron charge intensity the way delineated by said plots.

The assertion $D(r)=k^2 e^2/r$ tells us that the attractive force near the ground state is inversely proportional to the square of the distance separating the two objects under consideration (no matter whether or not it gets weakened much more sharply beyond the zone near the ground state). We shall elaborate on this. Next, we demonstrate that the constancy of the product *dissociation energy* $D(r) \times$ *interatomic distance* r is related to the scaling-symmetry properties of the Schrödinger Equation (section 4); this is a controversial problem, and will be given consideration accordingly. We bring up relatedly, Badger’s Rule, which is evoked along our approach, to frame an equivalent interesting relationship, as to the *vibration frequency of a diatomic molecule is proportional to the power of 3/2 of its dissociation energy, diminished by the square root of its reduced mass* (section 5). Finally, in section 6, we deliver our conclusions.

2. The product of dissociation energy and interatomic distance in relation to a straightforward categorization of diatomic molecules

In this section, we illustrate how the product $\mathcal{D} \times \mathcal{R}$ for diatomic molecules at the ground level appears to attain a relatively high and remarkable constant under a straightforward taxonomy, regardless of the complexity of the molecules involved. To track this intriguing finding, we present tables below which we drew for families of diatomic molecules composed of *alike atoms*.

What we refer to as “alike atoms” are atoms that display similar electronic configurations. One example is the family comprising alkali atoms; *i.e.*, Li, Na, K, Rb, Cs, Fr – they all bear a single electron at their outermost energy level. One other family made of alike atoms is that of the halogen group; *i.e.*, F, Cl, Br, I, At – all of these atoms lack one electron at their outermost shell.

Now, one can compose alkali molecules such as Li_2 , Na_2 , K, NaK, Rb_2 , RbK, Cs_2 , RbCs, Fr_2 , CsFr, *etc...* These constitute *alike molecules* – for, each of the alkali atoms share their *outermost solitary electron* with that of the companion atom. The created bond is, as is known, called a *covalent bond*.

Next to alkali molecules, and as a continuing example to alike diatomic molecules, we can now frame halogen pairs such as F_2 , Cl_2 , Br_2 , ClBr, I_2 , BrI, IAt, *etc...* They are alike molecules, too; for, in the case of each pair, the halogen atoms almost completely fill their outermost shell whilst lacking just a single electron that they seize from the outermost shell of the neighboring atom.

Another distinct family of alike molecules can be formed from an atom belonging to the family of alkali atoms and from elsewhere – *e.g.*, from one belonging to the family of halogen atoms; *ergo*, LiF, LiBr, NaF, NaBr, NaI, KCl, KBr, CsCl, CsBr, *etc...* The bond that comes into play is, as well-known, called an *electrovalent bond*.

In the last example, the halogen nucleus attracts the solitary electron of the alkali atom to “satisfy its appetite” for the single electron vacancy in its outermost shell; and by the same token, the electronic cloud of the halogen atom attracts the nucleus of the alkali atom – the resulting bond inundates, at the same time, the “near desolation of the alkali atom’s outermost shell”.

Within the framework introduced just above, we identify, at first hand, 18 families of alike diatomic molecules. They are shown in Index 1.

In addition to that, we assemble 10 more families of diatomic molecules each composed of *heavy metal atoms* belonging respectively to each of the ten columns drawn from the three rows of heavy metals under the Periodic Table; whereby we observe an even better conformance with respect to the delineated constancy. That is to say, they depict an ever increasing trend for the quantity $\mathcal{D}\hat{\mathcal{I}}\mathcal{R}$ versus the weight of the diatomic molecules under consideration.

By this token, [Sc₂, Y₂, La₂] is the first family of bimetallic diatomic molecules to be investigated. [Ti₂, Zr₂, Hf₂] and [Va₂, No₂, Ta₂] are then the next two families. [Zn₂, Cd₂, Hg₂] is the last family of heavy metal diatomic molecules of concern.

Cross combinations on the basis of any set of three heavy metal atoms are further considered, as long as data are available.

We further coined 5 more families made of heavy heavy metal hydrides, oxides, chlorides, and alkalines. These families are shown in Index 2.

Index 1, Index 2 (see end of text)

On the whole, we have 33 “alike families” altogether. Various parameters, including the dissociation energies (\mathcal{D}) and internuclear distances (\mathcal{R}), together with the products $\mathcal{D}\times\mathcal{R}$ for diatomic molecules belonging to each of these families, are shown in the subsequent Tables 1-33 (*cf. “supporting information”, annexed to this article*).

As can be visually tracked page after page, the quantity $\mathcal{D}\times\mathcal{R}$ strikingly remains *constant* for all of the chemical families we framed, no matter how much the complexity of the molecule at hand increases along with the ingress of more and more massive nuclei with their associated heavier and heavier electronic clouds. While the *constant* coming into play is different for each family, the important thing to emphasize in any event is that the *electrical interaction capability* reigns *strongly and commensurately* even for heavier, thusly more complex, bodies. It delineates, remarkably, an ever increasing trend versus *complexity* in especially some of the cases.

At this juncture, we have to discuss how we appraise the complexity of the object. One immediate answer is, we can assess it by the number of protons and associated electrons. The higher Z_1 and Z_2 (*i.e.*, the atomic numbers of the atoms making the diatomic molecule at hand) the more complex the object would be. The numbers Z_1 and Z_2 , when multiplied by 3, determine the *total number of coordinates* in the eigenfunction we introduced above for a diatomic molecule made of alike atoms; *i.e.*, when $Z_1=Z_2=Z$, the number of coordinates of becomes $2Z\times 3=6Z$, and, in general, it is $3\times(Z_1+Z_2)$. We could then propose to evaluate the complexity under scrutiny as the sum Z_1+Z_2 .

All the same, the product Z_1Z_2 gains priority in measuring the complexity of the diatomic molecule one deals with; after all, this product represents the number of interactions reigning in-between the protons of the first atom and the electrons of the second, were the diatomic molecule at hand not ionized.

This brings forth the possibility of considering straightly A_1A_2 – *i.e.*, the product of the atomic weights of the atoms constituting the molecule – *where the atomic numbers Z_1 and Z_2 are anyway included respectively in the atomic weights A_1 and A_2 .*

Having settled on this last consideration, we hence propose to plot our $\mathcal{D}\hat{\mathcal{I}}\mathcal{R}$'s versus A_1A_2 's. The reason for this is our insight which led us to anticipate right at beginning a *slight increase* in $\mathcal{D}\hat{\mathcal{I}}\mathcal{R}$ with respect to A_1A_2 for very large A_1A_2 's (*e.g.*, *much larger than those delineated by the entire body of diatomic molecules – no matter whether such A_1A_2 numbers are hypothetical or not*).

It is anyway rewarding to observe at the final stage that clues of such behavior clearly pop out of some of the figures we present below.* I strongly suggest to omit this footnote. It definitely represents a subject of a separate research, lying outside the scope of the paper.

Based on the foregoing deliberation, we draw each $\mathcal{D}\times\mathcal{R}$ with respect to each product A_1A_2 for all of the 33 families of alike diatomic molecules that we framed under this study. Related plots are drawn in Figures 1-33, which can be checked in the *supporting information (annexed to this article)*. All the same, herein, for easy visualization, also comparison, we reassemble them, under Sets 1-6, geared in harmony with similar scales.

What we observe throughout is practically the same behavior. That is to say, $\mathcal{D}\times\mathcal{R}$, with respect to the product A_1A_2 , maintains a relatively high value and remains astonishingly that way despite increasing complexities – *no matter whether or not the value of the investigated constant of concern changes from one family to the other*. This is so much so that, at the time we were drafting this paper, we entertained doubts about the validity of the values of a diatomic molecule which looked somewhat misplaced on a particular graph; and as an immediate remedy, a cursory search for *more recent data (or computed data whenever possible; cf. Ref. 5)* indeed benefitted us with a better-fit with regards to the overall distribution of points in the plot of concern.

As an example and a comparative aid, we drew some of the figures (such as Figure 1) with more recent data (black curves) superposed over the older data (blue curves) (see supporting information). This endeavor afforded us the possibility of determining which one of the two parameters out of the couple (\mathcal{D} , \mathcal{R}) for a diatomic molecule would better belong to a locale amongst the two representations of the diatomic molecules on our plot if the other one was adequately known.

In any case, regardless of how heavy the atoms making up the diatomic molecule are, they electrically still remain equally unopaque toward each other – if not even more transparent versus complexity for all groups composed of chemically-alike diatomic molecules. Therefore, the *persistent constancy*, and *even further, the ascending trend* of $\mathcal{D}\times\mathcal{R}$ for larger and larger

* Following our referee's righteous inquiry about more precision on our choice to plot $\mathcal{D}\hat{\mathcal{I}}\mathcal{R}$ with respect to A_1A_2 , and speaking *forthright*, we like to share with our readers that, we wished originally to see, as an *elementary exercise*, whether one can somewhat bridge *electric force*, via the examination of diatomic molecules, *with gravitational force*, which would thus possibly turn to be a *manifestation* of the former force at large distances. While we do not advocate here any claim on this at all [*for the magnitudes of A_1A_2 we could work with, do not go beyond 10^5 , whereas one needs to see, how the behavior of concern would be, at around $A_1A_2=10^{36}$, and even more fundamentally $D(r)$, say, for the H_2 molecule, falls much more sharply than $1/r$]; still, the information we forged out, together with the formulations we provided, herein, do not seem discouraging. In other words, we have originally anticipated that the slope of $\mathcal{D}\hat{\mathcal{I}}\mathcal{R}$ with respect to A_1A_2 would tend to assume the gravitational constant G , if not already for the heaviest diatomic molecules, still, for what could be tapped beyond, via extrapolation. Recall that the *product* of the *gravitational dissociation energy* of A_1 and A_2 by the *distance separating these two objects*, is proportional to G . Thereby frankly, we had predicted a fall of $\mathcal{D}\hat{\mathcal{I}}\mathcal{R}$ from its value at $p-e$, with respect to A_1A_2 , then, a more or less sustained value of it, and then a soft climb of it, to catch with its value at $p-e$, and eventually go beyond this ceiling. As it stands we happened to have tapped what we have originally predicted. So much so that, not only that heavy metals (Sets 5 and 6) show already an aggressive trend on that matter; but furthermore, the slope we coin between Fr_2 and $Unue_2$ (Set 1), intercepts the level $p-e$ of $\mathcal{D}\hat{\mathcal{I}}\mathcal{R}$, at $A_1A_2=10^7$ amu², all the same, promising to approach to the asymptote G , in a long hypothetical run. We would like to stress, we have no claim, on any kind of demonstration of our original insight, over here. We save the analysis of all of the physico-chemical information deployed herein, for a follow-up work, some of the clues of which are painted in the text. In any case, as discussed right above, the product A_1A_2 , is not far at all, from representing the product Z_1Z_2 . Our original insight may lead to a result complying with Nature or not, and both of these results, no matter which of the two, is the correct one, would surely be precious. In any case, herein we simply tried to answer in full sincerity our referee's relevant query.*

complexities may bear a profound meaning when plotted versus A_1A_2 as we intimated right above.

Actually, it is but a question of the attraction of the two atoms of concern that are candidates to form a diatomic molecule. The attraction, just like we deliberated on the basis of the H_2 molecule, results from the summation of four interactional potential energy terms. Despite this fact, we propose (though without any loss of generality) to simplify things not only for the H_2 molecule, but also for diatomic molecules of even highest complexities; and, as a means of easy conceptualization, to suppose that the attraction is governed by just the *cross-attractional terms*.

As a matter of fact, it is non-challenging to understand this in the light of polarization, which happens, for instance, with regards to alkali halides such as LiF, LiBr, NaF, NaBr, *etc...* (cf. Group 2, Index 1). Such a diatomic molecule can indeed well behave, on the whole, as a pair of positive and negative charges with the intensity of each being close to e . This already constitutes a strong argument to adopt our general proposition of handling diatomic molecules based only on the terms of mutual attraction in-between the nuclei and the proximate electronic clouds. Further on, under the given circumstances, $\mathcal{D}\times\mathcal{R}$ for such molecules would be expected to arise at a magnitude not far from e^2 ; which, at least for the given set of molecules, could explain the reigning constancy of $\mathcal{D}\times\mathcal{R}$.

All the same, though, it was not expected *a priori* that $\mathcal{D}\times\mathcal{R}$ would remain at the e^2 order of magnitude for all diatomic families; *but it conspicuously does, and even exceeds it in some cases* – which makes that we can effectively *conceptualize* the attraction force term between the atoms of diatomic molecules as comprising just the *cross-attractional force terms*.

3. Approximate representation of the dissociation energy $\mathcal{D}(r)$ at small interatomic distances vis-à-vis the constancy of $\mathcal{D}\times\mathcal{R}$

To make easier the reception of our idea, one may initially carry the exercise over to the H_2 molecule and suppose henceforth that the attraction is generated merely by *i) first proton-second electron* coupling, and *ii) second proton-first electron* coupling; where, with the denominations *first* and *second*, we mean the *first H atom* and the *second H atom* making the H_2 molecule. We can afterwards reduce the resulting attraction force by a given constant to take into account the forces of repulsion.

At any rate, the idea we propose facilitates the expression of the magnitude of the attractional potential energy, especially near the ground state, as $k_0^2e^2/r$ – where k_0 is a *reduction factor* associated with the charge e , which we can well calculate as such. It will be seen below that this is, in effect, quite plausible.

Thus, the dissociation energy \mathcal{D} at the ground level becomes

$$\mathcal{D} = k_0^2e^2/\mathcal{R} . \quad (1)$$

We would like to call the quantity $k_0^2e^2$ the “*product of effectively attractive charges*”.

While we have written eq. (1) at the start for the H_2 molecule, we will soon see that it can be considered quite valid in general.

The fact remains that the coefficient k_0^2 is expected to behave *nearly as a constant* for alike diatomic molecules – *i.e.*, with similar electronic configurations, which already provides an explanation as to the constancy of $\mathcal{D}\times\mathcal{R}$ we conjecture for the given molecules.

Thus we propose to represent the product *dissociation energy* $\hat{\mathcal{I}}$ *interatomic distance* by a constant in the proximity of the ground state; which is indeed the case given that the product

$\mathcal{D} \times \mathcal{R}$ exhibits a “plateau” around the interatomic distance \mathcal{R} . Therefore, in the zone near the ground state, we propose to express the dissociation energy $D(r)$ of the molecule with respect to r (i.e., separation distance between the nuclei) as

$$D(r) = k_0^2 e^2 / r, \quad (2)$$

insofar as involving the *same constant* k_0 . Thus, under the given circumstances, one may assume that $D(r)$ displays a *hyperbolic* dependence on r near the ground state.

We dealt with yet the H_2 molecule. In the meantime, let us stress the fact that eq. (2) can be rephrased to be more generally valid. It is so much so that the heavier the molecule under consideration, the wider will be the *plateau* of concern delineated by $D(r) \times r$ near the ground state; for, the wider will evidently be the interatomic distance, and, by the same token, the smaller will be its dissociation energy – meaning the shorter will be the occupied space of the *dissociation process*. We would even expect that a giant molecule made of huge atoms of the given kind, if one could ever manufacture it, would thusly demarcate a very wide interatomic distance.

Therefore, not only can we confidently rely on eqs. (1) and (2) for our purposes at this stage of the present work, but, extraordinarily enough, we soon come to discover that the dissociation energy for the heaviest molecules will tend to behave in accordance with eq. (2) beyond the ground state (*given that there is hardly any room left for any excited state beyond that*).

Let us come back to the H_2 molecule. The known fact that dissociation energy falls much more acutely than the $1/r$ dependence under the usual circumstances, thusly at $r > \mathcal{R}$, should anyway be emphasized. Nevertheless, eq. (2) can still be considered valid in the zone near the ground state.

As is known, the ground dissociation energy \mathcal{D} of the H_2 molecule is 4.52 eV at room temperature. On the other hand, the magnitude of the potential energy of a proton and an electron ($p-e$) bound at the distance of a Bohr Radius (0.529 Å) from each other is $2 \times 13.6 = 27.2$ eV.

That is to say, the dissociation energy \mathcal{D} of the H_2 molecule is already quite high, while its average internuclear distance is 0.742 Å. Under these circumstances, k_0^2 , in reference to the dissociation energy of $p-e$ (*conjecturally held at rest at a distance equal to the Bohr Radius*) becomes

$$k_0^2 = 4.52 \times 0.742 / (27.2 \times 0.529) = 3.35 / 14.39 = 0.233;$$

which makes that, for the H_2 molecule, k_0 is about 0.5 near the ground state. This is how we propose to pin down the value of k_0 to be associated with the simplest isotope of the H atom near the ground state also.

By the proposed methodology, $\sqrt{k_0^2 e^2} = k_0 e$ comes first of all to betoken an *effective electric charge to be associated with both H atoms* and characterizing the pull between these atoms in an H_2 molecule. Thereby, it is this *equivalent charge* which, for one thing, governs the net attractional electric field created by the H atoms on each other near the H_2 molecule’s ground state [see eq. (1)].

The reason we considered the hypothetical static bound system of $p-e$ versus the H_2 molecule is that the dissociation path of both systems is rectilinear – thus, similar; whereas, the dissociation energy of the H atom is half of that of the $p-e$ system. Therefore, the dissociation of

the hypothetical static p - e bond and of the dissociation of the H_2 molecule can well be considered side by side for purposes of comparison.[†]

In that sense, the statically held proton and electron in the suppositional p - e setting constitutes the simplest attractional binary system delineating $k=1$ pursuant to our abridged framework about the attractional mechanism for the H-H molecule; whereby, all other diatomic molecules can follow suit.

It is surely interesting to unveil that, despite all the interelectronic screening the heavy diatomic molecules are thought to undergo, the $\mathcal{D} \times \mathcal{R}$ value associated with some of them can turn out to be as high as that of the p - e system, and manifestly even higher...

This means the electrical field transmission in-between complex atoms making up the given diatomic molecules is virtually as important as the electrical field transmission created between a bare electron and a bare proton; which is remarkable once tapped from the enterprise advanced herein that could prospectively encompass the entire body of diatomic molecules.

Thus, we now propose that, on the whole, the dissociation energy may be written essentially based on the sum of i) the dissociation energy of the attraction between the first atom's nucleus and the electronic cloud of the second atom, and ii) the dissociation energy of the attraction between the second atom's nucleus and the electronic cloud of the first atom – whereby, eqs. (1) and (2) can, in general, be re-formulated as

$$\mathcal{D} = \frac{(Z_1 e)(z_2 e)}{K \mathcal{R}} + \frac{(Z_2 e)(z_1 e)}{K \mathcal{R}} = 2 \frac{(Z_1 e)(z_2 e)}{K \mathcal{R}}; \quad (3)$$

with Z_1 and Z_2 being the respective number of protons that reside in the nuclei of the atoms constituting the diatomic molecule at hand, and where z_1 and z_2 are respectively the numbers of the corresponding electrons (*for neutral atoms, we naturally have $Z_1=z_1$ and $Z_2=z_2$*), while \mathcal{R} represents a constant which takes care of the weakening of the potential energy as referred to what one would, in cases where point-like charges $Z_1 e$ and $z_2 e$ are considered, have to face, and K is a constant that reduces the outcome due to the repulsion between respectively the nuclei and the electronic clouds under consideration. All the while, the former constant reigns naturally with regards to the interaction of $Z_2 e$ with $z_1 e$.

No matter how complicated the situation might become, we still propose, at this stage, to write eq. (3) as

$$\mathcal{D} = k_{10} k_{20} \frac{e^2}{\mathcal{R}} \quad (4a)$$

for alike molecules at the ground state – with k_{10} and k_{20} getting associated with the first and second atoms making the diatomic molecules of concern, so that $k_{10} k_{20}$ then reads as

$$k_{10} k_{20} = 2 / K. \quad (4b)$$

Similarly to $k_0^2 e^2$ associated above with the H_2 molecule, we call $k_1 k_2 e^2$ the “*generalized product of effectively attractive charges*” associated, in general, with any diatomic molecule of concern; where $k_1 e$ and $k_2 e$ are their respective “*equivalent attractional charges*”.

[†] The p - e bond may not, after all, be hypothetical: The water molecule H-O-H, for instance, constitutes a dipole made of $2e^-$ and $2e^+$ separated by a distance of about 1 Angström.

In any case, the value of the product $k_1 k_2$ can now be derived from eq. (3) after knowing \mathcal{D} and \mathcal{R} in just the way we did for the H_2 molecule above.

As the next step, we are going to express the dissociation energy $D(r)$ of the given molecule whose nuclei are separated by a distance r at the zone near the ground state – *i.e.*, around \mathcal{R} , [see eq. (2)] – as

$$D(r) = k_{10} k_{20} e^2 / r, \quad (5)$$

which still contains the same constants k_{10} and k_{20} .

One can quickly check the validity of eqs. (2)-(5) on the basis of the H_2 molecule. We thus draw Table 34,¹² we then plot $D(r) \hat{=} r$ with respect to r in Figure 34 (*cf. supporting information*).

Thus, it can be observed in Figure 34 that, as one approaches $2\mathcal{R}$ (or more precisely, as one comes within the interval $1.5 \text{ amu} < \mathcal{R} < 2.5 \text{ amu}$, where amu is 0.529 \AA), one encounters a *plateau*. (Recall that the maximum for $D(r)$ occurs at $\mathcal{R} = 0.74 \text{ \AA}$; *i.e.*, 1.4 amu).

Therefore, we anticipate that, in the *vicinity of the ground state*, first eq. (2) written for the H_2 molecule, and then eq. (5) written for any of the heavier diatomic molecules, can be considered as plausible representations of the dissociation energy with respect to r .

The mentioned approach may be even more plausible for diatomic molecules of higher complexity, because the dissociation energy happens to be much less at those levels, and the path of dissociation one should pay attention to is relatively shorter.

One can further demarcate a guideline as regards the validity of eq. (5) and, in effect, with respect to the validity of eq. (4). Indeed, if this latter equation is valid, then one should be able to write

$$\mathcal{D}_{ii} \mathcal{R}_{ii} = k_{i0}^2 e^2, \quad (6a)$$

$$\mathcal{D}_{jj} \mathcal{R}_{jj} = k_{j0}^2 e^2, \quad (6b)$$

along with the following trivial definitions:

- \mathcal{D}_{ii} : Dissociation energy of the molecule i-i
- \mathcal{D}_{jj} : Dissociation energy of the molecule j-j
- \mathcal{R}_{ii} : Internuclear distance of the molecule i-i
- \mathcal{R}_{jj} : Internuclear distance of the molecule j-j
- k_{i0}^2 : The constant associated with the molecule i-i
- k_{j0}^2 : The constant associated with the molecule j-j

Let us further indicate the following available definitions:

- \mathcal{D}_{ij} : Dissociation energy of the molecule i-j
- \mathcal{R}_{ij} : Internuclear distance of the molecule i-j

We now write eq. (5) for the molecule i-j:

$$\mathcal{D}_{ij}\mathcal{R}_{ij} = k_{i_0}k_{j_0}e^2 \quad ; \quad (6c)$$

and then we square it:

$$D_{ij}^2R_{ij}^2 = k_{i_0}k_{j_0}e^2k_{i_0}k_{j_0}e^2 \quad . \quad (6d)$$

This leads to

$$D_{ij}^2R_{ij}^2 = D_{ii}\mathcal{R}_{ii}D_{jj}\mathcal{R}_{jj} \quad . \quad (6e)$$

Therefore, if this latter equation holds, it would mean that eq. (5) would hold. Here, we have no room to show any details. All the same, eq. (6e) can be ascertained to remain valid within an error margin of roughly 10% and, for some cases such as Rb-Cs and Br-Cl, within an error margin of around 1% or even less (cf. Te-Se).

Thence, first things first, we propose to express the dissociation energy $D(r)$ of any diatomic molecule around the *ground state* the way given in eq. (5).

Effectively, we disclose through Figs. 1-33 that $\mathcal{D}\hat{\mathcal{R}}$ stays constant for a particular family – *even starting from comparably light diatomic molecules all the way up to the heaviest ones*.

This means several important things:

- Eq. (5) is already valid near the ground state for each member of any family.
- A figure similar to Figure 34 (*cf. supporting information*) that we would draw for the first member of a given family, when displaced appropriately, becomes virtually identical to similar figures we would draw for the next members of the family – though with ever smaller dissociation energies and shorter dissociation pathways.
- Eq. (5) then becomes valid for the entire range of space covered by the respective ground states.
- It is so much so that the heavier the molecule under consideration, the smoother the *plateau* of concern will be near the ground state, for the wider evidently will be the interatomic distance.
- Thence, surprisingly, electrical field transmission capability turns out to be unexpectedly high even for atoms of extreme complexity.
- Eq. (5) operates very adequately for the entire body of diatomic molecules – albeit with the condition that it should be fixed for each chemical family separately.

What is just as exciting is the following:

Suppose one hypothetically keeps making more and more massive a molecule of a given kind; let us consider as an example the set composed of Li_2 , Na_2 , K_2 , Rb_2 , Cs_2 , Fr_2 – we can then conceive of molecules made of atoms heavier than Francium (Fr) and obeying the alkali atom rules. Can we not? Surely it is plausible and apparently realistic; even if any exotic isotope we end up with is exceedingly unstable (seeing as the heaviest available alkali Francium’s most stable isotope has a half-life of merely 22 minutes)... But why do we do this, actually? We do it because we propose to apprehend atomic interactions in-between such putative heavy atoms as not any different than atomic interactions in-between the lighter atoms of the given kind.

Next, it will be conjectured that, as we keep on piling nucleons and negatrons at just the right admixture onto our hypothetical alkali atoms, the positive charge of the nucleus of concern and the negative charge of the corresponding electronic cloud will quantum mechanically interfere more and more with each other to the extent that, after crossing a certain weight threshold, we may be entitled to speak of an altogether “homogeneous distribution” of all

charges inside each giant atom – inasmuch as denoting a strict algebraic neutrality of electric charge.

The essential idea here is that an attractional electric field of source charge ke will still leak out of these giant atoms where k approaches and perhaps even surpasses unity. The heavier the molecule at hand, the more rigorously will its dissociation energy obey eq. (5).

Suppose now that the two giant atoms of the given kind form, however fleetingly, a giant molecule. We would expect it to endure under an enormously wide interatomic distance (*as we will quantify right below*) across which eq. (5) will rigorously reign. And there will further on be no change in the dissociation energy versus the interatomic distance, for recombination and dissociation would meet at practically the same interatomic distance; there would, in effect, be no room for any vibrational excited levels after a certain point.

Therefore, we can i) confidently rely on eqs. (4b) and (5), and ii) remarkably come to disclose that the dissociation energy for the heaviest molecules will tend to behave approximately in accordance with eq. (5) all the way through.

Looking at the general ascending behavior of the $D\chi\mathcal{R}$ plots for chiefly the heavy molecules, there appears hence a *postulatory universal neutral atom of mass $M_{Universal}$* , or M_U for short, which would leak an attractional electric field of source charge of intensity e , for which the coefficient k would assume the value of just unity.

This trend is most apparent for heavy metal molecules (*cf. Figures 19-33, or Sets 5 and 6*); M_U for them occurs, for instance, at an even lighter upperbound. In any case, via writing $GM_U=e^2$, with G standing for the gravitational constant, one derives $M_U=(\frac{1}{f_{sc}})^{1/2}M_{Planck}$, where f_{sc} is the *fine structure constant* and M_{Planck} is the Planck Mass at 2.18×10^{-8} kg, whereby M_U becomes 2.04×10^{-10} kg.

All the same, a group of, say, hydrogen atoms whose total mass amounts to the delineated universal mass M_U too will be expected to leak an attractional electric field of source charge of intensity e . This, though, is a peculiar problem: H atoms in an H-H molecule do not, for one thing, attract each other in accordance with e^2/r^2 , and the dissociation energy of the H-H molecule appears to die away with a spatial dependency much more enhanced than $1/r$.

The question then becomes “if a test H atom is subjected to the force F vis-à-vis a source H atom sitting at a given distance from the former one, will, “said test atom” be subject to the force of strength $\mathcal{N}F$ vis-à-vis \mathcal{N} number of H source atoms sitting together at the same distance?”. The answer to this question, is not trivial, for the test atom’s proton and electron now interact with \mathcal{N} protons and \mathcal{N} electrons belonging to the set of source $\mathcal{N}H$ atoms. This problem should moreover be posed quantum mechanically and solved accordingly to understand how the dissociation energy $D(r)$ of $\mathcal{N}H$ -H at large distances shall behave with respect to the distance r between $\mathcal{N}H$ and H. We leave such a problem for a future study (*and here effectively, may be a clue, with respect to our insight, as to one can bridge electric force with gravitation*).

In any case, let us go back to our thought experiment of enlarging, say, an alkali atom until it reaches the mass M_U , wherefore this atom will supposedly leak an attractional electric force of charge e . Let us thence call R_U the radius of our giant alkali atom of mass M_U .

We now propose to determine the radius R_U .

For this purpose, we can trace the radii of alkali atoms versus their weights and then extrapolate the sloping behavior to the weight M_U . This neatly leads to an r of about 0.1 mm.

Such a finding resumes many crucial discussions:

- The conjectural giant alkali atom of mass M_U and radius $r=0.1$ mm is supposed to leak an attractional electric field of source charge of intensity e whilst behaving in full accordance with eq. (5).
- It appears that, remaining at this juncture at a macroscopic distance, the giant atom in question will not act with regards to just its immediate vicinity in accordance with eq. (5), but (*as discussed*) will act the same all the way through.

- A neutral mass of anything weighing as much as M_U is expected to act identically.

4. The constancy of $D(r) \times r$ for alike electronic configurations out of the Schrödinger Equation or Dirac Equation (whichever is appropriate)

In order to authenticate our eq. (5), we now present a derivation on the basis of quantum mechanics. T. Yarman had previously shown that, were the “mass” of an entity – the way described by the Schrödinger Equation or the Dirac Equation (*whichever is appropriate for the case under consideration*) – increased by an arbitrary number, then the eigenvalue (*total energy*) in said description (*irrespective of whether it is relativistic or non-relativistic*) is identically increased and all sizes are contrariwise identically decreased [13,14,15,16, 6-9]. This property is thoroughly general and is valid for any quantum mechanical description no matter how complex.

Remarkably, such an outlook yields the *invariance* of the spatiotemporal combination $mass \hat{\Gamma} energy \hat{\Gamma} size^2$ (for any size that one might pick) with respect to a *hypothetical change in mass* injected to the quantum mechanical description of the entity at hand.

We have to emphasize that we maintain this reflects a series of fundamental properties about matter – such as, first of all, a “*symmetry property*” in the Schrödinger Equation or the Dirac Equation with regards to a *mass change* input. It is primarily this “rest mass change contingency” that we are interested in over here.

So, we embark upon the hypothesis that such a “*rest mass change*” is *real*. It may consist of a *mass increase* when the object of concern is brought to a uniform translational motion [13]; or, it may consist of a *mass decrease* when the object at hand is embedded in a field it can interact with – such as a *gravitational field* [16]. In any case, we posit that the combination $mass \hat{\Gamma} energy \hat{\Gamma} size^2$ will stay invariant no matter what.

If there is more than one mass involved with the quantum mechanical description at issue, care is required to *identify* which “mass” is to be inputted to the spatiotemporal combination of concern for further processing. Here, we can overlook this peculiarity, for, we propose to apply the property under consideration to just the *electronic description* of a diatomic molecule extracted from the overall Schrödinger description of the molecule on the basis of the *Born and Oppenheimer approximation* [2]. As described in the Introduction part above, this *electronic description* is written for the pair of *fixed nuclei* separated by the distance r ; whereby the “energy” quantity of interest becomes its eigenvalue and we call the magnitude of this energy $D(r)$ – *i.e.*, the dissociation energy the molecule exhibits from the interatomic distance r onward.

In such a case, *mass* becomes the mass m of the electron, while the *size* to be focused on is particularly the interatomic distance r . Therefore, according to Yarman, and later on his colleagues too, *with respect to any mass change injected to the electronic description under consideration*, we must have

$$mD(r)r^2 = \text{Invariant.} \quad (7)$$

The invariant coming into play ought, after all, to relate to a *universal quantity* bearing the same dimensions and necessarily encompassed by the *Schrödinger Equation* or the *Dirac Equation* under scrutiny. This “*quantity*” cannot then be anything else but something proportional to the square of the Planck Constant h^2 , which is the *pivotal quantity* of any quantum mechanical description.

Therefore we arrive at

$$mD(r)r^2 \sim h^2. \quad (8)$$

Yarman had further argued in [6,9] that the *proportionality constant* coming into play must be commensurate with a constant g_n characterizing the *electronic configuration* of the molecule.

The presence of h^2 moreover necessitates, alongside itself, quantum numbers after supposing that r can only be changed incrementally.

To cut a long story short, for, say, an H_2 molecule, one can assume that two quantum numbers n_1 and n_2 will emerge; whereby, the product $n_1 n_2$ would be expected to multiply h^2 . We may, for simplicity, denote this product by the overall number n^2 . Recall that the quantum numbers we introduced are primarily mathematical artefacts tuned towards a simplified derivation. Therefore, we can rewrite eq. (8) via a self-explanatory notation – *at the quantum state which we will represent by just the number “n” (no matter whether or not this is even an integer)* – as

$$mD_n g_n r_n^2 = n^2 h^2. \quad (9)$$

Note that such a relationship can already be formulated within the framework of the Bohr Atom Model; and, had we written $\delta^2 mD_n g_{nBohr} r_n^2 = n^2 h^2$, the coefficient g_{nBohr} turns out to be simply *unity* in this case.

Based on the general eq. (9) written for any entity of concern, Yarman had, in addition, argued in [13, 16] that multiplying h^2 by n^2 is equivalent to dividing the *mass* m by n^2 in the corresponding quantum mechanical description; in which case, the interatomic distance r_n will get stretched as much as n^2 compared to the interatomic distance \mathcal{R} at the ground level [17,18,10,11]. Thus,

$$n^2 = r_n / \mathcal{R}. \quad (10)$$

Note that this relationship is exact. With this in mind, one can now rephrase eq. (9) as

$$mD_n g_n r_n \mathcal{R} = h^2 \quad (11)$$

to land at

$$D_n r_n = h^2 / m g_n \mathcal{R}. \quad (12)$$

This relationship is rigorous and is valid for any diatomic molecule. The only point to be remembered is that, we landed at it based on the Born & Oppenheimer (B&O) approximation, sketched in the Introduction above [2].

At this stage, we do not know how g_n would vary with the quantum state characterizing number n . One thing looks certain though; g_n is expected to stay the same for alike configurations [17,18].

This is a prized disclosure; not only does it work within the frame of excited states configured similarly within a given molecule, but it also works with regards to, say, *the ground states of a set of molecules* belonging to any of the families we assembled, which are also configured similarly.

Thusly, the foregoing derivation is well capable of clarifying the *nearly constant value* $\mathcal{D}\mathcal{X}\mathcal{R}$ we revealed in Sets 1-6 (*made out of Figures 1-33, which are in turn presented in supporting information*) with regards to similarly configured diatomic molecules. This already points to the *validity* of eqs. (1-5).

The nearly constant value (*which we qualified in the title of this article as “enigmatic”*) of $\mathcal{D}\mathcal{X}\mathcal{R}$ must generally be understood, as the constancy of the magnitude of it, yet still, remain-

ning within a rather narrow band, the way Sets 1-6, we present below, witness. While eq. (12), is rigorous as precised, along the B&O approximation, still, *tolerable oscillations* of $\mathcal{D}\chi\mathcal{R}$, are most likely due to i) the said approximation, also ii) to the fact that the electronic configurations we expected to be the same, with regards to the members of chemical families, we worked on, might not, as it appears, exactly the same.

One, further on, is inclined to inquire whether, say, Hydrogen (H) atoms of an H-H molecule may delineate the same constant g_n when separated by large distances from each other. It seems this would hold for the H_2^+ molecule (which for sure is interesting to investigate);¹⁹ valid with regards to the standard H-H molecule.²⁰

All the same, and even more importantly, here, as introduced above, one should more fundamentally handle, the *quantum mechanical dissociation problem* of $\mathcal{M}\text{H}$ atoms (\mathcal{N} tending to infinity), on the one side, and just a single H atom situated far from $\mathcal{M}\text{H}$, on the other side.

Such a situation seems to denote a peculiar problem which we plan to further elaborate on, in a subsequent study.

5. Badger's Rule

At this point, we like to call on the empirical Badger's rule,²¹ as might be in effect evoked, through this dissertation. It states in brief that the *strength of a bond is correlated with its vibrational frequency* ν_n at the given n th state.

We can represent the bond strength, *roughly* with the dissociation energy D_n ; we would, following Badger's rule, more carefully, propose to write

$$D_n^k \sim \nu_n \quad (13)$$

where k is an exponent to be determined.

The present framework, allows us to derive something similar, and accordingly fix k , through Yarman's earlier approach [19, 20].

Indeed, for a given diatomic molecule, at the n th excited level, one can accordingly write,[‡]

$$\epsilon_n \sim \sqrt{r_n} r_n^{-2} = r_n^{-3/2} . \quad (14)$$

Since we landed through eq. (12), and this rigorously, at,

$$D_n r_n = C_1 ; \quad (14)$$

where C_1 is a *constant*, furnished by eq. (12), we can thereby write,

$$\epsilon_n \sim D_n^{3/2} . \quad (15)$$

This becomes equivalent to the Badger's rule, which yet we coined through the present approach, for a given diatomic molecule, and k of eq. (13), thusly turns out to be 3/2.

We can furthermore state that Yarman's approach [19,20], allows us to transpose the foregoing derivation, to members of any of the chemical families, we shaped above, where n ,

[‡] The rigorous Yarman relationship is this [19,20]:

$$T_n \sim \frac{4f^2 r_0}{h r_n} \sqrt{g_n M m_e r_n^2} ;$$

T_n is the vibrational frequency at the n th level; r_n is the internuclear distance, r_0 is the internuclear distance, at the ground level, g_n is a constant characterizing the electronic configuration of the bond, M is the reduced mass of the given atoms, and m_e is the electron's mass.

instead of n th quantized level in a given diatomic molecule, will now be associated with the i th member of the chemical family at hand. Under the circumstances, say, for alkali molecules, eq. (15), will read as,

$$\epsilon_i \sim \frac{D_i^{3/2}}{M_i^{1/2}}, \quad i=Li_2, Na_2, K_2, Rb_2, \dots; \quad (16)$$

here M_i is the *reduced mass* of the diatomic molecule belonging to the i th member of the given family, and takes place there, given that the vibration frequency is inversely proportional to it [19,20] (cf. the footnote below).

As a conclusion, we can affirm that Badger's rule does not seem to add any significant information to the present approach. So much so that; whereas it is empirical; eqs. (15) and (16), we came out with, are certainly rooted to a deeper quantum mechanical ground. The investigation of chiefly eq. (16) will be, no doubt interesting, which we already have checked out quickly, and it indeed works very fine.

6. Conclusion

It has been shown herein that, with respect to the body of diatomic molecules comprising such items as "strictly alkali pairs" or "strictly halogen pairs" or "mixed alkali-halogen pairs" or even "heavy metal pairs", etc... – each thus composed of diatomic molecules formed of atoms bearing similar electronic configurations – their *dissociation energy* (\mathcal{D}) \times *interatomic distance* (\mathcal{R}) products delineate a relatively high and perplexingly constant value.

More precisely, the $\mathcal{D}\mathcal{R}$'s versus the products A_1A_2 of the weights of atoms making up the molecules at hand decreases for light molecules, then acquires a value that remains fairly constant for intermediately heavy molecules, and then – were the span of A_1A_2 sufficient to track it – keeps on gently increasing for the heaviest molecules.

The increase in $\mathcal{D}\mathcal{R}$ with respect to A_1A_2 for some of the diatomic molecules we considered under the present study, such as the domain around W_2 (which climbs even beyond e^2), is, on the other hand, strikingly aggressive.

We thusly disclosed the *fairly constant* behavior of $\mathcal{D}\mathcal{R}$ at an unexpectedly high value very near e^2 (in *esu*) for each of the 33 families we arranged from chemically-alike diatomic molecules (cf. *Indexes 1 and 2 at the end of the text, and Tables 1-33, presented in supporting information*).

As a matter of fact, it is easy to think of this in reference to polarization – which takes place, for instance, in the case of alkali halides such as LiF, LiBr, NaF, NaBr, etc... as well as other halides (cf. Index 1, Group 2; and also Groups 4, 6, 8, 11, 15, 16, 17, 18). In suchlike situations, the diatomic molecule at hand can indeed behave, on the whole, as a pair of positive and negative charges where the intensity of each charge is close to e .

This already by itself constitutes a strong argument to adopt our general proposition as to the handling of diatomic molecules based on solely the attractive terms for mutual interactions between electronic clouds and nuclei alone.

In addition, $\mathcal{D}\mathcal{R}$ for such molecules would, under the given circumstances, be expected not to deviate far from e^2 ; which, at least for the mentioned sets of molecules, could explain the near constancy of $\mathcal{D}\mathcal{R}$.

Yet, it might appear hard to guess beforehand that $\mathcal{D}\mathcal{R}$ would remain at the e^2 order of magnitude, let alone at a value very close to it, for all the other diatomic families we dealt with and which we constructed upon one, two, or even three covalent bonds (cf. Index 1, Groups 1, 3,

7, 9, 10, 12, 13). But it well does so (*Tables 1-33, together with Figures 1-33 presented in supporting information*). Take a further look, as an extreme case, at the Si_2 and C_2 molecules: $\mathcal{D} \times \mathcal{R}$ for them takes the values of 7.2 and 7.7 eV \times Å (along with $A_1A_2=784$ and $A_1A_2=144$) respectively [4]. It so happens that the value of $\mathcal{D} \times \mathcal{R}$ for these molecules – *which are far from delineating electrovalent bonds* – comes to be strikingly at more than half of that of the pair of p - e .

This picture is further reinforced by the common behavior of diatomic molecules made of transition metals (heavy metals) presented in Sets 5 and 6 (Figures 19-33 of supporting information).

The sharply escalating trend in many of them versus the heaviest molecules is quite noticeable.

These observations allow us to presume that we can visualize the attraction force term between the atoms constituting the diatomic molecules as made of just the *cross-attractional force terms*; *i.e.*, the nucleus of the first atom attracting the electrons of the second and vice versa, in contrast to the nucleus of the second atom attracting the electrons of the first one and vice versa – no matter how much the coincident nuclei and electronic clouds mutually repel each other.

Thusly, we come to the following conclusions:

- The dissociation energy $D(r)$ behaves *hyperbolically* near the ground state with respect to r . This seems understandable on the basis of the plot we drew for molecular hydrogen displaying a *plateau* near the ground state (cf. Figure 34 of supporting information).
- It appears that this property remains practically valid for other diatomic molecules, too.
- An important point is that, the wider the atoms making the diatomic molecule, the wider will be the size of the *plateau* of $D(r)r$ (cf. Figure 34).
- This, *quantum mechanically* evokes that, as the size of the atoms, making the diatomic molecule at hand, though hypothetically, tends to practically infinity, through a longer and longer range, $D(r)r$, will remain constant, versus r .
- Without any further anticipation, still, the electrical field transmission capability becomes henceforth unexpectedly high for atoms of even very high complexity.
- We have figured out that a giant atom occupying, however fleetingly, a radius of around 0.1 mm , and remaining neutral on the whole, would leak an attractional electric field of source charge of intensity e whilst behaving in full accordance with eq. (5).
- Likewise, a neutral mass of anything weighing at a similar $M_U=2.04 \times 10^{-10} \text{ kgs}$ is expected to act the same.
- The fact that a neutral W (Tungsten) atom, having an atomic number equal to 184 ($184 \times 10^{-23} \text{ g} / 6 = 3 \times 10^{-25} \text{ kg}$), already behaves that way vis-à-vis another neutral W atom is surely worth deliberating in this regard.
- A bunch of, say, Hydrogen atoms weighing altogether as much as M_U would be expected to delineate the same behavior, too. This is surely controversial, for H atoms in an H-H molecule do not attract each other, for one thing, in accordance with $\sim e^2/r^2$, and the dissociation energy of the H-H molecule appears to vanish with a spatial dependency much more enhanced than $1/r$. The question then becomes “if a test H atom is subjected to the force F vis-à-vis a source H atom sitting at a given distance from the former one, will, “said test atom” be subject to the force of strength $\mathcal{N}F$ vis-à-vis \mathcal{N} number of H source atoms sitting together at the same distance?”. The answer to this question, is not trivial, for the test atom’s proton and electron now interact with \mathcal{N} protons and \mathcal{N} electrons belonging to the set of source $\mathcal{N}H$ atoms. This problem should moreover be posed quantum mechanically and solved accordingly to understand how

the dissociation energy $D(r)$ of the system $\mathcal{N}H-H$ at large distances shall behave with respect to the distance r between $\mathcal{N}H$ and H .

- In any case, one would tend to think that the opacity with respect to the attractional field transmission of a neutral atom will be diminished if an increased number of protons inside the nucleus are screened by an equal number of electrons residing in the electronic cloud surrounding the nucleus. This remarkably does not happen. Consider, for instance Set 4 presented below, and, pay in particular attention, to the red plot comprising the behavior of the Dissociation Energy x Interatomic Distance ($\mathcal{D}\times\mathcal{R}$) of Be-H, Mg-H, Ca-H, Sr-H, and Ba-H versus A_1A_2 (*the product of the atomic weights of the atoms making up the given molecules*). The nuclei of the neutral atoms Be, Mg, Ca, Sr, Ba, are screened by 4, 12, 20, 38, 56 electrons, respectively (*if one does not count the neutrons which, evidently, would not come into the description of the electrical attraction of the hydride in question in any meaningful way*). The fact remains that $\mathcal{D}\times\mathcal{R}$ – composed with regards to the hydrides of said atoms – delineates an increasing trend with respect to A_1A_2 . We observe that for even halogenic acids.

Thereby, if not an “increasing trend”, the “near constancy” of $\mathcal{D}\times\mathcal{R}$ with respect to A_1A_2 we revealed for particularly the diatomic molecules made of heavy atoms points *electric-wise* to i) the *non-opacity* of strictly neutral bodies, and thusly ii) an *attractional electric property of neutral matter*, regardless how heavy the mass of concern may be. With all restraint, and upon the skillful inquiry of our referee, we like to mention that, our original intuition consisted in the fact that, all this, may constitute a clue with respect to bridging electric force with gravitational force, which, in turn would become to be the manifestation of the former, at large distances.

If we want the acceptance of the paper, the indicated text must be removed. I am sure that the problem about representation of gravity via the latter idea must be much more better verified, before making this claim.

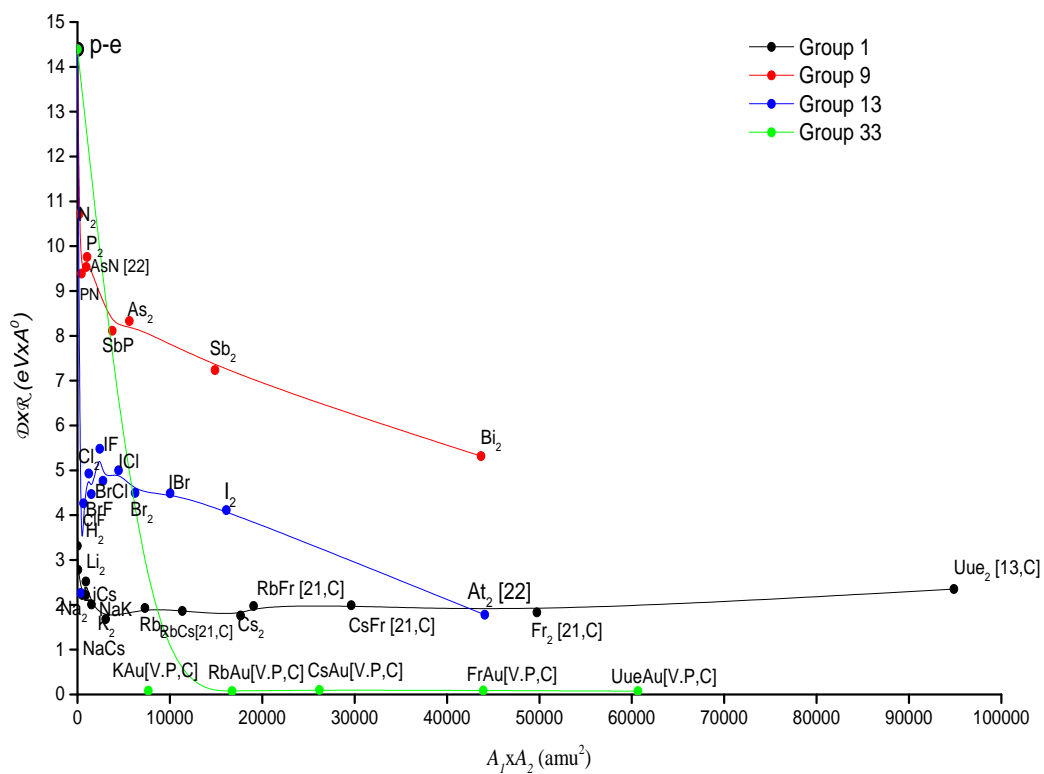
All of these enthusiastic aspects shall be elaborated on in a further work where we propose to check our arguments via plausible experiments.

Index 1 Alike families of diatomic molecules

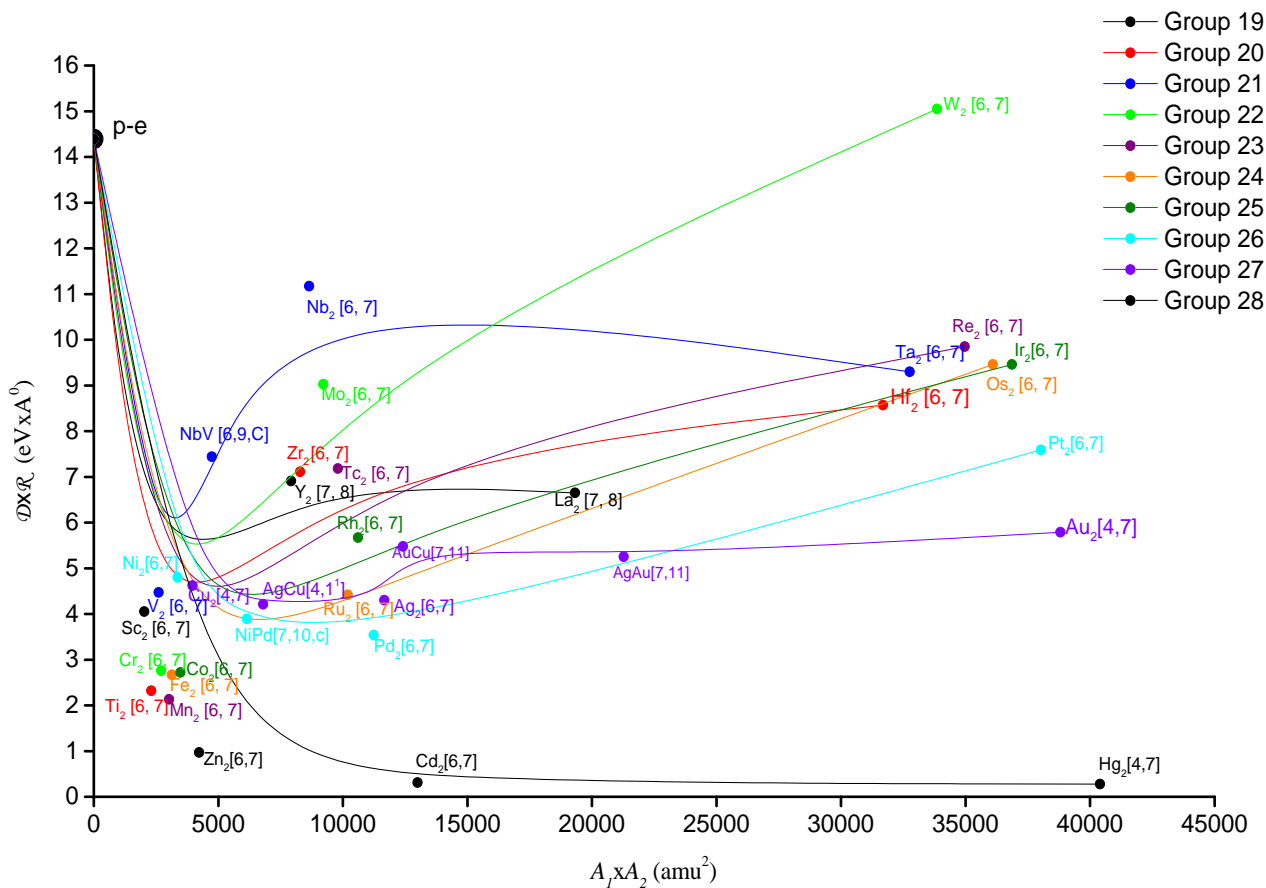
Group Number	Molecules made of Atoms belonging to columns [i, j] of the Table of Elements	Molecules belonging to the Group
1	[1,1]	H ₂ , Li ₂ , Na ₂ , K ₂ , Rb ₂ , Cs ₂ , Fr ₂ , Uuue ₂ , LiCs, NaK, NaCs, RbCs, RbFr, CsFr,
2	[1,7]	LiF, LiCl, LiBr, LiI, NaF, NaCl, NaBr, NaI, KF, KCl, KBr, KI, RbF, RbCl, RbBr, RbI, CsF, CsCl, CsBr, CsI
3	[2,6]	BeO, MgO, CaO, SrO, BaO
4	[2,7]	BeF, BeCl, BeBr, MgF, MgCl, MgBr, CaF, CaCl, SrF, BaF
5	[3,6]	BO, BS, AlO, AlS, GaO
6	[3,7]	BF, BCl, BBr, AlF, AlCl, AlBr, AlI, GaF, GaCl, GaBr, GaI, InF, InCl, InBr, InI, TlF, TlCl, TlBr, TlI
7	[4,6]	CO, CS, CSe, SiO, SiS, SiSe, GeO, GeS, GeSe, GeTe, SnO, SnS, SnSe, SnTe, PbO, PbS, PbSe, PbTe
8	[4,7]	CF, CCl, CBr, Cl, SiF, SiCl, SiBr, SiI, GeF, GeCl, GeBr, SnF, SnCl, SnBr, PbF
9	[5,5]	N ₂ , P ₂ , PN, As ₂ , AsN, Sb ₂ , SbP, Bi ₂
10	[5,6]	NO, NS, NSe, PO, PS, AsO, AsS, SbO, BiO, BiS
11	[5,7]	NCl, NBr, PF, AsF, SbF, BiF, BiCl, BiBr, McF, McCl
12	[6,6]	O ₂ , S ₂ , SO, Se ₂ , SeO, Te ₂ , TeO, TeS, TeSe
13	[7,7]	F ₂ , Cl ₂ , ClF, Br ₂ , BrF, BrCl, I ₂ , IF, ICl, IBr, At ₂
14	[1,7] <i>(Hydrogen Halides)</i>	HF, HCl, HBr, HI, HAt,
15	[1,2] <i>(Beryllium Group Hydrides)</i>	BeH, MgH, CaH, SrH, BaH
16	[1,3] <i>(Boron Group Hydrides)</i>	BH, AlH, GaH, InH, TlH
17	[1,4] <i>(Carbon Group Hydrides)</i>	CH, SiH, GeH, SnH, PbH
18	[1,5] <i>(Nitrogen Group Hydrides)</i>	NH, PH, AsH, BiH

Index 2 Alike families of diatomic molecules
composed of Heavy Metals

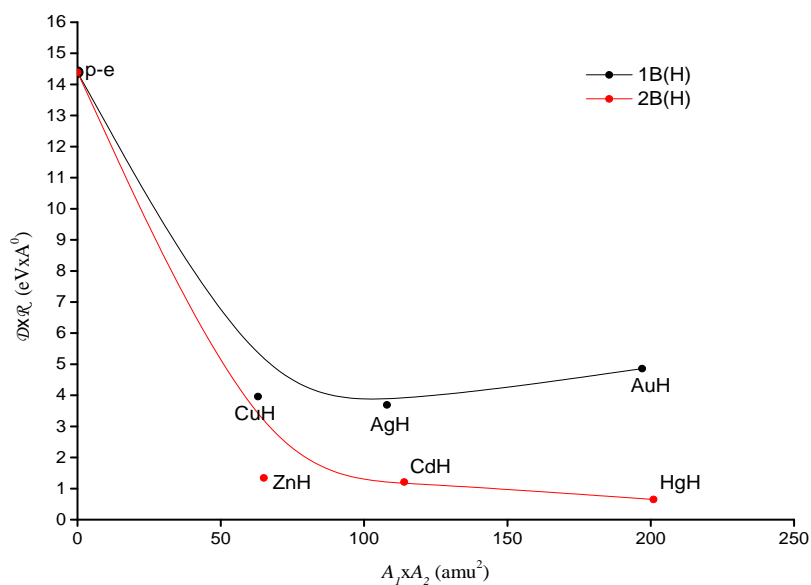
Group Number in the Periodic Table	Molecules made of Atoms belonging to the Said Group
IIIB	Sc ₂ , Y ₂ , La ₂
IVB	Ti ₂ , Zr ₂ , Hf ₂
VB	V ₂ , Nb ₂ , NbV, Ta ₂
VIB	Cr ₂ , Mo ₂ , W ₂
VIIB	Mn ₂ , Tc ₂ , Re ₂
VIII(Fe)	Fe ₂ , Ru ₂ , Os ₂
VIII(Co)	Co ₂ , Rh ₂ , Ir ₂
VIII(Ni)	Ni ₂ , Pd ₂ , NiPd, Pt ₂
IB	Cu ₂ , Ag ₂ , AgCu, AgAu, AuCu, Au ₂
IIB	Zn ₂ , Cd ₂ , Hg ₂
IB-Hydride	CuH, AgH, AuH
IIB-Hydride	ZnH, CdH, HgH
IVB-Chloride	TiCl, ZrCl, HfCl
VB-Oxide	VO, NbO, TaO
IB-Alkaline	KAu, RbAu, CsAu, FrAu, UueAu



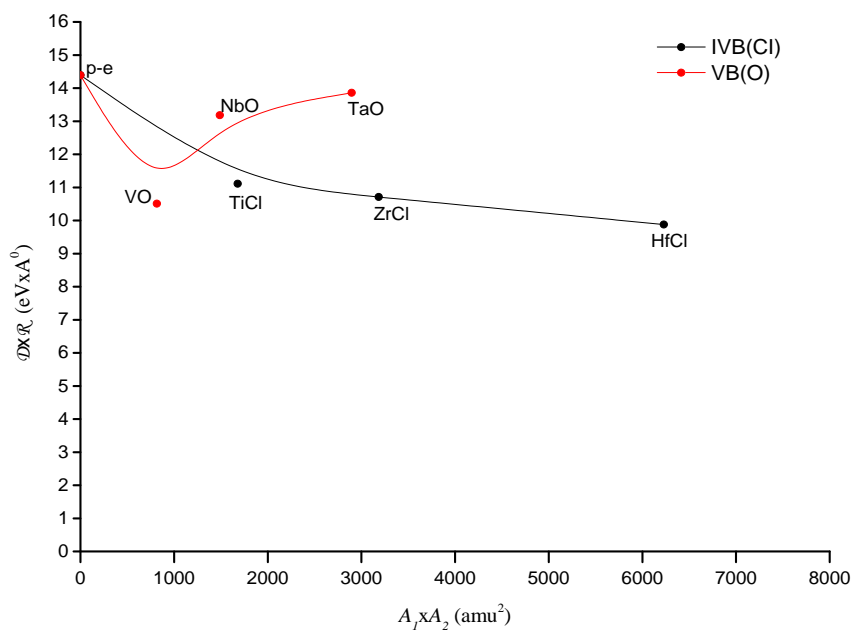
Set 1 Data is generally picked from [4]. Otherwise, for RbCs [²²:C], CsFr [22], RbFr [22], Fr₂ [22:C], for Uue₂ [²³:C], for AsN [²⁴], for At₂ [24,²⁵], for KAu, RbAu, CsAu, FrAu, UueAu [²⁶:C], it is picked from references indicated right next to the said molecules. “C” means, data is *computed*. Data for Li₂, is, versus its measured value [4], further computed [²⁷], in good harmony with what is previously reported.



Set 5 Data is generally picked from [4]. Otherwise, for Sc₂ [5], for Y₂, La₂ [6, 7], for Ti₂, Zr₂, Hf₂, for V₂, Nb₂, Ta₂ [5, 6], for NbV [6, 8:C], for Cr₂, Mo₂, W₂, Mn₂, Tc₂, Re₂, Fe₂, Ru₂, Os₂, Co₂, Rh₂, Ir₂, Ni₂, Pd₂, Pt₂ [5, 6], for NiPd [6, 9:C], for Cu₂ [6], for Ag₂ [5, 6], for Au₂ [6], for AgCu [10], for AgAu, AuCu [6, 10], for Zn₂, Cd₂ [5, 6], for Hg₂ [6], it is picked from references indicated right next to the said molecules. “C” points to the fact that the data of concern is computed.



Set 6a Data is generally picked from [4]. Otherwise, for CuH, ZnH [11:C], it is picked from the reference indicated right next to the said molecules. “C” means, data is *computed*.



Set 6b Data is generally picked from [4]. Otherwise, for TiCl [11:C], for ZrCl [31,32], for HfCl [33,34:C], for VO [11], it is picked from the references indicated right next to the said molecules. “C” points to the fact that the data of concern is computed.

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REFERENCES

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- ¹ J.C. Davis Jr., *Advanced Physical Chemistry: Molecules, Structure, and Spectra*, Chapter 6 (The Ronald Press Company, New York, 1965).
 - ² M. Born, R. Oppenheimer, *Zur Quantentheorie der Molekeln*, *Ann. Physik*, **84**, 457 (1927).
 - ³ G. Herzberg, *Molecular Spectra and Molecular Structure* (Van Nostrand Company, 1964).
 - ⁴ K. P. Huber, G. Herzberg, *Molecular Spectra And Molecular Structure (Vol. 4): Constants of Diatomic Molecules*, Website: <http://www.qfa.uam.es/qcomp/libros/16.pdf> (online access: 20 September 2020) (Van Nostrand Reinhold Company, New York, 1979).
 - ⁵ J.L. Jules, J. R. Lombardi, *Transition Metal Dimer Internuclear Distances from Measured Force Constant*, *J. Phys. Chem. A*, **107**, 1268 (2003).
 - ⁶ Luo, Y.R. *Comperensive Handbook of Chemical Bond Energies* (CRC Press, Boca Raton, FL, 2007).
 - ⁷ R. J. Meyer, E. H. E. Pietsch, A. Kotowski, M. Becke-Goehring, *Gmelin Handbook of Inorganic Chemistry* (8th ed., Springer-Verlag, Berlin, 1987).
 - ⁸ J.L. Bao, X. Zhang, X. Xu, D.G. Truhlar, *Predicting Bond Dissociation Energy and Bond Length for Bimetallic Diatomic Molecules: A Challenge for Electronic Structure Theory*. *Phys. Chem.* **19**, 5839 (2017).
 - ⁹ K. Li, Z. Zhou, Y. Wang, Z. Wu, *A Theoretical Study of CH₄ Dissociation on NiPd(111) Surface*, *Surface Science*, 612, **63** (2013).
 - ¹⁰ J. L. Jules, J. R. Lombardi, *Toward an Experimental Bond Order*. *J. Mol. Struct: THEOCHEM*, **664–665**, 255 (2003).
 - ¹¹ Z. Fang, M. Vasiliu, K. A. Peterson, D. A. Dixon, *Prediction of Bond Dissociation Energies/Heats of Formation for Diatomic Transition Metal Compounds: CCSD(T) Works*, *J. Chem. Theory Comput*, 2017, 13, 1057.

-
- ¹² L. Wolniewicz, *Relativistic Energies of the Ground State of the Hydrogen Molecule*, Int. J. Chem. Phys., **99**, 3 (1993).
- ¹³ T. Yarman, *Revealing the Mystery of the Galilean Principle of Relativity – Part I: Basic Assertions*, Int. J. Theor. Phys. **48**, 2235 (2009).
- ¹⁴ T. Yarman, *Scaling Properties of Quantum Mechanical Equations Working as the Framework of Relativity: Principal Articulations about the Lorentz Invariant Structure of Matter*, Phys. Essays, **26**, 473 (2013).
- ¹⁵ T. Yarman, *Scaling Properties of Quantum Mechanical Equations Working as the Framework of Relativity: Applications Drawn by a Unique Architecture, Matter is Made of*. Phys. Essays, **27**, 558 (2014).
- ¹⁶ T. Yarman, *The Quantum Mechanical Framework Behind the End Results of the General Theory of Relativity: Matter Is Built on a Matter Architecture* (Nova Publishers, New York, 2010).
- ¹⁷ T. Yarman, *An Essential Approach to the Architecture of Diatomic Molecules: 1. Basic Theory*, Optics and Spectroscopy: Molecular Spectroscopy, **97**, 683 (2004).
- ¹⁸ T. Yarman, *An Essential Approach to the Architecture of Diatomic Molecules: 2. How are Size, Vibrational Period of Time, and Mass Interrelated?*, Optics and Spectroscopy: Molecular Spectroscopy, **97**, 581 (2004).
- ¹⁹ G. Jaffé, *Zur Theorie des Wasserstoffmoleküls*. Z. Physik, **87**, 535 (1934).
- ²⁰ J. Liu, E. J. Salumbides, U. Hollenstein, J. C. J. Koelemeij, K. S. E. Eikema, W. Ubachs, F. Merkt, *Determination of the Ionization and Dissociation Energies of the Hydrogen Molecule*, Int. J. Chem. Phys, **130**, 174306 (2009).
- ²¹ R. Badger, "A Relation Between Internuclear Distances and Bond Force Constants" (PDF), *The Journal of Chemical Physics*. **2** (3): 128 (1934).
- ²² M. Aymar, O. Dulieu, F. Spiegelman, *Electronic properties of Francium diatomic compounds and prospects for cold molecule formation*, arXiv:quant-ph/0604144v1 (2006).
- ²³ J. Cameron, P. Mountford, A. Stasch, M.P. Blake, "*s*-block Metal-Metal Bonds". In Liddle, Stephen T. (ed.). *Molecular Metal-Metal Bonds: Compounds, Synthesis, Properties*. John Wiley and Sons. pp. 23–24, 2015, ISBN 9783527335411.
- ²⁴ J. A. Dean, A. L. Norbert, *Lange's Handbook of Chemistry*, "Properties of Atoms, Radicals, and Bonds" (McGraw-Hill, 1992), <https://labs.chem.ucsb.edu/zakarian/armen/11---bonddissociationenergy.pdf> (online access: 19 September 2020).
- ²⁵ Royal Society of Chemistry, *Periodic Table*, <http://www.rsc.org/periodic-table/element/85/astatine> (online access: 19 September 2020).

-
- ²⁶ V. Pershina, A. Borschevsky, J. Anton, "Fully relativistic study of intermetallic dimers of group-1 elements K through element 119 and prediction of their adsorption on noble metal surfaces", *Chemical Physics*. Elsevier. **395**: 87–94 (2012).
- ²⁷ A. Das, E. Arunan, Chemical bonding in Period 2 Homonuclear Diatomic Molecules: A Comprehensive Relook, *J. Chem. Sci.* 2019, 131, 120.
- ²⁸ R. T. Santiago, R. L. Haiduka, Determination of molecular properties for Moscovium Halides (McF and McCl), *Theoretical Chemistry Accounts*, Vol: 139, 60 (2020).
- ²⁹ Texas A&M University's Dept. of Chemistry, *Selected Bond Energies and Bond Lengths*. Website: www.chem.tamu.edu/rgroup/Connell/linkfiles/bonds.pdf. Original link broken; working link is <https://pdf4pro.com/view/selected-bond-energies-and-bond-lengths-55eb06.html> (online access: 19 September 2020). Suggested citations: J. E. Huheey et al., "*Inorganic Chemistry: Principles of Structure and Reactivity*", Chapters A-21 to A-34 (Pearson, India, 2008); T. L. Cottrell, "*The Strengths of Chemical Bonds*", (2nd ed., Butterworths, London, 1958); B. deB. Darwent, "*National Standard Reference Data Series (Nr. 31)*", National Bureau of Standards (Washington DC, 1970); S. W. Benson, *Bond energies*, *J. Chem. Educ.*, **42**, 502 (1965).
- ³⁰ E.J. Baran, *Vibrational Properties of Hydrogen Astatide*, *Z. Naturforsch.* **59A**, 133 (2004).
- ³¹ M.G.M. van der Vis, E.H.P. Cordfunke, R.J.M. Konings, Thermochemical properties of zirconium halides: Aa Review, *Thermochimica Acta* 302 (1997) 93-108.
- ³² R. B. Nevarez, E. Kim, B. C. Childs, H. Brabarand, L. Bigler, U. Stalder, R. Alberto, P. F. Weck, F. Poineau, *SN Applied Sciences*, 1:392 (2019), <https://doi.org/10.1007/s42452-019-0410-y>.
- ³³ E.N. Moskvitina, P.I. Stepanov, O.B. Shakkovkin, The Electron Absorption Spectrum of Hafnium Monochloride, *Spectroscopy Letters: An International Journal for Rapid Communication*, Pages 1639-1647 (1993).
- ³⁴ R. S. Ram, A. G. Adam, A. Tsouli, J. Lie´vin, P. F. Bernat, High-Resolution Spectroscopy and Ab Initio Calculations on HfCl, *Journal of Molecular Spectroscopy* 202, 116–130 (2000), doi:10.1006/jmsp.2000.8120.