

Why much of Chemistry may be indisputably non-bonded?

Porque grande parte da Química pode ser indiscutivelmente não ligada?

Boaz Galdino de Oliveira¹

Abstract

In this compendium, the wide scope of all intermolecular interactions ever known has been revisited, in particular giving emphasis the capability of much of the elements of the periodic table to form non-covalent contacts. Either hydrogen bonds, dihydrogen bonds, halogen bonds, pnictogen bonds, chalcogen bonds, triel bonds, tetrel bonds, regium bonds, spodium bonds or even the aerogen bond interactions may be cited. Obviously that experimental techniques have been used in some works, but it was through the theoretical methods that these interactions were validate, wherein the QTAIM integrations and SAPT energy partitions have been useful in this regard. Therefore, the great goal concerns to elucidate the interaction strength and if the intermolecular system shall be total, partial or non-covalently bonded, wherein this last one encompasses the most majority of the intermolecular interactions what leading to affirm that chemistry is debatably non-bonded.

Keywords: intermolecular interactions; periodic table; theoretical methods; non-bonded.

Resumo

Neste compêndio, o amplo escopo de todas as interações intermoleculares já conhecidas foi revisitado, em particular dando ênfase à capacidade de muitos dos elementos da tabela periódica de formar contatos não covalentes. Podem ser citadas tanto ligações de hidrogênio, ligações de di-hidrogênio, ligações de halogênio, ligações de pnictogênio, ligações de calcogênio, ligações de triel, ligações de tetrel, ligações de regium, ligações de espódio ou mesmo as interações de ligações aerogênicas. Obviamente que técnicas experimentais têm sido utilizadas em alguns trabalhos, mas foi através dos métodos teóricos que estas interações foram validadas, onde as integrações QTAIM e as partições de energia SAPT têm sido úteis neste sentido. Portanto, o grande objetivo é elucidar a força de interação e se o sistema intermolecular deve ser total, parcial ou não covalentemente ligado, sendo que este último engloba a maioria das interações intermoleculares o que leva a afirmar que a química é discutivelmente não ligada.

Palavras-chave: interações intermoleculares; tabela periódica; métodos teóricos; não-ligado.

¹ Prof. Dr., Chemistry Depto., UFOB, Barreiras, BA, Brazil; E-mail: boazgaldino@gmail.com

Introduction

Once all together in cooperation, the atoms, the chemical bonds hitherto known, and electronic structure compose the foundation responsible for the functioning of the chemical reactions, and this is validated either by kinetic or thermodynamic viewpoint (FULTZ, 2014; NÄTHER *et al.*, 2013; PISANO *et al.*, 2002) and even some events arising from electrochemical nature are also included in this context (MAGNUSSEN; GROß, 2019).

Historically, it is known that the studies of Boyle about gaseous substances have inspired Newton to propose its corpuscularism presented in the form of 'ultimate particles of the matter' (VIANA; PORTO, 2007). However, the association between Henry and Dalton promulgated the first contemporary atomic theory (FILGUEIRAS, 2007), and later, the discoveries of both Thomson and Rutherford (MANSOOR, 2009) have opened wide horizons to understand the electronic arrangement around the atomic nuclei (EVANS, 1942). Until more recent times, the atomic profile was definitively established through the solving of the 'Schrödinger' equation for the hydrogen atom (KURNIAWAN *et al.*, 2019) as well as to other systems based on formalism of the Born-Oppenheimer approximation ruled by the postulates of the quantum mechanics (MÁTYUS, 2019; VEIS *et al.*, 2016).

This scenery give support to the knowledge about the molecular structure and electronic structure (ŠTĚPÁNEK *et al.*, 2017), where the first concept is used to delineate the position of the atoms and the last one specifies the way by which they interact as well as shall be linked each other.

Methods

The chemical interaction interpreted ob the basis of theoretical premises

In a broad analysis between the vision of the molecular geometry and its relationship with the chemical bond (GILLESPIE; POPELIER, 2003), the contribution of the Valence-Shell Electron-Pair Repulsion (VSEPR) model proposed by Gillespie is irrepressibly notorious (GILLESPIE, 1963). Despite bonding term express mutuality or interactivity, it is not similar to linkage. Indeed, it means that something binds or restrains. For too long, since there was no analytical protocol to unveil how the atoms bond each another, and this was treated as an undefined physical observable until the improvement of some spectroscopy techniques (ZHANG *et al.*, 2013).

Well, it is the electronic density (MACCHI, 2013) makes real the interatomic contacts (IRIBARREN *et al.*, 2021), and as aforesaid, an irrefutable mathematic formalism to described it still remains as one of the greatest interdisciplinary challenges for the physics and chemistry (HELLIWELL, 2017). So, the absence of mathematic foundation limits the truly recognition of the electronic density as feasible natural observatory for the chemistry. However, it is remarkable to emphasize that some proposals were divulged in order to equate a relationship between electronic density and chemical stability (HIRSHFELD, 1977a; KAMAL *et al.*, 2020; PIETSCH; HANSEN, 1996), and with all the credits, truly the contributions of Hirshfeld (HIRSHFELD, 1977b) and Hubbard-Holstein (HOLSTEIN, 1959; VON DER LINDEN; BERGER; VALÁŠEK, 1995) were essentials in this regard.

The most used quantum approaches for interaction studies

Turning out to the practice, since the formulation of the Lewis theory of the lone pairs of electrons (FILGUEIRAS, 2016; GILLESPIE; ROBINSON, 2007; LEWIS, 1916; SEABORG, 1984) widely used as response to the behavior of polar compounds in aqueous solution and, mediated by the Pauling's empirical electronegativity (MURPHY *et al.*, 2000; TANTARDINI; OGANOV, 2021), until the content of the Generalized Valence Bond (GVB) method (GODDARD III *et al.*, 1973) and Molecular Orbital (MO) (ROOTHAAN, 1951) theory calculations, as well as the more recent statement of the Quantum Theory of Atoms in Molecules (QTAIM) (AYERS; FRENKING, 2012; BADER, 1991), a wide range of molecular structures and chemical bonds have been studied in order to unveil the phenomenology that exist within them (FARRUGIA *et al.*, 2009; FRONTERA; BAUZÁ, 2021; MATTA, 2013; OLIVEIRA, 2020; PADASH; ESFAHANI; RAD, 2021; REGO; OLIVEIRA, 2020; ROJAS *et al.*, 2020; SUMA *et al.*, 2020).

The QTAIM proposal is dedicated to a quantum view of the chemical bond based on the quantification of the electronic density through the algebraic equations (BADER; NGUYEN-DANG, 1981) and physical approaches (BADER, 2011), some of them revolutionary due the fact to model open systems conception as those that exchanges charge and momentum with their neighbors (BADER; HERNÁNDEZ-TRUJILLO; CORTÉS-GUZMÁN, 2007; BADER, 2001). It is, in this point that, QTAIM focuses greatly the description of the chemical

bond, and of course justly by means of the electronic density taken as physical quantity for topological integrations on molecular surface (BIEGLER-KÖNIG; BADER; TANG, 1982). Moreover, it should be noticed that many other singular contributions have been documented (RODRÍGUEZ *et al.*, 2016), either from the theoretical insights as aforesaid or even those based on experimental procedures (CHOPRA, 2012), all of them greatly important along the genealogy of the chemical bond (HUNTER; RODRIGUEZ; BECKER, 2022; RITTER, 2016), so to speak.

Besides the QAIM capabilities devoted to locate bond paths in order to estimate the flux of charge density between two atoms (BADER, 2009; JABŁOŃSKI, 2021), the intermolecular researches are also supported by an useful strategy of electronic partition of energy by which the interaction strength is accounted (UMEYAMA; MOROKUMA, 1977). On this foregoing, the nature and source of the electronic energy in terms of the electrostatic (elest), exchange (exc), polarization (pol), charge transfer (ct) and dispersion (disp) contributions frame the intermolecular system as weak or strongly bound (PHIPPS *et al.*, 2015). This is amazing cause a lot of parameters are ruled by the interaction strength (OLIVEIRA; ARAÚJO, 2012), such as the frequency shifts in the infrared spectrum (HEINDEL; KNODEL; SCHOFIELD, 2018), for instance.

Nowadays, the mostly used protocol for partition of energy is the Symmetry-Adapted Perturbation Theory (SAPT) developed by Jeziorski; Moszynski; Szalewicz (1994) and Szalewicz (2012), and due its importance many others works and revisions have been published in recent years (GARCIA; PODESZWA; SZALEWICZ, 2020; HAPKA *et al.*, 2020; PATKOWSKI, 2020). It is through the computing of the SAPT energies labeled as E_{elest} , E_{exc} , E_{pol} , E_{ct} and E_{disp} for modeling of the interaction strength that some intermolecular covalent profiles have been discovered (GRABOWSKI, 2016).

More specifically in a revision signed by Grabowski (2011), the intermolecular covalence is clearly treated and discussed, and from SAPT energies, the induction/electrostatic ratio in a relationship with the intermolecular distance defines if the intermolecular system may be total, partial or noncovalent. In other words, the induction or delocalization (polarization and charge transfer) is the responsible by the covalent character that is so much looking for.

The IUPAC manifestation to refine some definitions

In the midst of importance whether the atoms are bonded or even under interaction condition (RZEPA, 2009), a mandatory conception to cite the non-bonded forms is well-known upon the hydrogen bond formation (VAN DER LUBBE; GUERRA, 2019). Among the scientists, however, the hydrogen bond is discerned indistinctly as theme worthy of Nobel prize (KOJIĆ-PRODIĆ; MOLČANOV, 2008), and in face of this scenario, an IUPAC document elaborated by a group of great experts in area delineated a new profile to this interaction (ARUNAN *et al.*, 2011). So, the historical background recognizes Lewis as one of the hydrogen bonding pioneers due to its famous studies focused on the elucidation of the acid/base behavior wherein intermolecular interaction phenomena are invoked (ABRAHAM *et al.*, 1990; GIMENO; HERRERA, 2020; RAHAMAN; DOREN; DI TORO, 2014). After him, it is worthy to emphasize that Pauling was one of the greatest “hydrogen bond scientist” due his work based on the electronegativity scale of the elements applied in important intermolecular researches.

Well, some years later, Pimentel and McClellan (1971) have discussed the nature of the hydrogen bonds, where some conflicting interpretations in regards to the electronegativity of the carbon when bonded to oxygen ($\text{H}\cdots\text{O}=\text{C}$) were highlighted (VARGAS *et al.*, 2000). The model idealized by Pauling affirms that the carbon is not enough electronegative to be taken into account in the intermolecular context (GRABOWSKI, 2020a). On the other hand, Pimentel and McClellan (1971) argue that hydrogen bond occurs if specifically involves a hydrogen atom bonded to another atom. All of these informations are often reported and serves as support for elucidation of several chemical and physical questions in their own ways (MONDAL; DATTA, 2017).

The types of intermolecular interactions derived from a large part of the elements of the periodic table

Traditionally, the oxygen, fluorine and nitrogen are the most known proton acceptors in systems stabilized at light of the $\text{H}\cdots\text{F}$ and $\text{H}\cdots\text{N}$ hydrogen bonds (ADHIKARY *et al.*, 2014; URNER *et al.*, 2022). However, the protonic condition is well acceptable, and thereby, the hydrogen bond framework leads to the $\text{X}-\text{H}\cdots\text{Y}$ model (DESIRAJU, 2011). It can be perceived a separation of electronic density interpreted as charge transference between HOMO and LUMO orbitals of the proton acceptor and donor (CHENG *et al.*, 2019), respectively.

Therefore, it was established that other types of proton acceptors can be useful, such as the unsaturated hydrocarbon centers, by which the $X-H\cdots\pi$ hydrogen bonds emerged with great evidence (CARVALHO; BUENO; OLIVEIRA, 2019; GRABOWSKI; LIPKOWSKI, 2011; SAGGU; LEVINSON; BOXER, 2012).

In this scenery, it become stated that a single element is not answerable for the formation of the hydrogen bond, but ideally the cornerstone of this interaction is a site with high electronic density (ZHANG *et al.*, 2018), which can be elements with high or median electronegativity or even unsaturated bonds. The magnificence of the π centers is consolidated upon the formation of the $\pi^-\cdots\pi$ sandwich stacking (ZHUANG *et al.*, 2019), whose profile is known as one of the weakest interactions with energy in range of 1-3 kcal.mol⁻¹, being considered then as London dispersion forces. However, the acceptor of protons, in these cases the π bonds, certainly these centers does not turn out as a single source of high electronic density upon the formation of intermolecular interactions.

In some studies, the halogen center attained the independency status thereby yielded the halogen bond formation (CAVALLO *et al.*, 2016). As halogen atoms F, Cl, I and Br and their correspondent anions F⁻, Cl⁻, I⁻, and Br⁻ provide very strong hydrogen bonds, in regards to halogen bonds they interact among each other and form $Y^{-\delta}\cdots Y^{-\delta}$ (TURUNEN; ERDÉLYI, 2020). Normally, the halocarbons function as mediator in the halogen bonds wherein the halogen itself is an electron density acceptor.

It can be quoted that electronic density is the key role to form intermolecular interactions, and the halogen atoms and π bonds are the benchmark sites in this regard (IBRAHIM; MOUSSA, 2020; JALILOV *et al.*, 2020; PRASANNA; ROW, 2000; SHISHKINA *et al.*, 2022). Independently, this is a non-covalent interaction with absence of Lewis or Brønsted's proton donators, and despite this, it is noted that positive and negative molecular sites bind one to another in a stable form (LU *et al.*, 2007). It is through the polar region wherein occur nucleophilic attacks, i.e., the interaction with electronic density centers, or actually, the π bonds of the hydrocarbons, and thereby the formation of the $Y^{-\delta}\cdots\pi$ halogen- π (SHAH *et al.*, 2017) bond come true, and note that, some of these with covalent evidence (KELLETT; KENNEPOHL; BERLINGUETTE, 2020).

Obviously that the contributions of the hydrogen or halogen atoms are not suppressed, but the literature reports the existence of others intermolecular interactions types (CHAŁASIŃSKI; SZCZEŚNIAK, 2000).

In this intermolecular chemistry world, however, a new and in certain respects intriguing contact arisen as being formed by hydrogen atoms interacting mutually.

From the researches of Crabtree (2011) and (2016), the so-called dihydrogen bonds $X-H^{+\delta}\cdots H^{-\delta}-W$ looks like contradictory in principle, although the separation of charge is motivated by the high electropositive character of W often assumed as an alkaline-earth metal. In some cases, $H^{-\delta}-W$ is taken as a base specie, but this affirmation is quantitatively validated in agreement with topological analysis and electronic profiles (DIXIT; RATHI; BHARATAM, 2010).

The inclusion of alkaline elements in the context of the intermolecular interactions led to one more model symbolized as $X-H^{-\delta}\cdots H^{+\delta}$ namely by the authors as hydride bond (GRABOWSKI; SOKALSKIC; LESZCZYNSKI, 2006). In this case, X means to hydrides (HBe, HMg, Li, and Na) (WANG *et al.*, 2012), whereas $Y^{+\delta}$ represents cationic species. Once again, it is worthy to mention that $H^{-\delta}$ and $Y^{+\delta}$ behave not as acceptor and donor of protons, but as a typical base-acid pair (GRABOWSKI, 2020b). Thus, the great appeal is dedicated to the negative character of $H^{-\delta}$, what is often observed in the 'beryllium bonds' formed by beryllium hydride (BeH₂) (YÁÑEZ *et al.*, 2009) and earth-alkaline ions Li⁺, Na⁺, and Mg²⁺ (GRABOWSKI; SOKALSKIC; LESZCZYNSKI, 2006). This is not a merely revolutionary interaction at some extent, but the presence of metals leads to an extreme complexity of ideas. In addition, another dismember chemical contact formed by earth-metal alkaline is the 'lithium bond' (LIU *et al.*, 2019; SANNIGRAHI *et al.*, 1990), which plays a key role in very interesting studies reported recently (CHEN *et al.*, 2020).

The hydrogen atom action within the context of the intermolecular interactions should be necessarily revisited, once its contact with metal mediated by a carbon atom yields the so-called agostic bond (BROOKHART; GREEN; PARKIN, 2007). By taking into account the content of the IUPAC gold book in this regard, we must think in a multifaceted chemical interaction understood as 'to clasp or hold to oneself' (IUPAC, 2019).

In an overview, it is natural that the agostic bond formed by a hydrogen covalently bonded to both a carbon and transition metal atom occurs. However, a redefinition to agostic bond whose title is "distortion of an organometallic moiety which brings an appended C-H bond into close proximity with the metal center" has been reported by (SCHERER; MCGRADY, 2004).

At last, it can be quoted a lot of possibilities to intermolecular interaction in regular conditions through the contact of molecular and/or ionic subunits (MEOTNER, 2005; SCHNEIDER, 2022). In a purely contradictory interaction, halogen bound to carbon groups present a positive profile by which interact with hydride compounds in a stable way. This kind of interaction is so-called halogen-hydride bond (JABŁOŃSKI; PALUSIAK, 2012; LI *et al.*, 2010).

In a statement of Rzepa (2009), the importance of being bonded is the benchmark of the modern chemistry, and in the intermolecular context, the number of interactions is ever increasing beyond the conventional vision hitherto known (FABBRIZZI, 2022; GOYMER, 2012; VLADILLO; HASSANALI, 2018). In this sense, a recent work elaborated by Alkorta, Elguero and Frontera (2020) clarified the magnitude of the non-covalent interactions world in all types and sub-types studied so far. In this sense, one of the commented interactions is the chalcogen bond, which in according to Vogel, Wonner and Huber (2019) it can be defined as formed by the contact between a positive chalcogen element and a Lewis base, and actually this statement can be extended to the elements belonging to the 16th family of the periodic table.

The origin of the chalcogen bonds O...S, O...Se and S...S has been studied by Pascoe, Ling and Cockcroft (2017), wherein the charge density receptor center possesses a ρ -hole that is fundamentally found in halogen bonds (MURRAY *et al.*, 2007). In other words, due to the interaction between the lone pairs of electrons and the positive ρ -hole or even with the ρ^* anti-bonding orbital, amazingly, the chalcogen bond strength resembles or outweighs to that of other conventional interactions (DONG; LI; SCHEINER, 2018).

The chalcogen bond has been explored by many authors (VARADWAJ; VARADWAJ; MARQUES, 2020), and indeed, the strong character of this interaction has been consolidated (HABERHAUER; GLEITER, 2020).

Giving continuity to the other groups of the periodic table, in particular the nitrogen family also well-known as 15 group, another kind of intermolecular interaction was established, namely as pnictogen bond (MAHMUDOV *et al.*, 2020; SANTOS *et al.*, 2021; WYSOKINSKI *et al.*, 2020). Among all interaction known already commented here and other ones to be revisited subsequently, the pnictogen bond is a classical non-covalent type (VARADWAJ *et al.*, 2022a). From the systems hitherto studied (OLIVEIRA, 2014), mainly those ones represented as $\text{PH}_3 \cdots \text{NFH}_2$, $\text{H}_3\text{CPH}_2 \cdots \text{H}_3\text{CNH}_2$, and $\text{H}_2\text{FP} \cdots$

H_3CNH_2 and $\text{H}_3\text{CPH}_2 \cdots \text{NFH}_2$, all of them exhibit a median interaction strength (DEL BENE *et al.*, 2011). Similar to halogen bonds, the electrostatic ρ -hole effect can also be evidenced upon the formation of pnictogen bonds in systems derived from arsenic bound with unsaturated structures (VARADWAJ *et al.*, 2022b). As an indispensable citation, this interaction was also recognized as a new noncovalent force (SCHEINER, 2011).

The tetrel bond is another singular intermolecular interaction whose structure is composed by the elements group 14 or the carbon family (SCHEINER, 2019). In recent publication Scheiner (2021) has elected the basic principles of the tetrel bond as being the vacancy of orbitals, electrostatic potential and electronic density (BAUZÁ; SETH; FRONTERA, 2019) in order to discuss the capability to form supramolecular structures depending of this interaction, although regardless the interaction strength, the carbon has been included as a special participant on tetrel bonds between *N*-Methylacetamide and the FHSCH_3^+ cation (SCHEINER, 2021), for instance. Very interesting is the fact of strong tetrel bonds are formed by cations (ESRAFILI; MOUSAVIAN, 2018), and, specifically, the cation- π centers have already been validated in this context (ESRAFILI; MOHAMMADIAN-SABET, 2016).

Because cannot be fail to mention, the π clouds with sp^2 -hybridization allows to arises the π -hole, by which become susceptible to carbon interact with nucleophilic species (WANG *et al.*, 2019). From the elements of the 13th group, called of boron family, Grabowski (2014) another kind of intermolecular interaction titled of triel bonds was established. Similar to halogen and tetrel bonds, the triel requires the existence of the π -hole to interact with Lewis bases, wherein, the molecules constituted by the B, Al and Ga elements are the corresponding acids. In BF_3 structure, for instance, the empty p -orbital perpendicularly aligned to the molecular plane yields a π -hole (GRABOWSKI, 2020c).

One of the main characteristics of the triel bonds is the hypervalent profile due to the vacancy of electrons (KARACHI; ESKANDARI, 2021), and thereby, the systems formed by this interaction are so strongly stabilized to the extent that can be classify them as highly covalent (WANG *et al.*, 2021). It can be cited the very short triel bond distance in range of 1.55-1.63 Å and interaction energies reaching values of up to -100 KJ.mol^{-1} or higher (GRABOWSKI, 2020c), such as is known for the $\text{BI}_3 \cdots \text{NCH}$ and $\text{BCl}_3 \cdots \text{NH}_3$ complexes.

In a recent innovation, the elements of the 10, 11 and 12 groups Alkorta, Elguero and Frontera (2020) were also involved in intermolecular studies with formation of stable structures (BAUZÁ *et al.*, 2020). Notably, the unsaturated centers are also presents with respect to the interaction make up from the elements of the 10 and 11 groups, i.e., the regium- π bonds (PIÑA; FRONTERA; BAUZÁ, 2020).

At a high-level computational level, the regium bond strength was evaluated theory through a comparison with hydrogen bonds in a same contextualization (SÁNCHEZ-SANZ *et al.*, 2019) with HF, HNC, HCl and H₂O linking with gold. Indeed, by using a highly sophisticate *ab initio* level of theory, Wang *et al.* (2021) carried out a full study of Au...P and Au...N regium bonds in systems with cis/trans geometries, and, in fact, announcing the importance of these interactions to elucidate the most stable configuration.

In another point of view and besides the region bond, it was demonstrated that gold also forms hydrogen bond in the form of Au...H in cluster structures (BAKAR *et al.*, 2017) as well as in model systems (SCHMIDBAUR; RAUBENHEIMER; DOBRZAŃSKA, 2014).

Through the elements belonging to the 12 group, i.e., zinc, cadmium, mercury and copernicium, it is from them that the spodium bonds has appeared (BISWAL *et al.*, 2021; PIÑA; FRONTERA; BAUZÁ, 2020). In small systems, Xia, Li and Cheng (2020) presented a theoretical study of the HgCl₂...O(CH₃)₂, HgCl₂...(CH₃)₂, HgCl₂...Se(CH₃)₂ and HgCl₂...Te(CH₃)₂ spodium dimers whose concluding remarks pointed out the presence of coulombic effects and existence of covalent interactions. Lastly, the extreme right placed family of the periodic table, in which holds the inert gases, these elements also have contributed to the cutting-edge world of the intermolecular interactions. Just like also formerly dedicated to pnictogen bond (SANTOS *et al.*, 2021), the interaction engaged with inert gases nominated as aerogen bond, it was also considered as a new force in the molecular environment (BAUZÁ; FRONTERA, 2015).

According to Zierkiewicz, Michalczyk and Scheiner (2018), the aerogen bond was studied in systems formed by xenon and kryptonium in contact with diazines. From this same research group, it has been shown that the aerogen bond may be widely dynamic by forming interactions with chalcogen (WANG *et al.*, 2020) and in the anionic forms (GRABARZ *et al.*, 2021). As pictured in Figure 1, the intermolecular interactions cover a much part of the elements of the periodic table.

Development and discussion

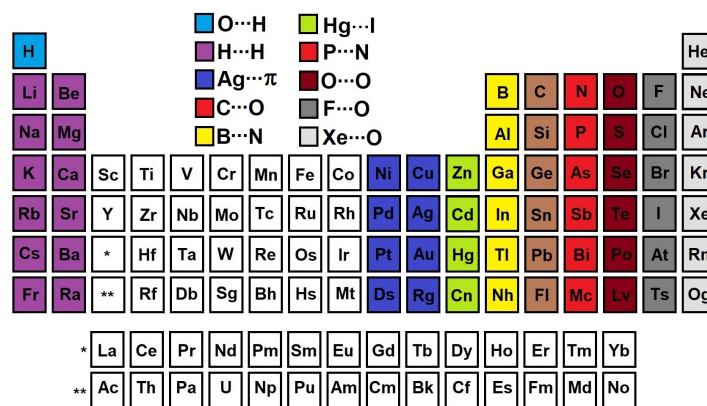
Theoretical methods vs intermolecular interactions: the turning point in the non-bonded chemistry

From the large set of theoretical methods often used for studying of intermolecular systems (JABŁOŃSKI, 2020), and even so as it has been slightly argued early here, the use of SAPT decomposition calculations have an enormously impact (DUARTE; ANGELINA; PERUCHENA, 2014; SZALEWICZ, 2012).

For the whole group of intermolecular interactions cited throughout this review, of course that QTAIM integrations jointly with the SAPT decomposition calculations shall display an accurate elucidation of the intermolecular phenomenology (BANKIEWICZ; MATCZAK; PALUSIAK, 2012; JIMÉNEZ-GRÁVALOS; SUÁREZ, 2021).

In couple of last decades, the maority contribution of the electrostatic potential to form the hydrogen bounded-complexes has been authenticated (HOJA; SAX; SZALEWICZ, 2014; UMEYAMA; MOROKUMA, 1977). In a provocative work, Hoja, Sax and Szalewicz (2014) argument that only the electrostatic potential is not enough to stabilize hydrogen-bonded dimers, and this statement is in line with the findings of Emamian *et al.* (2019), wherein the dispersion is also intrinsically participative in association with the electrostatic effect in neutral and anionic conditions, whereby, for the last one, the charge transfer also manifests very forcefully. Moreover, the induction term shows a satisfactory correlation with QTAIM parameters (GRABOWSKI, 2011), namely as the ratios between the sum of the potential and kinetic electronic energy, $H_{(r)}$, and electronic density, $\rho_{(r)}$, by taking into account a measurement of the covalent character. This leads to a recognition of the interaction strength, from weak up to strongly bound, and in practice, it impacts in other parameters, such as the vibrational frequency shifts (OLIVEIRA, 2017), for instance. The nature of the dihydrogen bond interaction appraised at the light of the SAPT scheme was consolidated by Hong and Chen (2007). Complexes formed by beryllium and monoprotic acids present interaction energies with values reaching up to $-14.46 \text{ KJ.mol}^{-1}$, which with positive results for the Laplacian of the electronic density, the values of the $E_{\text{elst}}^{(10)}$ and $E_{\text{ind}}^{(20)}$ are negatives, although the repulsion outweigh separately these two ones.

The study of formation of halogen bonds conditioned to the SAPT analysis was orientated by Hill (2014), when studied the context of small heterocyclic structures.

Figure 1 – Periodic table of elements and the indication of the intermolecular interactions.

Source: The author.

A comparison between hydrogen and halogen bonds was primarily stated, and either through the interaction between thiirane (C_2H_4S) or oxirane (C_2H_4O) with chlorine fluoride (ClF) or hydrochloric acid (HCl), the halogen bonds are more stable than hydrogen bonds with certain considerations, in particular whenever the $C_2H_4O \cdots ClF$ and $C_2H_4O \cdots HCl$ complexes are cited. Even the $C_2H_4S \cdots ClF$ presenting the higher interaction energy with the value of $-55.35 \text{ KJ.mol}^{-1}$, the SAPT examination shows that the E_{exc} is excessively overestimated.

Well, the interaction energy is often high, and as such, the contribution of the dispersion is minima in all systems. Since the interaction strength even could be overestimated in these complexes, the electrostatic contribution is roughly higher than the inductive, by which, as is widely known, the expectation by the appearing of intermolecular covalent character could be clearly realised. In other words, no arguments to assure the presence of covalence. In other aspect, however, as in a theoretical study developed by Riley and Hobza (2008) involving halohydrocarbons and formaldehyde with formation of halogen bonds, it was demonstrated that the inductive effect is the smallest attractive contribution, whereas the dispersion accounts the highest one. It can be seen, this is a scenario quite distinct from that documented by Hill (2014), and in addition, the repulsive exchange outweighs all SAPT contributions, either electrostatic or inductive and even the dispersive.

One of the foundational prerequisites to form halogen bonding is the characterization of the ρ -hole (IBRAHIM; MOUSSA, 2020; MURRAY *et al.*, 2007; NZIKO; SCHEINER, 2016; STENLID; JOHANSSON; BRINCK, 2018; WANG *et al.*, 2019), and based in a QTAIM study signed by Syzgantseva, Tognetti and Joubert (2013), be-

sides the $Br \cdots O$ halogen bond in the $CH_2CHBr \cdots OCH_2$ complex, a secondary interaction between the bromine and hydrogen was also cogitated, and therefore, a new cyclic structure would be formed among $Br-O-C-H$. In fact, the $Br \cdots H$ hydrogen bond was validated upon the formation of a Bond Critical Point (BCP) (BADER, 1991, 2001, 2009; BADER; NGUYEN-DANG, 1981) along the nuclear axis between bromine and hydrogen, and besides, this interaction is less stable than prime halogen bond because the electrostatic interaction is much higher in $Br \cdots O$. This can be understood in terms of the ρ -hole emerged on the electronic structure of the bromine, what may lead to a certain repulsion with the hydrogen.

Still with respect to heterocyclics, although treating the formation of chalcogen bonds in these structures and submitting them to the SAPT calculations, Haberhauer and Gleiter (2020) have studied the supermolecular complexes formed by the tellurium involving aromatics compounds. The SAPT analysis has no evidenced any significance of the electrostatic or induction energies, and exclusively, the steric repulsion is that rules the formation of strong chalcogen bonds hitherto observed. By taking into account the SAPT formalism, the steric repulsion conditionates the exchange energy, E_{exch}^1 , and this term represent nothing less than the Pauli repulsion (RACKERS; PONDER, 2019), and in the tellurium complexes, the E_{exch}^1 , varies in close dependence with the dihedral angles. Very important, the contribution of E_{exch}^2 is prominent in strong chalcogen interactions, whereas in weak ones, the electrostatic is that dominates and drives the intermolecular orientation (HABERHAUER; GLEITER, 2020).

In another set of systems, e.g., $F_2O \cdots NH_3$, $Cl_2O \cdots NP$ and $FNCO \cdots N_2$, Varadwaj (2019) showed that weak or strong chalcogen complexes are merely stabilized with domain of the exchange repulsion.

The QTAIM intermolecular BCPs of the O...N and O...O chalcogen bonds contains small charge density concentration with positive Laplacian, as it expected for. In pnictogen bonds, the SAPT analysis was carried out with a multiple comparison with halogen and chalcogen bonds (TRUJILLO *et al.*, 2015). The systems, more precisely the following homodimers (FNO₂)₂, (ClNO₂)₂, (BrNO₂)₂ and (INO₂)₂, all of them yield several structures with formation not only of pnictogen bonds, but also halogen bonds. In the best of our knowledge, here is devoted attention to the systems formed exclusively by pnictogen bonds, in which the exchange energy separately stands out among the remaining ones. Nevertheless, even the results of dispersion overcoming the electrostatic term, it is justly with the association in between them that the attractive force to stabilize the supermolecule is consolidated.

For these set of complexes, the QTAIM investigation display the results of electronic density and its corresponding Laplacian. According to that and as is widely known (BADER, 1991; GRABOWSKI, 2011), the framework of the pnictogen bonds is of closed-shell type due to the positive values of the Laplacian and small charge density amounts. Moreover, because the intermolecular distances varying softly, the QTAIM charge density remains essentially unchanged.

The tetrel bonds has been also undergone to the SAPT analysis. In a series of complexes of FCN...NH₃, ClCN...NH₃, BrCN...NH₃ and ICN...NH₃ (NZIKO; SCHEINER, 2016), the tetrel bonds is aligned with π -hole of the carbon-halogen bond. For all of these systems, the exchange energy is dominant followed by inductions and electrostatic, which match up one another. A close look to the strongest bonded complex, the E_{exch} reaches up to 13.30 Kcal.mol⁻¹ as well as the E_{elst} and E^{ind} which represent -6.52 and -6.03 Kcal.mol⁻¹, respectively. In terms of intermolecular distances, the values often exceed the 3.0 Å, what is typical of weak contact. The N...C tetrel bonds were confirmed by the QTAIM modeling with the identification of BCPs and bond paths of charge density between nitrogen and carbon.

A remarkable point concerning to all BCPs was registered, wherein directly the authors affirm that this topological parameter cannot guarantees of existence of such interaction (NZIKO; SCHEINER, 2016), even if is covalent or non-covalent. For the next interaction, the triel bonds, it can cite the report of Yourdkhani, Korona and Hadipour (2015) that handles about a comparison with tetrel bonds through the SAPT and QTAIM calculations.

Directly among a large sort of systems studied, the triel bonds are existent within the SiF₃CN...BF₃ and GeF₃CN...BF₃ complexes while the tetrel bonds in C₆H₅CN...SiF₃CN and C₆H₅CN...GeF₃CN ones. Of course, by the discrepancy of structures, i.e., the C₆H₅CN cyclic, the SAPT values are enormously distinct in magnitude.

Firstly, and in accordance with the structural and energetic results, the N...B triel bond lengths are 2.481 (SiF₃CN...BF₃) and 2.514 Å (GeF₃CN...BF₃), which are in agreement with the values of the interaction energies of -22.70 and -20.34 KJ.mol⁻¹, respectively. For the strongest bonded complexes being formed by tetrel bonds, the shorter length values of 2.271 and 2.222 Å for the N...Si and N...Ge interactions points out that, C₆H₅CN...SiF₃CN and C₆H₅CN...GeF₃CN respectively, whose results of the interaction energies are -69.60 and -88.48 KJ.mol⁻¹, these systems are much more strongly bound rather than those ones formed by triel bonds.

From SAPT results, indeed this statement is confirmed because the induction energies values of -210.07 (C₆H₅CN...SiF₃CN) and -411.92 KJ.mol⁻¹ (C₆H₅CN...GeF₃CN) are greater than the repulsive exchange amounts of 196.75 and 238.41 KJ.mol⁻¹, respectively. As is widely known and established in the specialized literature (OLIVEIRA; ARAÚJO, 2012; UMEYAMA; MOROKUMA, 1977), the SAPT inductive contribution is responsible for the trend to appears the covalency (GRABOWSKI, 2011), and an opposite behavior is observed in the triel-bonded complexes, wherein the E_{exch} values of 48.54 and 43.23 KJ.mol⁻¹ have overcome the induction energies of -29.43 and -25.48 KJ.mol⁻¹ of the SiF₃CN...BF₃ and GeF₃CN...BF₃ complexes respectively. Note that, it was only in these last two systems that the electrostatic character stood out. The QTAIM analysis revealed a partial covalent character for the tetrel complexes, C₆H₅CN...SiF₃CN and C₆H₅CN...GeF₃CN, while the triel ones are closed-shell structures with full absence of any trend of covalency.

To treat the remaining groups of the periodic table under the intermolecular context, and remarkably with appreciation by SAPT and QTAIM calculations, firstly it may be cited the work of Bauzá and Frontera (2018) about regium- π bonds formed between substituted aromatic rings and AgCl. It is, then, the systems of C₆H₆...AgCl, C₆H₃F₃...AgCl and C₆F₆...AgCl undergone to SAPT and QTAIM analyses.

Initially, the introduction of another computational methods, namely Natural Bond Orbitals (NBO) (GLEN-DENING; LANDIS; WEINHOLD, 2012; WEINHOLD; LANDIS; GLENDENING, 2016), the NBO $E^{(2)}$ energy results of 7.0, 3.52 and 4.04 Kcal.mol⁻¹ indicate a sequential interaction strength as follows $C_6H_6 \cdots AgCl > C_6F_6 \cdots AgCl > C_6H_3F_3 \cdots AgCl$. Even with the Eexch contribution dominating the electronic partition, e.g., the value of 59.4 Kcal.mol⁻¹ for $C_6H_6 \cdots AgCl$, it is through the electrostatic energy value of -39.4 Kcal.mol⁻¹ that the most stable profile of this complex is justified. Moreover, it can be seen that the dispersion energy is slightly manifested and the induction is moderately participative. The QTAIM topology located BCPs that bind the silver atoms to each carbon of the aromatic ring, and in all paths, the Laplacian is positive as typical for closed-shell for non-covalent interactions.

Hereinafter, the hydrogen and halogen bonds conjointly in systems of $ZnCO_3 \cdots HF$ and $ZnCO_3 \cdots F_2$ were theoretically examined by Yang *et al.* (2022), and properly, how these interactions are influenced by spodium bonds dignify this research even more. From classical intermolecular parameters, the interaction energy values of -11.27 and -1.80 Kcal.mol⁻¹ reveal how relatively much strong is the $ZnCO_3 \cdots HF$ complex, and of course, this is due to its hydrogen bond rather than the halogen bond of $ZnCO_3 \cdots F_2$. Because the increase of the H-F bond length is larger to that computed to F-F, amazingly, the vibrational red-shifts are not in line with this scenario because these bonds oscillate in up to -488.4 and -910.6 cm⁻¹, respectively.

From SAPT results, the electrostatic energy of -18.53 Kcal.mol⁻¹ of the hydrogen bond ($ZnCO_3 \cdots HF$) is much greater than the corresponding value for the halogen bond ($ZnCO_3 \cdots F_2$). Due to this, not surprisingly, the total interaction energy with hydrogen fluoride is higher to that of fluorine upon the formation of the spodium bond in the trimer with hydrogen cyanide.

From NBO calculations, the $E^{(2)}$ results of 16.33 ($ZnCO_3 \cdots HF$) and 0.09 Kcal.mol⁻¹ ($ZnCO_3 \cdots F_2$) increasing up to 30.66 and 0.11 Kcal.mol⁻¹ unrestrainedly prove the influence of the spodium bond. Ideally, and no contestations else, the results of low QTAIM charge density followed by the positive Laplacian show that all interactions wither hydrogen and halogen bonds are closed-shell interactions. The ultimate contact, the arogen bond, and reciting the work of Zierkiewicz, Michalczyk and Scheiner (2018), the Kr \cdots N and Xe \cdots N arogen bonds possess a massive contribution of the Pauli's repul-

sion, being it unquestionably, the greatest one. The others, mainly the electrostatic, that is the second more important energy is followed by the orbital interaction. Regarding the dispersion energy, it accounts the smaller participation. About the QTAIM applied for the Kr \cdots N and Xe \cdots N arogen bonds, the non-covalent character was testified in all topological criteria known ever.

Conclusions

The state-of-the-art of the non-covalent interaction world was revisited. Among the eighteen groups of the periodic table (CHAVERRI, 1953; GIUNTA; MAINZ; GIROLAMI, 2021; SCERRI, 2012), it is known that elements of ten of these ones can form intermolecular models, whose definitions were reviewed at the light of the most modern quantum computational approaches. On the basis in the energetic context, the strength of these interactions is broadly varied with distinct contributions of electrostatic, induction, and in some cases, the repulsive exchange energy. With respect to the QTAIM topography, really is demonstrated that hydrogen bonds, dihydrogen bonds, halogen bonds, chalcogen bonds, pnictogen bonds, tetrel bonds, triel bonds, regium bonds, spodium bonds and arogen bonds are essentially non-covalent interactions.

In view of the most of what is known about the properties of the elements of the periodic table, a great part of them behaves suitable to form intermolecular interactions with a single and authentic non-covalent requisite.

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