


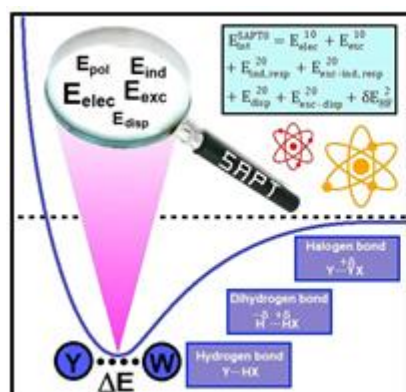
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The Quantum Electronic Partitioning as Modernization in the Studies of the Intermolecular Interactions

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Throughout the years, the evolution in the works involving hydrogen bond based on the direct determination of the interaction energy has become limited in order to characterize the electronic nature and interaction strength of the intermolecular system. Through a quantum mechanical formalism, the electronic partitioning has been considered a modernizing methodology in the studies of intermolecular interactions, unveil it at the light of electrostatic, Exchange, dispersion and induction contributions.

Graphical abstract



The Quantum Electronic Partitioning Studies of the Intermolecular Interactions

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1. Introduction

Even after more than one century of studies involving a conceptual evolution [1] and applicability in the most diverse fields and research lines [2], the hydrogen bond keeps on evidence as scientific target and questions about it still are highlighted [3], either on structural [4], electronic [5] or thermodynamic [6] points of view. It is widely known that some others more specific areas, such as the spectroscopy [7], for instance, the hydrogen bond has become a mandatory benchmark [8], and it is in this context that the interaction strength rises as one of the main parameters in intermolecular investigations [9].

In an overview, the interaction strength, and of course the minimum required energy for stabilizing the intermolecular system through the hydrogen bond formation, it is a clear mention to hydrophobic and hydrophilic extremes [10], in

particular those manifested in biomacromolecular analyses [11]. The polarity, in fact, it satisfies one of the electronic conditions to form interactions when often it is ruled by their distance values [12], which, in this structural vision, it is routinely attributed to the hydrogen bonds [13] but also can be evidenced in other interaction type. Nevertheless, it is of crucial relevance to focus in the source of the electronic energy [14].

In a couple of last decades, an alert took on relevance in the community of hydrogen bond researchers [15], especially regarding to a lack by a firm criterion that offers an accurate study of properties and parameters as well as the phenomenology of the intermolecular interactions [16]. To the best of our knowledge, it was well established that the hydrogen bond recognition was carried out on the basis of the

Lennard-Jones potential function (Eq. 1) [17], wherein the repulsive term differs a hydrogen bond from the less stable ones, such as those whose London dispersion forces are the reigning term [18]. In other words, even though this condition has been widely used, the threshold of its applicability can be summarized in the determination and analysis of the interaction strength if the hydrogen bond or van der Waals interaction with London dispersion is accounted [19], and no exams about the origin of the interaction strength is performed [20]. In line with the bibliography sources, there is a clear differentiation based on knowledge of the dispersion forces, wherein the interactions have been classified as hydrophobic and hydrophilic if, and only if, their polarities frame the nonpolar and polar effects [21], although contextualizing the intermolecular forces, there is, indeed, a math formalism by which these two profiles of intermolecular contacts can be defined.

$$V = 4\epsilon \left[\left(\frac{\sigma}{d} \right)^{12} - \left(\frac{\sigma}{d} \right)^6 \right] \quad (1)$$

With the dawn of the quantum mechanics, however, the hydrogen bond study was catapulted to a new level [22], wherein it needs to be highlighted, the viability to quantify the electronic energy, and mainly, the own and lower interaction energy. Incredibly composed by a small energy portion (ΔE , in accord with the Eq. 2 to subtract from the energy of the complex the amounts of the monomers) assigned to the intermolecular contact region [23]:

$$\Delta E = E_{\text{complex}} - \sum E_{\text{monomers}} \quad (2)$$

It was in this scenario that since the performing of the first quantum chemical calculations [24], up to the most sophisticated computational approaches that the quantification of the hydrogen bond energy, and evidently its interaction strength, all of these parameters often appreciate the intermolecular energy, and no scrutinizes in order to justify the origin of this energy could be performed. Thus, it is necessary an improvement of the theoretical methods to furnish a punctual detailing of how and where the supermolecule intermolecular energy comes from, and therefore can be useful to justify the interaction strength and related phenomena [25]. Once again, it is important to emphasize that the intermolecular energy is a small portion, and even as such, some kinds of events, in particular those from spectroscopy, even so can be unleashed. So, it is through the decomposition of the electronic energy that becomes reliable to attribute a better criterion to unveil the source of the interaction energy, and in the case of the hydrogen bonds, it was also established that the electrostatic attraction nor always is the dominant contribution to the intermolecular stabilization of the supermolecules.

The electronic partitioning implemented beyond the primary existence of the electrostatic potential also reveal the presence of spin exchange as a truly repulsive effect, which, in fact, it contributes to the destabilization of the system. By taking into account the quantum mechanics approach for the electronic structure regarding the wave function of the molecular orbital, the estimation of the gaps derived from the charge transfer trend to provide a substantial stabilization, which composes the electronic induction in cooperative association with the polarization. In view of this, it must be highlighted that the induction is the main parameter to analyze

the interaction strength and prediction of the intermolecular covalence even being rarely evidenced, although it has been demonstrated when the intermolecular distance is reduced down to 1.7 Å [26].

Otherwise, weakly bound systems present a subtle interaction potential, and since that minima fluctuations in the molecular polarity are observed, it is thereby then that the dispersion is manifested. In practice, the pioneer proposal to quantify these terms, or more properly the energies derived from the electrostatic nature (elec), the spin exchange (exc), charge transfer (ct), polarization (pol), induction (ind) and dispersion (dis) was divulged by Umeyama and Morokuma in the 70 years [27] titled as Energy Decomposition Analysis (EDA):

$$\text{Energy} = E_{\text{elec}} + E_{\text{exc}} + E_{\text{ct}} + E_{\text{pol}} + E_{\text{dis}} \quad (3)$$

$$\text{Energy} = E_{\text{elec}} + E_{\text{exc}} + E_{\text{ind}} + E_{\text{dis}} \quad (4)$$

It is known, but also must be routinely revised, the definitions of these terms as follows [28]: *electrostatic*, from characteristics of the multipolar momenta of the bound species when the punctual charge densities emerge and overlap; *induction*, derived from the *polarization* effect between the molecules involved in the interaction, wherein the rising of an electric field affects the permanent dipole moments of the species whether the isolated condition is taken into account, and also the *charge transfer* between the frontier molecular orbitals; *dispersion*, it encompass the correlation effects and charge density fluctuations in the surface of the intermolecular system, whose attractive nature is typical of the weakly-stabilized complexes; *exchange*, it is a direct consequence of the Pauli exclusion principle, and once being from repulsive nature, which, in practice, provides a contribution to the destabilization of the electronic system.

With the evolution of the electronic structure methods, which if is based on the *ab initio* formalism or in accord with the Density Functional Theory (DFT) [29], for which the theoretical geometry is optimized and consequently the electronic energy for the determination of the intermolecular amount, of course it is required indeed, new energy partition models have been developed beyond the EDA of Umeyama and Morokuma [27]. In this context, the energy terms of the Eq. 1 were expanded in order to get a better accuracy, and as such the Symmetry-Adapted Perturbation Theory (SAPT) [30] and psi4 [31] have arisen, for instance. In according to that is well established in the specialized literature, the SAPT built by Szalewicz and co-authors [30] is defined as a practical computational method to calculate the interaction energy under the physical point of view, that is represented by the contributions contained in the Eq. 3 and Eq. 4 [28].

It should to be considered, indeed, that in the universe of the intermolecular interactions, since being noteworthy to mention the 'non-covalent' condition [32] as often used when intermolecular complexes are weakly bound stated [33], there is a low energy frame, assuming, in an overview, the dominance of the London dispersion forces into the nature of the hydrogen bond, if applicable. Although is present every matte, the diversity of the intermolecular systems shows that there is no exclusivity to the dispersion, and in view of this foregoing is clear justified the importance of the quantum electronic partitioning.

2. SAPT Formalism: brief revision

As in any type of quantum mechanical protocol [34], the electronic perturbation of the SAPT partition requires an intermolecular potential, either attractive or repulsive, which embodies the zero-order Hamiltonian operator (H_0) for the Schrödinger equation, and in this case for the isolated monomers, follows:

$$H_0 = \sum H_{\text{monomers}} \quad (5)$$

with

$$H_X \Psi_X^{(0)} = E_X^{(0)} \Psi_X^{(0)} \quad (6)$$

where $X = A$ or B , which are the representativity of the monomers. Naturally that the product of the wave function as well as the cooperative energy ($\sum E_{\text{monomers}}$) are both of them considered. At the light of the Pauli exclusion principle, however, the spin permutation in the wave function cannot be considered in the Rayleigh-Schrödinger equation for the unperturbed Hamiltonian H_0 , and it is through the potential operator (V) that the first order energy can be obtained by means of the Eq. 7:

$$E^{(1)} = \langle \Psi_A^{(0)} \Psi_B^{(0)} | V | \Psi_A^{(0)} \Psi_B^{(0)} \rangle \quad (7)$$

By the quadratic wave function and the electrostatic operator, it is natural to consider the interaction between the electronic densities non-overlapping of the monomers ($\rho_A^{(0)}$ and $\rho_B^{(0)}$), where the latter term is used in the exemplification of the Eq. 8, and the energy whose nature is purely electrostatic, see Eq. 7, it results in the Eq. 9:

$$\rho_A^{(0)}(r_1) = \sum_{A \in A} Z_A \delta(r_1 - R_A) - N_A \sum_{\sigma_1} \int \Psi_A^{(0)*}(1, 2, \dots, N_A) \Psi_A^{(0)}(1, 2, \dots, N_A) d\tau_1' \quad (8)$$

$$E_{\text{elec}}^{(1)} = \iint \rho_A^{(0)}(r_1) \frac{1}{|r_1 - r_2|} \rho_B^{(0)}(r_2) dr_1 dr_2 \quad (9)$$

Even though the non-overlapping has been cited, the Eq. 9 can be also used for overlapping conditions, what potentiates the formation of interactions involving multipoles with penetration in the charge densities of A and B , and vice-versa, well-founded by more negative and stable energies. Other formalisms bring expressions for higher perturbations, by which energetic contributions are generated to induction and dispersion, namely as $E_{\text{ind}, A \rightarrow B}^{(2)}$ and $E_{\text{ind}, B \rightarrow A}^{(2)}$. Still regarding in the treatment for the first order energy, nonetheless, the contribution of exchange (exc) in the approximation of the Schrödinger equation has a participation of a symmetrizer, A , for the wave function, wherein the energy ES is displayed by the Eq. 10 and Eq. 11. In both, specifically the first one, there is a positive contribution for the energy derived from the repulsive interaction of the closed-shell systems.

$$E_S^{(n)} = E^{(n)} + E_{\text{exc}}^{(n)} \quad (10)$$

$$E_S = \frac{\langle \Psi_A^{(0)} \Psi_B^{(0)} | V A | \Psi_A^{(0)} \Psi_B^{(0)} \rangle}{\langle \Psi_A^{(0)} \Psi_B^{(0)} | A | \Psi_A^{(0)} \Psi_B^{(0)} \rangle} \quad (11)$$

and, this same symmetrizer A results in the wave function

for the induction and dispersion of first order, $\Psi_S^{(1)} = \Psi_{\text{ind}}^{(1)} + \Psi_{\text{disp}}^{(1)}$, whose equations are placed below:

$$\Psi_{\text{ind}}^{(1)} = \sum_{i \neq 0} \frac{\langle \Psi_A^{(0)} \Psi_B^{(0)} | V | \Psi_A^{(i)} \Psi_B^{(0)} \rangle}{E_A^{(0)} - E_A^{(i)}} \Psi_A^{(i)} \Psi_B^{(0)} + \sum_{i \neq 0} \frac{\langle \Psi_A^{(0)} \Psi_B^{(0)} | V | \Psi_A^{(0)} \Psi_B^{(i)} \rangle}{E_B^{(0)} - E_B^{(i)}} \Psi_A^{(0)} \Psi_B^{(i)} \quad (12)$$

$$\Psi_{\text{disp}}^{(1)} = \sum_{i, j \neq 0} \frac{\langle \Psi_A^{(0)} \Psi_B^{(0)} | V | \Psi_A^{(i)} \Psi_B^{(j)} \rangle}{E_A^{(0)} + E_B^{(0)} - E_A^{(i)} - E_B^{(j)}} \Psi_A^{(i)} \Psi_B^{(j)} \quad (13)$$

Therefore, the equipartition of the wave function $\Psi^{(1)}$ into the induction ($A \rightarrow B$ and $B \rightarrow A$) dispersion terms, and from the Eq. 10 the repulsive energy can be obtained:

$$E_{\text{exc}}^{(2)} = E_S^{(2)} - E^{(2)} \quad (14)$$

$$E_{\text{exc}}^{(2)} = E_{\text{exc-ind}, A \rightarrow B}^{(2)} + E_{\text{exc-ind}, B \rightarrow A}^{(2)} + E_{\text{exc-disp}}^{(2)} \quad (15)$$

Taking a brief outlook in the basis of the quantum mechanical, the zero-order Hamiltonian consists in sum of the Fock operators from the monomers, F_A e F_B :

$$H = F_A + F_B + \xi(W_A + W_B) + \lambda V \quad (16)$$

wherein, the terms labeled as ξ e λ are parameters for insertion of the electronic correlation, and $E_{\text{SAPT}}^{(mn)}$ implies that the indexes m (values of 1, 2,...) and n (values of 0, 1, 2,) describe the order of the electrostatic potential V while W accounts the expansion of the perturbation. So, the simplest model, SAPT0, is recognized, although disregarding, yet, the intramonomeric correlation:

$$E_{\text{int}}^{\text{SAPT0}} = E_{\text{elec}}^{(10)} + E_{\text{exc}}^{(10)} + E_{\text{ind, resp}}^{(20)} + E_{\text{exc-ind, resp}}^{(20)} + E_{\text{disp}}^{(20)} + E_{\text{exc-disp}}^{(20)} + \delta E_{\text{HF}}^{(2)} \quad (17)$$

The $E_{\text{elec}}^{(10)}$ and $E_{\text{exc}}^{(10)}$ terms above correspond the electrostatic interaction at the Hartree-Fock level of theory for the charge density of the monomer and the spin exchange resulting from the symmetrization described in the Eq. 11. The following terms, $E_{\text{ind, resp}}^{(20)} + E_{\text{exc-ind, resp}}^{(20)}$, encompass the induction energy at second order by the compensation of the exchange, and herein deserves a commentary that these energies are computed as a response (resp) to the electrostatic potential of the monomers acting one to another.

Regarding the electronic correlation, this is represented by the $E_{\text{disp}}^{(20)}$ and $E_{\text{exc-disp}}^{(20)}$ terms, and at last, the $\delta E_{\text{HF}}^{(2)}$ terms is the responsible by the calculation of the inductive effects and exchange in higher orders concerning the supermolecule approximation of the Eq. 2.

$$\delta E_{\text{HF}}^{(2)} = E_{\text{int}}^{\text{HF}} - E_{\text{elec}}^{(10)} - E_{\text{exc}}^{(10)} - E_{\text{ind, resp}}^{(20)} - E_{\text{exc-ind, resp}}^{(20)} \quad (18)$$

$$E_{\text{int}}^{\text{SAPT0}} = E_{\text{int}}^{\text{HF}} + E_{\text{disp}}^{(20)} + E_{\text{exc-disp}}^{(20)} \quad (19)$$

By combining the equations, (18) and (19), it is obtained,

beyond the Eq. 17, the final expression for the SAPT0 energy, although for corrections of double order perturbations ruled by the effects of the intermolecular potential (V), the equation to the SAPT2 energy, for instance, assumes the following form:

$$E_{\text{int}}^{\text{SAPT2}} = E_{\text{int}}^{\text{SAPT0}} + E_{\text{elec,resp}}^{(12)} + E_{\text{exc}}^{(11)} + E_{\text{exc}}^{(12)} + {}^tE_{\text{exc}}^{(22)} + {}^tE_{\text{exc-ind}}^{(22)} \quad (20)$$

Since is necessary to execute a electronic structure calculation involving correlation, a the MP2 level, for instance, similarly to the Hartree-fock approach, the Eq. 21 reveals that the higher order terms to quantify the induction and repulsion increments the SAPT accuracy when is applied to weakly-bonded complexes. Not only with respect to the MP2, but the Kohn-Sham formalism for the DFT molecular orbitals, the SAPT method presents also calculation specificity.

$$\delta E_{\text{MP2}} = E_{\text{int}}^{\text{MP2}} - E_{\text{int}}^{\text{SAPT2}} \quad (21)$$

It is with the calculation of all these terms that the physical nature of the intermolecular system can be unveiled regardless of the interaction energy ruled by the Eq. 2.

3. SAPT and intermolecular systems: a novel vision

When it comes of the exploration of the electronic origin of the intermolecular interactions [35], undeniably that the studies of hydrogen bonds are pioneers [26]. In a vast work elaborated by Emanian and collaborators [36], the SAPT analysis for neutral, anionic and cationic complexes formed by $Y \cdots X$ hydrogen bonds with $Y = \text{N}, \text{O}, \text{S}$ and F as well as $X =$ basically hydrocarbons ($\text{H}_3\text{CH} \cdots \text{NCH}$), sulfides ($\text{HSH} \cdots \text{SH}_2$), water ($\text{HOH} \cdots \text{OH}_2$) and ammonia ($\text{NH}_3 \cdots \text{HF}$) (see Fig. 1), and it is uncontested that 52.2% computed to the electrostatic character largely dominates the interaction energy of these systems and other ones also studied. Likewise, it was also presented the results by which the dispersion and induction also contribute for the stabilization of a serial of complexes, such as, in particular, $\text{H}_3\text{CH} \cdots \text{NH}_3$ and $[\text{H}_2\text{OH} \cdots \text{SH}_2]^+$ (see Fig. 1), respectively. In a comparison, it is suitable to highlight that the induction accounts a greater contribution rather than the dispersion upon the formation of the ionic complexes, wherein, their interaction energies is higher, what it can be in some cases, reach levels of partial covalence [26], as is observed in the classical system ($\text{F} \cdots \text{H} \cdots \text{F}$).

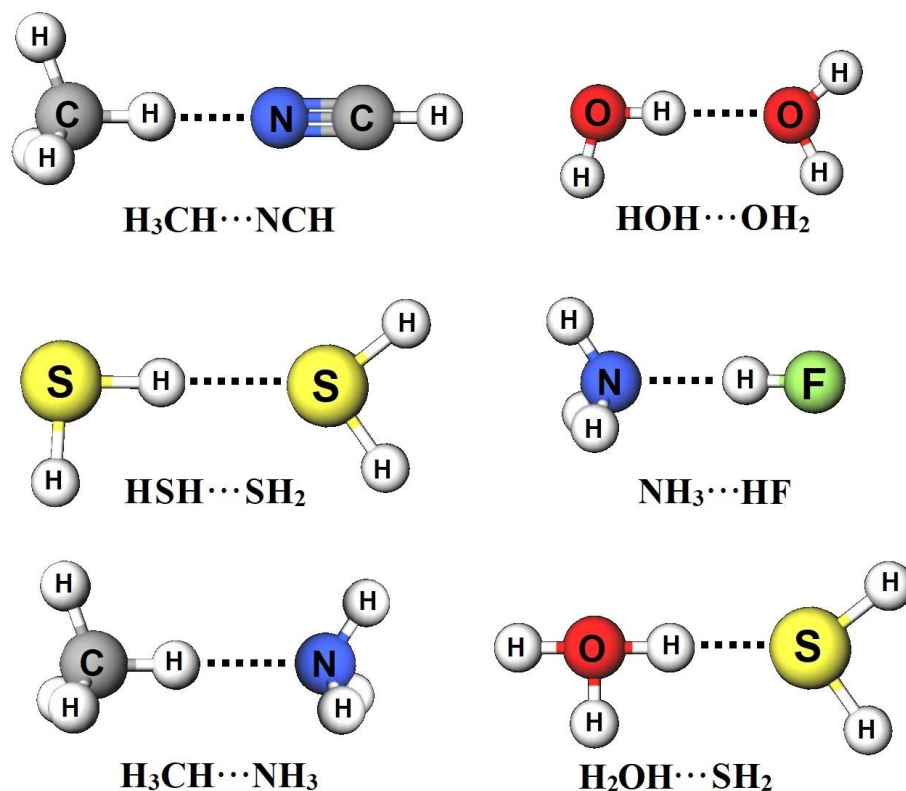


Fig. 1. Illustration of the $\text{H}_3\text{CH} \cdots \text{NCH}$, $\text{HSH} \cdots \text{SH}_2$, $\text{HOH} \cdots \text{OH}_2$, $\text{NH}_3 \cdots \text{HF}$, $\text{H}_3\text{CH} \cdots \text{NH}_3$ and $[\text{H}_2\text{OH} \cdots \text{SH}_2]^+$ complexes [36].

Lastly and expected, the dispersion with 28.6% stands out in neutral complexes in comparison with the value of 19.1% of the induction. Traditionally, it can be seen that the interaction energies scan a large spectrum with results from -0.60 up to -65.47 Kcal/mol, there is no any detailed explanation with respect to origins of these interaction energies. In complexes whose structure bring the presence of inert gases, e.g., xenon, in a study signed by Cukras and co-authors [37], it is not the

dispersion that stands out, but truly the spin exchange bringing its destabilization in many cases, e.g., $\text{HXeOH} \cdots \text{H}_2\text{S}$ and $\text{HXeSH} \cdots \text{H}_2\text{S}$ (see Fig. 2), wherein it outweighs or equivalents with the electrostatic character due to the values of 73.22 ($E_{\text{exch}}^{(10)}$) and -59.17 KJ/mol ($E_{\text{elec}}^{(10)}$) as well as 46.11 ($E_{\text{exch}}^{(10)}$) and -35.46 KJ/mol ($E_{\text{elec}}^{(10)}$).

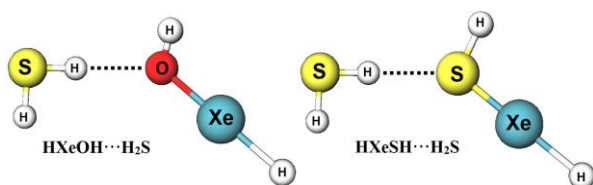


Fig. 2. Illustration of the HXeOH...H₂S and HXeSH...H₂S complexes [37].

As abovementioned the Y...X model, it shall be better discussed that X encompass the molecules or functional groups able to form hydrogen bonds, but it is also important to temper that the most refined model for hydrogen bonds shall be Y...HX [16], wherein the intermolecular requirement is that Y and X must contain empirical electronegativity values higher to that for the hydrogen atom [38]. However, the Y...HX model also can be extended to another interaction type, such as the dihydrogen bond [39], whose scaffold is H^{δ+}...H^{δ-}X. In this case, X represents elements belonging to the alkaline or alkaline earth metals, in which the electropositivity is such intensive that H^{δ+} presents an enough charge density to act as a base in order to interact with hydrogen of the acid species [35]. According to results divulged by Hong and Chen [40], the spin exchange potential domains the contributions to the interaction energy of the dihydrogen-bonded complexes of BeH₂...HX with X = F, Cl, Br and I, as illustrated in Fig. 3.

The systems formed by bromide and iodine present quite close results approximately of -11.00 and 17.00 KJ/mol for the $E_{elec}^{(10)}$ and $E_{exch}^{(10)}$, although for BeH₂...HF and BeH₂...HCl the results are -21.29 and 24.44 KJ/mol as well as -14.23 and 19.02 KJ/mol, respectively. In a direct comparison with a model system formed by hydrogen bond, HF...HF, the results of -27.70 KJ/mol for $E_{elec}^{(10)}$ demonstrates the stronger character of the hydrogen bond.

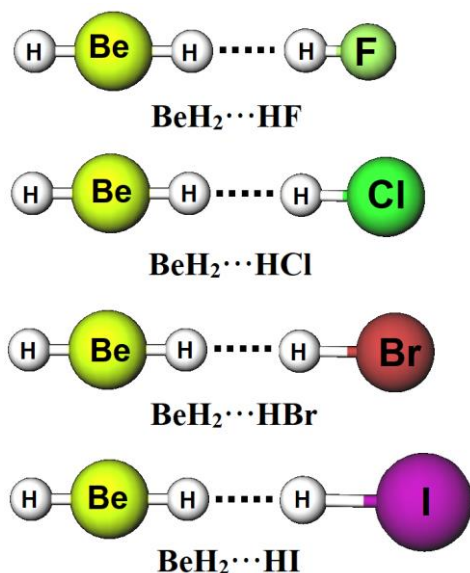


Fig. 3. Illustration of the BeH₂...HF, BeH₂...HCl, BeH₂...HBr and BeH₂...HI complexes [40].

In the fluoric acid dimer, the participation of -10.95 KJ/mol from the inductive term reasonably approximates this system of the BeH₂...HF whose result of -17.22 KJ/mol for $E_{ind,r}^{(20)}$ corroborates with the higher interaction energy values of -14.46 and -16.94 KJ/mol. With respect to inductive and dispersive contributions uniquely for the dihydrogen-bonded

complexes, these electronic partitions are lower, repressing, therefore, any possibility to exist intermolecular covalency.

In this relatively vast universe of the intermolecular interactions [41], another kind of contact entered the spotlight of the scientific community, the halogen bond [42]. By the format of the Y...X model, Y and X indicate the presence of halogen interacting with each other [43] or with any element with high charge density. Undeniably that enough electronic density to be transferred between the HOMO/LUMO not brings any hindered to the conception and understanding of the halogen bond, but is through the formation of a positive electrostatic potential named σ -hole [44], that an able center to interact with a Lewis base, for instance, become feasible.

Holding as reference the work of Riley and Hobza [45], which explore the formation of Y...O halogen bond in the H₃CCl...OCH₂, H₃CBr...OCH₂ and H₃CI...OCH₂ complexes (see Fig. 4), the SAPT analysis emphasizes that dispersion is salient even though in different calculations levels.

At the MP2 with Dunning basis sets [46], the interaction energies values from -1.11 up to the -2.34 Kcal/mol, a range very below of the halogen bond and dihydrogen bond energies. Regarding the SAPT results, the dispersive contributions are -1.81 and -1.98 Kcal/mol followed by -2.31 Kcal/mol for the abovementioned complexes, although only in the dimer formed by H₃Cl that the electrostatic energy presents a higher value of -2.61 Kcal/mol distinguishing solely in -0.30 Kcal/mol more stable in comparison to the dispersive amount.

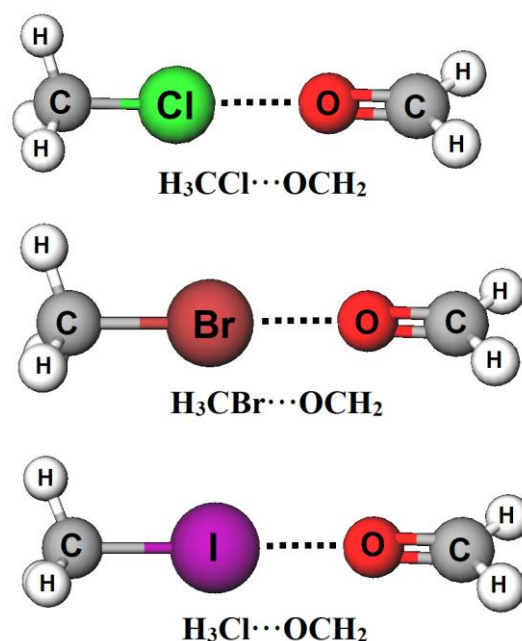


Fig. 4. Illustration of the H₃CCl...OCH₂, H₃CBr...OCH₂ and H₃CI...OCH₂ complexes [45].

4. Conclusions

In view of all exposed here about the modernization for the hydrogen bond studies [47], although from the emergence of other types of intermolecular interactions, it is established a recognition concerning the application of a quantum mechanical formalism, for instance, initially for determining of geometries and spectroscopy parameters [48], but the necessity to the executability of the electronic partitioning, especially via SAPT method, in fact it becomes truth. The

determination of the interaction energy on the basis of the traditional supermolecule approach deprives the real understanding of the electronic nature of the intermolecular interactions, wherein, surely, it consists on physical properties from electrostatic, dispersive, spin exchange, inductive nature, basically. To determine the contribution of each one of these terms has become more and more inclusive in any kind of hydrogen bond study and ideally extended to the more recently discovered interactions, such as the dihydrogen and halogen bonds.

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