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Study Of Non-Covalent Interactions In The Building Blocks Of Biomolecules And Materials: A Critical Review

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Abstract
Weak non-covalent interactions are interactions between molecules that are not based on the sharing of electrons between atoms, but rather arise due to electrostatic, van der Waals, or other types of forces. These interactions are generally weaker than covalent bonds, which involve the sharing of electrons between atoms. The most common types of weak non-covalent interactions include: Van der Waals interactions: These are weak electrostatic forces between molecules arising from temporary dipoles. Hydrogen bonds: These are weak interactions between a hydrogen atom and an electronegative atom such as oxygen or nitrogen. Ionic interactions: These are interactions between oppositely charged ions. Dipole-dipole interactions: These are interactions between molecules with permanent dipoles. π-π interactions: These are interactions between aromatic rings in molecules. Hydrophobic interactions: These are interactions between non-polar molecules in aqueous solution, due to the tendency of non-polar molecules to aggregate together in water.
Weak non-covalent interactions are important in many areas of chemistry and biology, including the formation and stability of supramolecular structures, protein-ligand interactions, and the properties of materials such as polymers. Understanding the nature and strength of these interactions is essential for predicting and controlling the behavior of molecules and materials in various contexts.

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I. Introduction

Weak non-covalent interactions play a crucial role in the building blocks of biomolecules and materials.[1-5] Proteins are composed of long chains of amino acids that fold into specific three-dimensional structures that are critical to their biological function.[5-7] Weak non-covalent interactions such as hydrogen bonds, van der Waals forces, and electrostatic interactions play a crucial role in determining protein structure and stability. For example, hydrogen bonds help to stabilize the alpha helices and beta sheets that make up the backbone of protein structures, while van der Waals forces and electrostatic interactions contribute to the packing of the protein core.

DNA is a double-stranded helix composed of nucleotides that are held together by weak non-covalent interactions such as hydrogen bonds and van der Waals forces. These interactions allow for the precise pairing of complementary nucleotides, which is critical for DNA replication and the transmission of genetic information. Enzymes are proteins that catalyze biochemical reactions in the body. Weak non-covalent interactions play a crucial role in enzyme catalysis, helping to position substrate molecules in the active site of the enzyme and stabilizing the transition states of the reaction. Weak non-covalent interactions are critical for the specific recognition and binding of molecules in biological systems. For example, the complementary shape and electrostatic properties of ligands and receptors allow for the formation of specific non-covalent complexes that underlie many biological processes.

Weak non-covalent interactions also play a crucial role in the properties of materials, such as polymers and supramolecular assemblies.[8] For example, hydrogen bonding and van der Waals forces can contribute to the self-assembly and stability of supramolecular structures, while electrostatic interactions can control the solubility and reactivity of polymers.

Experimental determination of weak non-covalent interactions is challenging, as these interactions are typically weaker than covalent bonds and may involve subtle changes in molecular geometry or electron density. However, there are several experimental techniques that can be used to study weak non-covalent interactions, including: X-ray crystallography: This technique involves analyzing the diffraction pattern of X-rays passed through a crystalline sample, which can reveal the arrangement of atoms and the nature of intermolecular interactions.[9] Nuclear magnetic resonance (NMR) spectroscopy: NMR can be used to study weak non-covalent interactions by monitoring changes in the chemical shift or relaxation times of molecules in solution. For example, hydrogen bonding can be detected by observing shifts in the NMR spectrum of a molecule in the presence of a hydrogen bond donor or acceptor.[10] Isothermal titration calorimetry (ITC): This technique involves measuring

the heat released or absorbed during a binding reaction, providing information about the thermodynamics of weak non-covalent interactions such as binding affinity and enthalpy. Surface plasmon resonance (SPR): This technique can be used to study binding interactions between molecules immobilized on a sensor chip and molecules in solution, providing information about binding kinetics and affinity. Circular dichroism (CD) spectroscopy: CD spectroscopy can be used to study the secondary structure of proteins and nucleic acids, as well as the effects of weak non-covalent interactions such as hydrogen bonding and electrostatic interactions on their conformation. Overall, a combination of these techniques and others can be used to gain insights into the nature and strength of weak non-covalent interactions and their effects on the properties and behavior of molecules in various contexts.

Theoretical methods have become increasingly important for the prediction and interpretation of non-covalent interactions, as they can provide insights into the electronic structure and energetics of molecules that are not easily accessible through experimental techniques. Some of the theoretical methods commonly used for the determination of non-covalent interactions include: Density functional theory (DFT): DFT is a widely used computational method that can provide accurate calculations of the electronic structure of molecules and materials. DFT can be used to calculate the energies and geometries of non-covalent interactions, including hydrogen bonds, van der Waals interactions, and electrostatic interactions. Molecular mechanics (MM): MM is a simplified approach to modeling molecular systems that considers the potential energy of the system based on the relative positions and orientations of the atoms. MM can be used to study the stability and structural properties of non-covalent complexes, including protein-ligand complexes.

Molecular dynamics (MD): MD simulations can be used to study the dynamics and thermodynamics of non-covalent interactions over time. MD can provide insights into the kinetics and thermodynamics of non-covalent processes such as ligand binding and protein folding. Quantum mechanics/molecular mechanics (QM/MM): QM/MM combines quantum mechanics and classical molecular mechanics, allowing for accurate modeling of both the electronic structure and the molecular environment. QM/MM can be used to study the energetics and dynamics of non-covalent interactions in complex systems, such as enzyme catalysis. Fragment molecular orbital (FMO) method: FMO is a quantum chemical method that can be used to study the interactions between different fragments of a molecule, including non-covalent interactions. FMO can provide insights into the nature and strength of non-covalent interactions in large biomolecules. These theoretical methods can be used to predict and interpret a wide range of non-covalent interactions, including hydrogen bonds, van der Waals interactions, ionic interactions, and π-π interactions. By combining experimental and theoretical approaches, researchers can gain a more complete understanding of the nature and importance of non-covalent interactions in various chemical and biological systems.

Inter and intra molecular hydrogen bonding

Hydrogen bonding is a type of intermolecular attraction between molecules containing hydrogen atoms bonded to electronegative atoms such as oxygen, nitrogen, or fluorine.[11-14] This attraction is due to the partial positive charge on the hydrogen atom and the partial negative charge on the electronegative atom.[15-18]

Intramolecular hydrogen bonding refers to the formation of hydrogen bonds within a single molecule. This occurs when a molecule contains two or more hydrogen bonding sites, such as an alcohol molecule where the -OH group can form a hydrogen bond with the oxygen atom within the same molecule.[19, 20] Intramolecular hydrogen bonding can affect the physical and chemical properties of a molecule, such as its boiling point and reactivity.

Intermolecular hydrogen bonding occurs between different molecules.[21-26] This occurs when the hydrogen bonding site in one molecule interacts with the electronegative atom in a neighboring molecule, forming a hydrogen bond. Inter-molecular hydrogen bonding plays an important role in many biological processes, such as protein folding and DNA base pairing.[26]

The strength of intermolecular hydrogen bonding depends on the distance and orientation of the interacting molecules, as well as the strength of the hydrogen bonding site and electronegative atom. In general, hydrogen bonding is a weaker intermolecular force compared to covalent or ionic bonding, but it is still an important contributor to the physical and chemical properties of many substances.[27-29]

Sigma hole interplay and its importance

The sigma-hole interplay refers to the interaction between the sigma-hole of an electron-deficient atom and the electron-rich region of a neighboring molecule.[30, 31] The sigma-hole is a region of positive electrostatic potential on the surface of an atom or molecule, which is located on the opposite side of the atom or molecule from the covalent bond.[31] This interaction is important because it can contribute to the formation of intermolecular interactions and can affect the properties of molecular systems.[31]

The sigma-hole interplay is particularly important in halogen bonding, a type of non-covalent interaction between a halogen atom (typically iodine, bromine, or chlorine) and an electron-rich species. In halogen bonding, the halogen atom acts as an electron-deficient site, with the sigma-hole located on the opposite side of the halogen

from the covalent bond. This sigma-hole can interact with the electron-rich region of a neighboring molecule, forming a stabilizing interaction that is similar to hydrogen bonding.

The sigma-hole interplay can also affect the reactivity of chemical reactions. For example, in organometallic chemistry, the sigma-hole of a metal atom can interact with the electron-rich region of an organic molecule, activating the molecule for reaction with other species.

Overall, the sigma-hole interplay is an important concept in chemistry that can contribute to the understanding of non-covalent interactions and the reactivity of molecular systems.

Halogen bond

A halogen bond is a type of non-covalent interaction between a halogen atom (typically iodine, bromine, or chlorine) and an electron-rich species, such as an oxygen, nitrogen, or sulfur atom.[32-34] Halogen bonds are similar to hydrogen bonds in that they involve an interaction between a donor and an acceptor, but the donor in this case is the halogen atom, which has a partially positive region known as a sigma-hole.[32, 34]

The sigma-hole is located on the opposite side of the halogen atom from the covalent bond, and it is created by the electronic structure of the halogen atom, which has a low-lying vacant orbital with positive electrostatic potential. This positive region can interact with the electron-rich region of a neighboring molecule, forming a stabilizing interaction that is similar to a hydrogen bond.[32-34]

Halogen bonds are important in many areas of chemistry, including crystal engineering, materials science, and drug design. In crystal engineering, halogen bonds can be used to control the packing arrangement of molecules in the solid state, leading to novel properties and functions. In materials science, halogen bonds can contribute to the mechanical properties and self-assembly of materials. In drug design, halogen bonds can be used to optimize the binding of small molecules to protein targets, leading to improved potency and selectivity.

Overall, the halogen bond is a relatively new and rapidly evolving area of research in chemistry, with many potential applications in various fields of science and technology.

Chalcogen bonds

Chalcogen bonds are a type of non-covalent interaction between a chalcogen atom (typically sulfur, selenium, or tellurium) and an electron-rich species, such as an oxygen, nitrogen, or sulfur atom. Chalcogen bonds are similar to halogen bonds in that they involve an interaction between a donor and an acceptor, but the donor in this case is the chalcogen atom.[35]

The chalcogen atom has a partially negative region, created by the electronic structure of the atom, which allows it to interact with the electron-rich region of a neighboring molecule, forming a stabilizing interaction that is similar to a hydrogen bond or a halogen bond.[36, 37]

Chalcogen bonds have been found to play an important role in many areas of chemistry, including crystal engineering, materials science, and biochemistry.[36-38] In crystal engineering, chalcogen bonds can be used to control the packing arrangement of molecules in the solid state, leading to novel properties and functions. In materials science, chalcogen bonds can contribute to the mechanical properties and self-assembly of materials. In biochemistry, chalcogen bonds are believed to play a role in protein folding and enzyme catalysis.[39]

Overall, chalcogen bonds are a relatively new and emerging area of research in chemistry, with many potential applications in various fields of science and technology.[36, 37, 39, 40]

Pnictogen bond

Pnictogen bonds are a type of non-covalent interaction between a pnictogen atom (typically nitrogen, phosphorus, arsenic, or antimony) and an electron-rich species, such as an oxygen, nitrogen, or sulfur atom.[41] Pnictogen bonds are similar to halogen bonds and chalcogen bonds in that they involve an interaction between a donor and an acceptor, but the donor in this case is the pnictogen atom.[42]

The pnictogen atom has a partially positive region, created by the electronic structure of the atom, which allows it to interact with the electron-rich region of a neighboring molecule, forming a stabilizing interaction that is similar to a hydrogen bond, halogen bond, or chalcogen bond.[42]

Pnictogen bonds have been found to play an important role in many areas of chemistry, including crystal engineering, materials science, and biochemistry.[43] In crystal engineering, pnictogen bonds can be used to control the packing arrangement of molecules in the solid state, leading to novel properties and functions. In materials science, pnictogen bonds can contribute to the mechanical properties and self-assembly of materials. In biochemistry, pnictogen bonds are believed to play a role in protein-ligand interactions and enzyme catalysis.

Overall, pnictogen bonds are a relatively new and emerging area of research in chemistry, with many potential applications in various fields of science and technology.

Tetral bond

Tetrel bonds are a type of non-covalent interaction between a Group 14 element (carbon, silicon, germanium, tin, or lead) and an electron-rich species, such as an oxygen, nitrogen, or sulfur atom. The name "tetrel" comes from the fact that these elements belong to the same column (Group 14) in the periodic table.[44, 45]

Tetrel bonds are similar to other non-covalent interactions, such as hydrogen bonds, halogen bonds, chalcogen bonds, and pnictogen bonds, in that they involve an interaction between a donor and an acceptor.[46] The donor in this case is the Group 14 element, which has a partially positive region on the opposite side of the covalent bond, known as a sigma-hole. The acceptor is typically an oxygen, nitrogen, or sulfur atom, which has a lone pair of electrons that can interact with the sigma-hole of the Group 14 element.

Tetrel bonds have been found to play an important role in many areas of chemistry, including crystal engineering, materials science, and biochemistry. In crystal engineering, tetrel bonds can be used to control the packing arrangement of molecules in the solid state, leading to novel properties and functions. In materials science, tetrel bonds can contribute to the mechanical properties and self-assembly of materials. In biochemistry, tetrel bonds are believed to play a role in protein-ligand interactions and enzyme catalysis.

Overall, tetrel bonds are a relatively new and rapidly evolving area of research in chemistry, with many potential applications in various fields of science and technology.

II. π-π interaction

π-π interactions are a type of non-covalent interaction between two aromatic or conjugated systems. In an aromatic or conjugated system, the electrons in the pi orbitals are delocalized over the entire system.[47, 48] When two such systems are brought close together, the electron clouds can interact, leading to a π-π interaction.

The strength of the π-π interaction depends on the orientation, distance, and size of the two interacting systems. If the two systems are parallel and the distance between them is less than the sum of their van der Waals radii, the interaction can be strong and stabilizing. In addition to being found in molecules, π-π interactions are also important in supramolecular chemistry, where they can be used to control the assembly and properties of materials.

In biochemistry, π-π interactions play an important role in the structure and function of biomolecules. For example, in DNA, the stacking of the base pairs is stabilized by π-π interactions, which help to maintain the double helix structure. In proteins, π-π interactions between aromatic amino acid residues can play a role in stabilizing the three-dimensional structure of the protein.

Overall, π-π interactions are an important type of non-covalent interaction in chemistry and play a significant role in a wide range of chemical and biological phenomena.

III. Van der Waals interactions

Van der Waals interactions are weak non-covalent interactions between molecules, resulting from the fluctuating electrostatic forces between them. These interactions arise due to the temporary dipoles that occur as electrons move around atoms or molecules, which can induce a dipole in a nearby molecule.[49, 50] There are three types of Van der Waals interactions:

Dipole-dipole interactions: These occur between molecules with permanent dipoles. The positive end of one dipole attracts the negative end of another, resulting in an attractive force.

Dipole-induced dipole interactions: These occur between molecules with a permanent dipole and a nearby molecule with no dipole. The dipole of the first molecule induces a temporary dipole in the second, resulting in an attractive force.[51, 52]

London dispersion forces: These occur between all molecules, even those with no permanent dipole. As electrons move around atoms or molecules, temporary dipoles are created, leading to an attractive force between the two molecules.

Van der Waals interactions are important in determining the physical and chemical properties of molecules, such as boiling point, melting point, and solubility. They also play a significant role in the structure and function of biomolecules, such as proteins and nucleic acids, as well as in the formation and stability of supramolecular structures.

Overall, Van der Waals interactions are a type of non-covalent interaction that arise due to fluctuating electrostatic forces between molecules and play an important role in many areas of chemistry and biology.

IV. Conclusion

There are several types of non-covalent interactions that occur between molecules, including:

- Hydrogen bonds: These are strong electrostatic interactions between a hydrogen atom and an electronegative atom such as nitrogen, oxygen, or fluorine.
- Ionic interactions: These are electrostatic interactions between oppositely charged ions, which can be strong in the presence of charges of high magnitude and low distance.
- Van der Waals interactions: These are weak interactions between two or more molecules due to fluctuating electrostatic forces, which include dipole-dipole interactions, dipole-induced dipole interactions, and London dispersion forces.
- π-π interactions: These are non-covalent interactions between two aromatic or conjugated systems that are parallel and close to each other, and can be strong and stabilizing.
- Hydrophobic interactions: These occur between non-polar molecules or regions of molecules that are insoluble in water and can result in the exclusion of water from the vicinity of the non-polar surface.
- Halogen bonds: These are non-covalent interactions between a halogen atom and an electronegative atom, such as oxygen or nitrogen.
- Chalcogen bonds: These are non-covalent interactions between a chalcogen atom (oxygen, sulfur, or selenium) and an electron-rich species.
- Pnictogen bonds: These are non-covalent interactions between a pnictogen atom (nitrogen, phosphorus, arsenic, or antimony) and an electron-rich species.
- Tetrel bonds: These are non-covalent interactions between a Group 14 element (carbon, silicon, germanium, tin, or lead) and an electron-rich species.

Overall, non-covalent interactions play a significant role in many areas of chemistry and biology, such as in the structure and function of biomolecules, the assembly of supramolecular structures, and the properties of materials.

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References

[1]. J. Antony, S. Grimme, Phys. Chem. Chem. Phys., 10, 2722 (2008); https://doi.org/10.1039/B718788B
[2]. L. Gráfová, M. Pitoňák, J. Řezáč, P. Hobza, J. Chem. Theory Comput., 6, 2365 (2010); https://doi.org/10.1021/ct1002253
[3]. K.E. Riley, M. Pitoňák, P. Jurečka, P. Hobza, Chem. Rev. (Washington, DC, U. S.), 110, 5023 (2010); https://doi.org/10.1021/cr1000173
[4]. S.E. Wheeler, Acc. Chem. Res., 46, 1029 (2013); https://doi.org/10.1021/ar300109n
[5]. Y. Zhao, D.G. Truhlar, J. Chem. Theory Comput., 3, 289 (2007); https://doi.org/10.1021/ct6002719
[6]. L.M. Salonen, M. Ellermann, F. Diederich, Angew. Chem., Int. Ed., 50, 4808 (2011); https://doi.org/10.1002/anie.201007560
[7]. A. Volbeda, E. Garcin, C. Piras, A.L. de Lacey, V.M. Fernandez, E.C. Hatchikian, M. Frey, J.C. Fontecilla-Camps, J. Am. Chem. Soc., 118, 12989 (1996);
[8]. E.B. Anderson, T.E. Long, Polymer, 51, 2447 (2010); https://doi.org/10.1016/j.polymer.2010.02.006
[9]. S. Williams et al., J. Biol. Chem., 278, 27138 (2003); https://doi.org/10.1074/jbc.M302260200
[10]. A. Nikolić, B. Jović, S. Csanady, S. Petrović, J. Mol. Struct., 834-836, 249 (2007); https://doi.org/10.1016/j.molstruc.2006.11.003
[11]. Y. Matsumoto, K. Honma, J. Chem. Phys., 127, 184310 (2007); https://doi.org/10.1063/1.2790894
[12]. S.E. Miller, N.R. Kallenbach, P.S. Arora, Tetrahedron, 68, 4434 (2012); https://doi.org/10.1016/j.tet.2011.12.068
[13]. A. Müller, S. Leutwyler, J. Phys. Chem. A, 108, 6156 (2004); https://doi.org/10.1021/jp049033h
[14]. G. Villani, J. Phys. Chem. B, 114, 9653 (2010); https://doi.org/10.1021/jp102457s
[15]. H.W. Roesky, M. Andruh, Coord. Chem. Rev., 236, 91 (2003);
[16]. M. Saeki, S.-i. Ishiuchi, M. Sakai, M. Fujii, J. Phys. Chem. A, 111, 1001 (2007); https://doi.org/10.1021/jp0668910
[17]. V. Stefov, L. Pejov, B. Šoptrajanov, J. Mol. Struct., 651, 793 (2003);
[18]. T.N. Wassermann, C.A. Rice, M.A. Suhm, D. Luckhaus, J. Chem. Phys., 127, 234309 (2007); https://doi.org/10.1063/1.2806181
[19]. R. Podeszwa, R. Bukowski, K. Szalewicz, J. Phys. Chem. A, 110, 10345 (2006); https://doi.org/10.1021/jp064095o
[20]. K.S.C. Reid, P.F. Lindley, J.M. Thornton, FEBS Lett., 190, 209 (1985);
[21]. H.S. Biswal, P.R. Shirhatti, S. Wategaonkar, J. Phys. Chem. A, 114, 6944 (2010); https://doi.org/10.1021/jp102346n
[22]. H.S. Biswal, S. Wategaonkar, J. Phys. Chem. A, 114, 5947 (2010); https://doi.org/10.1021/jp100439w
[23]. J.E. Braun, Grebner, H.J. Neusser, J. Phys. Chem. A, 102, 3273 (1998); https://doi.org/10.1021/jp980649e
[24]. J. Carney, F. Hagemeister, T. Zwier, others, J. Chem. Phys., 108, (1998);
[25]. J.R. Carney, F.C. Hagemeister, T.S. Zwier, J. Chem. Phys., 108, 3379 (1998); https://doi.org/10.1063/1.475356
[26]. G.R. Desiraju, Angew. Chem., Int. Ed., 46, 8342 (2007); https://doi.org/10.1002/anie.200700534
[27]. P. Zielke, M.A. Suhm, Phys. Chem. Chem. Phys., 8, 2826 (2006); https://doi.org/10.1039/b605926k
[28]. T. Zelený et al., J. Am. Chem. Soc., 134, 13662 (2012); https://doi.org/10.1021/ja3028845
[29]. Y. Yang, W. Zhang, Journal of Molecular Structure: THEOCHEM, 814, 113 (2007); https://doi.org/10.1016/j.theochem.2007.03.005
[30]. V. Elakkat, C.-C. Chang, J.-Y. Chen, Y.-C. Fang, C.-R. Shen, L.-K. Liu, N. Lu, Chem. Commun. (Cambridge, U. K.), 55, 14259 (2019); https://doi.org/10.1039/C9CC06731K
[31]. J.Y. Lim, P.D. Beer, Chem, 4, 731 (2018);
[32]. G. Cavallo, P. Metrangolo, R. Milani, T. Pilati, A. Priimagi, G. Resnati, G. Terraneo, Chem. Rev. (Washington, DC, U. S.), 116, 2478 (2016);
[33]. P. Politzer, P. Lane, M.C. Concha, Y. Ma, J.S. Murray, Journal of molecular modeling, 13, 305 (2007);
[34]. P. Auffinger, F.A. Hays, E. Westhof, P.S. Ho, Proc. Natl. Acad. Sci., 101, 16789 (2004);

[35]. L. Vogel, P. Wonner, S.M. Huber, Angew. Chem., Int. Ed., 58, 1880 (2019);
[36]. S. Benz, J. López-Andarias, J. Mareda, N. Sakai, S. Matile, Angew. Chem., Int. Ed., 56, 812 (2017);
[37]. W. Wang, B. Ji, Y. Zhang, J. Phys. Chem. A, 113, 8132 (2009);
[38]. P.C. Ho, J.Z. Wang, F. Meloni, I. Vargas-Baca, Coord. Chem. Rev., 422, 213464 (2020);
[39]. K.T. Mahmudov, A.V. Gurbanov, V.A. Aliyeva, M.F.C.G. da Silva, G. Resnati, A.J. Pombeiro, Coord. Chem. Rev., 464, 214556 (2022);
[40]. P. Scilabra, G. Terraneo, G. Resnati, Acc. Chem. Res., 52, 1313 (2019);
[41]. K.T. Mahmudov, A.V. Gurbanov, V.A. Aliyeva, G. Resnati, A.J. Pombeiro, Coord. Chem. Rev., 418, 213381 (2020);
[42]. P. Scilabra, G. Terraneo, G. Resnati, J. Fluorine Chem., 203, 62 (2017);
[43]. S. Benz, A.I. Poblador-Bahamonde, N. Low-Ders, S. Matile, Angew. Chem., 130, 5506 (2018);
[44]. T. Isozaki, Y.-i. Tsutsumi, T. Suzuki, T. Ichimura, Chem. Phys. Lett., 495, 175 (2010); https://doi.org/10.1016/j.cplett.2010.06.081
[45]. A. Bauzá, T.J. Mooibroek, A. Frontera, The Chemical Record, 16, 473 (2016);
[46]. A. Bauzá, T.J. Mooibroek, A. Frontera, Angew. Chem., Int. Ed., 52, 12317 (2013);
[47]. C. Chipot, R. Jaffe, B. Maigret, D.A. Pearlman, P.A. Kollman, J. Am. Chem. Soc., 118, 11217 (1996);
[48]. M.O. Sinnokrot, C.D. Sherrill, J. Am. Chem. Soc., 126, 7690 (2004);
[49]. F. Cozzi, R. Annunziata, M. Benaglia, K.K. Baldridge, G. Aguirre, J. Estrada, Y. Sritana-Anant, J.S. Siegel, Phys. Chem. Chem. Phys., 10, 2686 (2008); https://doi.org/10.1039/B800031J
[50]. M. Piacenza, S. Grimme, J. Am. Chem. Soc., 127, 14841 (2005); https://doi.org/10.1021/ja053613q
[51]. J. Gräfenstein, D. Cremer, J. Chem. Phys., 130, 124105 (2009); https://doi.org/10.1063/1.3079822
[52]. J.C. Amicangelo, B.W. Gung, D.G. Irwin, N.C. Romano, Phys. Chem. Chem. Phys., 10, 2695 (2008); https://doi.org/10.1039/B718722J