Review Article

Approaches for Special Characteristics of Chalcogen Bonding: A mini Review

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ABSTRACT

Chalcogen bonding, an intriguing and relatively new noncovalent contact, has drawn a lot of interest in the field of chemical bonding because of its special characteristics and possible uses in supramolecular chemistry, materials research, and drug development. An interaction between a chalcogen atom (sulphur, selenium, or tellurium) and a Lewis base, usually a lone pair donor or -electron-rich system, is referred to as a chalcogen bond. Chalcogen bonding, which is a fascinating replacement for conventional hydrogen and halogen bonds, demonstrates distinctive characteristics like a wide range of binding geometries, variable strength through substitution effects, and its involvement in numerous chemical and biological systems. An overview of the characterisation of chalcogen bonding is provided in this article, with an emphasis on the theoretical underpinnings, and experimental methods. To identify and analyze chalcogen bonds, experimental methods such as X-ray crystallography, spectroscopy, and thermodynamics are addressed. The identification of chalcogen atom, the makeup of the electron donors and acceptors, and the impact of solvents are the other aspects that affect chalcogen bonding. The article also discusses chalcogen bonding, including its function in supramolecular chemistry, crystal engineering, material design, and drug development. This article gives a thorough description of the characterisation of chalcogen bonding, stressing its potential for novel applications and illuminating its essential characteristics.

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1. Introduction

Molecules and materials structure, characteristics, and behavior are fundamentally shaped by noncovalent interactions. Non-covalent interactions are a class of weak bonding forces taking place between molecules or functional groups devoid of electron transfer or sharing. These interactions contribute to the stability, structure, and functionality of molecules and larger assemblies, and are also essential in a number of biological, chemical, and physical processes. Non-covalent interactions are more fleeting and reversible than covalent bonds, which involve the formation of chemical bonds through the sharing of electrons. This makes them crucial for dynamic processes and molecular recognition. Some of the non-covalent interactions include hydrogen bonding, halogen bonding, Van der Waals, ionic interactions, hydrophobic interactions and chalcogen bonding [1, 2]. These interactions, like halogen and hydrogen bonds, are crucial for self-assembly, molecular recognition, and the stability of diverse chemical systems. Chalcogen bonding, a particular kind of noncovalent contact, has recently become a fascinating area of research. Sulfur (S), selenium (Se), and tellurium (Te) are chalcogens, which have unusual bonding properties and may create potent attraction interactions with other atoms or molecules [3]. Similar to hydrogen bonding, chalcogen bonding is a non-covalent interaction between a chalcogen atom and an electron donor or acceptor that depends on the electrostatic attraction between a positively polarized region (the electrophilic chalcogen atom) and a negatively polarized region (the nucleophilic electron donor or acceptor). Comprehensive characterization is necessary to comprehend the nature and characteristics of chalcogen bonding. The structural characteristics, energetics, and variables affecting the directionality and strength of chalcogen bonding are all investigated. To clarify the specifics of chalcogen bonding and investigate its applications in chemistry and materials science, various experimental techniques and theoretical frameworks have been used [4]. X-ray crystallography is one of the experimental methods used to characterize chalcogen bonding because it offers important details on the distances and angles involved in bonds between chalcogens. The vibrational and electronic characteristics of chalcogen bonds may be studied using spectroscopic techniques including infrared and NMR spectroscopy. The energetics of chalcogen bonding is also revealed by thermodynamic studies like calorimetry and isothermal titration calorimetry [5]. The Lewis base serves as the donor and the chalcogen atom functions as the acceptor in a directed donor-acceptor interaction that defines chalcogen bonding. The Lewis base's electron-deficient area and the sole pair of chalcogen atom are attracted to one another by an electrostatic force in this interaction. The characteristics of the chalcogen atom, the type of the Lewis base, and the environment can all affect how strong the chalcogen bonding is. Researchers can adjust these variables to regulate the specificity and binding affinity of chalcogen bonding interactions. Different binding geometries, such as linear, T-shaped, and bifurcated configurations, can be used in chalcogen bonding. The development of intricate supramolecular structures and dynamic assemblies is made possible by this adaptability [6].

Theoretical methods, particularly computational ones, are crucial in the characterization of chalcogen bonding as a complement to experimental approaches. The electrical structure, energetics, and dynamics of chalcogen bonding interactions are examined using density functional theory (DFT)

computations and molecular dynamics simulations [7]. These theoretical techniques help in predicting and developing chalcogen bond-based systems as well as in understanding the variables affecting the strength and directionality of chalcogen bonds. To improve our understanding of this exceptional noncovalent interaction and its applications in diverse sectors, chalcogen bonding should be characterized. Chalcogen bonding's structural and energetic characteristics may be better understood, which will help researchers better understand how it functions in supramolecular chemistry, crystal engineering, materials design, and drug development. The creation of innovative materials and technologies based on the principles of chalcogen bonding will also be made possible by a greater comprehension of chalcogen bonding [8]. The aim of this article is to explore the characterization of chalcogen bonding, covering the theoretical background, experimental techniques, structural and energetic features, influencing chalcogen bonding. The scope of the study on chalcogen bonding approaches is to understand the nature, power, and uses of chalcogen bonding interactions. This is accomplished using various theoretical and experimental methods.

2. Characterization of Chalcogen Bonding

2.1. Theoretical background of chalcogen bonding

The electrical structure and bonding theories related to chalcogen atoms are the starting points for understanding chalcogen bonding. Chalcogens have six valence electrons and are a member of Group 16 of the periodic table. They easily share electrons with other atoms to create covalent bonds. The distribution of electron densities surrounding the chalcogen atom is very important in chalcogen bonding [9]. In chalcogen bonding, the chalcogen atom can act as both an electron donor and an electron acceptor. The chalcogen atom possesses a lone pair of electrons in its valence shell, which can function as an electron donor, forming a dative covalent bond with a Lewis base (electron pair donor). Charge transfer interaction is the basis for chalcogen bonding. Due to its greater electronegativeity compared to the other common electron donors (such as carbon, nitrogen, and oxygen), the chalcogen atom removes electron density from the donor atom or molecule, producing a positively polarized zone all around it. In turn, the electron donor goes through an induced negative polarization [10]. The electrostatic interaction that results between the nucleophilic electron donor and the electrophilic chalcogen atom creates the chalcogen bond [11]. The direction and strength of chalcogen bonding interactions are influenced by a number of variables. It is crucial to comprehend these elements to describe chalcogen bonding and forecast how it will behave in various situations. Here a few crucial ones are provided:

Identity and characteristics of the chalcogen atom: The strength of chalcogen bonds is greatly influenced by the chalcogen atom's nature (sulfur, selenium, or tellurium). In comparison to sulfur or selenium atoms, tellurium atoms often form stronger chalcogen bonds because of their bigger size and higher polarizability. The characteristics of the electron donor and acceptor affect chalcogen bonding, including electronegativity, polarizability, and steric effects [12, 13]. Stronger chalcogen bonds often result from electron donors with higher electronegativity or better polarizability. Steric effects can alter the strategy and alignment of chalcogen bonding, facilitating or impeding it. Chalcogen bonding can be considerably impacted by the presence of solvents or other environmental conditions. Chalcogen bonding may be hindered or facilitated by the polarity of solvent and the existence of hydrogen bonding interactions. The strength and directionality of chalcogen bonds can be affected by polarity and dielectric constant of the solvent [14].

2.2. Experimental techniques for characterizing chalcogen bonds

2.2.1. X-ray crystallography

X-ray crystallography is a popular method for characterizing the structural properties of chalcogen bonds. By examining the diffraction

patterns of X-rays flowing through a crystal, structures may be ascertained. Given that the intermolecular lengths and angles involved in chalcogen bonding interactions, X-ray crystallography is useful in the context of chalcogen bonding. The strength and geometry of chalcogen bonds may be evaluated by measuring the lengths between chalcogen atoms and their interacting partners as well as the angles generated by the interacting atoms [15]. By comparing chalcogen bonding to the other non-covalent interactions, such as hydrogen or halogen bonding, this approach enables researchers to get insight into the relative potency and structural characteristics of various interactions [16]. For example, the presence of chalcogen bonding between a selenium atom and a nitrogen atom in a molecule was discovered by an investigation of the crystal structure. It was found that the selenium atom's distance from the nitrogen atom was 2.8 (Å), pointing to a robust chalcogen connection. It was discovered that the angle created by the selenium-nitrogen interaction was around 160 degrees, illuminating the bent geometry present in chalcogen bonding (**Figure 1**) [17].

2.2.2. Spectroscopic approaches

By examining the vibrational and electronic characteristics of the molecules participating in the contacts, spectroscopic techniques provide important insights into the characterization of chalcogen bonding interactions.

Infrared spectroscopy

Infrared (IR) spectroscopy is a powerful technique frequently employed in the study of chalcogen bonding. It provides valuable information about the vibrational properties

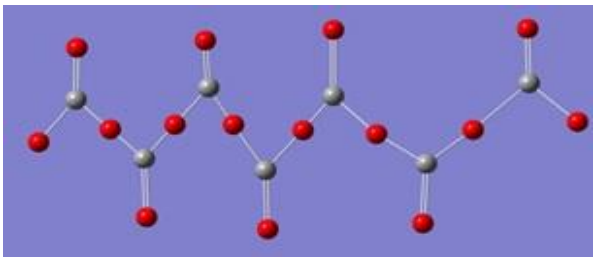

Figure 1. Chalcogen bonding in selenium [17]

and interactions of molecules involved in chalcogen bonds. By analyzing the IR spectra of chalcogen-bonded compounds, researchers can identify specific vibrational modes associated with chalcogen bonding interactions, allowing for the characterization and analysis of these interactions as shown in **Figure 2**. Chalcogen bonds exhibit distinctive vibrational frequencies related to the stretching and bending modes of the participating atoms [18].

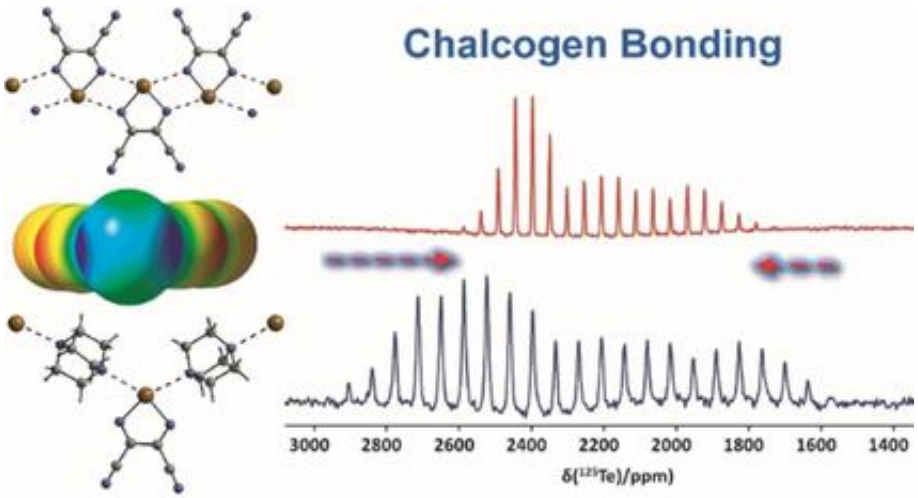

Figure 2. Chalcogen bonding in IR spectroscopy [18]

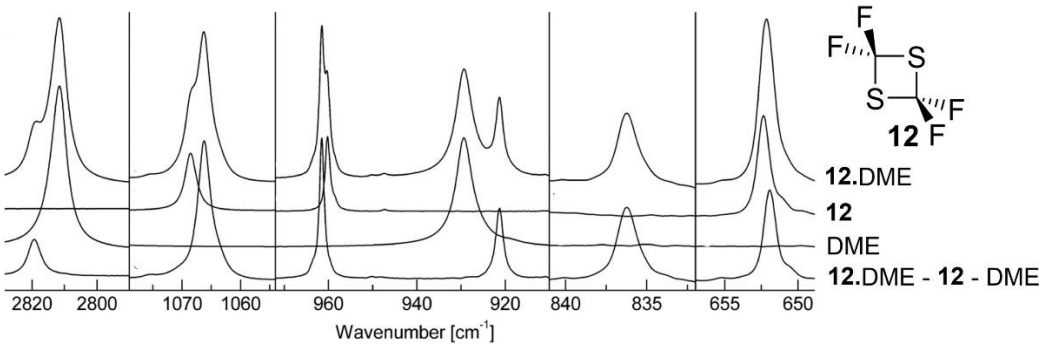

Figure 3. IR spectra of selected spectral regions for the mixtures of chalcogen with DME [20]

These vibrational modes are sensitive to the strength and nature of chalcogen bonding interactions. Changes in vibrational frequencies and intensities in the IR spectra provide valuable insights into the strength and composition of chalcogen bonds. For instance, a chalcogen-bonded complex between an oxygen atom and a sulfur atom was studied using IR spectroscopy [19]. In the IR spectrum, a characteristic vibrational band was observed at 1200 cm^{-1}. This vibrational band corresponded to the stretching vibration associated with the chalcogen bond. The presence and intensity of this band provided evidence for the formation of a chalcogen bond between the oxygen and sulfur atoms in the complex. the use of IR spectroscopy is very limited because of the complexity of the recorded spectra at room temperature. It was however successfully used to confirm the intramolecular ChB in 1-$COCH_3$. Indeed, IR stretching frequencies of the C=O bond in S- and Se-derivatives (1709 cm^{-1} and 1713 cm^{-1}) were significantly shifted compared to the O-derivative (1748 cm^{-1}), as expected from the weakening of the carbonyl bond arising from $n_O \rightarrow \sigma^*_{S/Se-C}$ delocalization. IR spectra can be simplified by working at very low temperature in liquid krypton (120 K) and with a rigid ChB donor such as 2,2,4,4-tetrafluoro-1,3-dithiethane. Under these conditions, simplified spectra could be obtained in the presence of 1,2-dimethoxyethane (DME), with appearance of several new bands associated with the Ch-bonded DME 1,1 dimer, as confirmed by theoretical calculations [20].

This example (shown in **Figure** 3) demonstrates how IR spectroscopy can be utilized to identify and characterize chalcogen bonding interactions. By analyzing the vibrational frequencies and intensities associated with chalcogen bonds, researchers can gain valuable insights into the strength, nature, and structural features of these noncovalent interactions. Such information is crucial for understanding the role of chalcogen bonding in various chemical and biological systems and for designing and manipulating chalcogen bond-based materials with desired properties [21].

NMR spectroscopy

NMR spectroscopy is a powerful technique for investigating chalcogen bonding interactions by analyzing changes in chemical shifts, coupling constants, and relaxation times. It provides valuable information about the electronic environment and dynamics of chalcogen-bonded systems [22]. In NMR spectroscopy, the applied magnetic field interacts with the nuclei of atoms, resulting in characteristic resonance frequencies. The chemical shift, expressed in parts per million (ppm), reflects the local electronic environment around a nucleus. In the context of chalcogen bonding, the presence of a chalcogen bond can induce changes in the chemical shifts of the atoms involved in the interaction. For instance, consider a chalcogen-bonded complex between a tellurium atom and an aluminum, nitrogen, and carbon atom (**Figure 4**) [23].

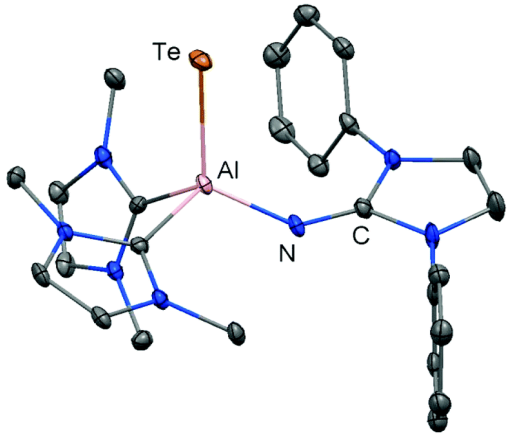

Figure 4. Chalcogen bond between tellurium and aluminium, nitrogen and carbon atom source [23]

In the NMR spectrum, the carbon atom involved in the chalcogen bond would exhibit a shifted chemical shift upfield. This upfield shift indicates a de-shielding effect, meaning that the electron density around the carbon atom is reduced due to the electron-withdrawing nature of the tellurium atom. The magnitude of the chemical shift change provides insights into the strength and polarity of the chalcogen bond. Coupling constants observed in the NMR spectrum are another important parameter for characterizing chalcogen bonding [24]. Coupling constants reflect the spin-spin interactions between neighboring nuclei. In the case of chalcogen bonds, the presence of the chalcogen atom can influence the coupling constants of the atoms involved in the bond. The magnitude and splitting pattern of the coupling constants provide information about the conformational preferences and dynamics of the chalcogen bond [24].

Some of the applications of NMR spectroscopy in characterizing chalcogen bonding include:

Changes in Chemical Shift

Chalcogen bonding has the ability to significantly alter the chemical shifts of adjacent nuclei. Chemical shifts in NMR spectroscopy are responsive to the local electronic environment of atoms. A chalcogen bond modifies the electron density surrounding the chalcogen atom, which affects the chemical shifts of nearby atoms. The presence of chalcogen bonding in a molecule can be determined by researchers by keeping track of these chemical shift shifts in NMR spectra [25].

a. *2D NMR Methods*: The spatial proximity and separation between the chalcogen bond donor and acceptor can be determined with the use of two-dimensional NMR techniques, such as NOESY (Nuclear Overhauser Effect Spectroscopy) and ROESY (Rotating-frame Overhauser Effect Spectroscopy). Cross-peaks in the 2D NMR spectra allow scientists to identify the presence of chalcogen bonding and clarify its mechanisms [26].

b. *J-Coupling Constants*: J-coupling constants in NMR spectroscopy are connected to the coupling between nuclei. Due to variations in bond lengths and angles, chalcogen bonding can have an impact on the J-coupling constants of the atoms engaged in the interaction. The J-coupling constants can be used to provide light on the structural alterations brought about by chalcogen bonding.

c. *Temperature Dependence*: Chalcogen bonding is more susceptible to temperature fluctuations than covalent bonds since it is often weaker. The strength of chalcogen bonding and its contribution to the overall stability of molecular system can be determined by observing the temperature dependence of chemical shifts and J-coupling constants, which can be done by performing NMR spectroscopy at various temperatures [27].

d. *Chalcogen Bond Strength*: NMR titration experiments can be used to quantitatively quantify the binding affinity and power of chalcogen bonding. The binding constants and thermodynamics of chalcogen bonding can be studied by titrating a chalcogen bond donor into a solution containing a chalcogen bond acceptor and observing the changes in NMR signals.

e. *Competitive Binding Investigations*: NMR spectroscopy can be used to examine if chalcogen bonding is preferred over other non-covalent interactions in competitive binding investigations. Researchers can learn more about the specificity of chalcogen bonding by concurrently examining a number of binding partners in the presence of a chalcogen bond donor or acceptor such as the ChB donor shown in **Figure 5** [28].

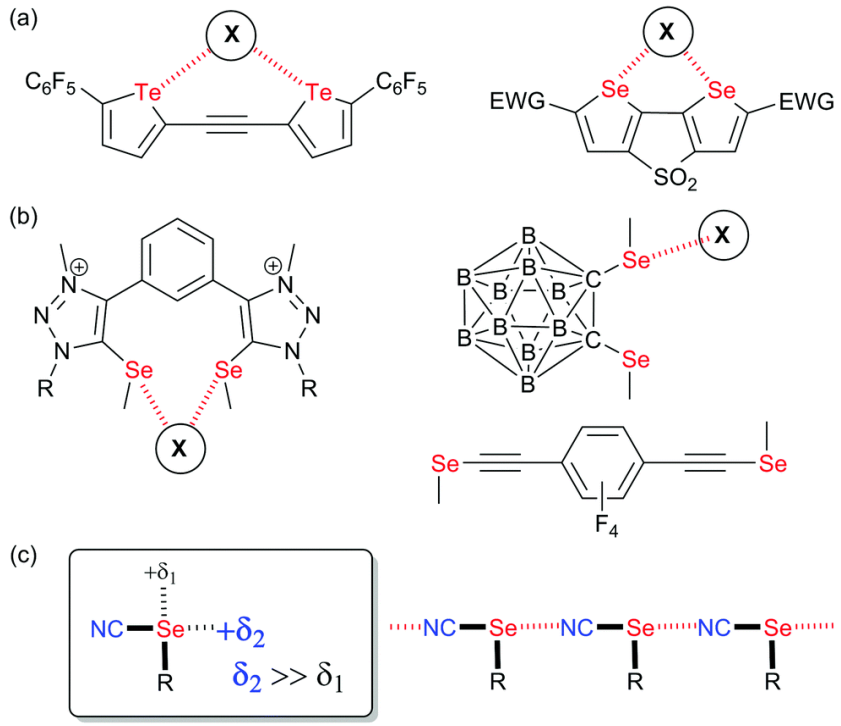

Figure 5. (a) Structures of reported ChB donors chelating halides, (b) Systems with strongly asymmetric selenium activation, and (c) Organic selenocyanates: Sigma-holes and solid-state association [31]

Vibrational circular dichroism (VCD)

A spectroscopic method called vibrational circular dichroism (VCD) can reveal important chiral details regarding chalcogen bonds. It characterizes the chiral characteristics of chalcogen-bonded complexes by measuring the differential absorption of left- and right-circularly polarized light [29]. Due to the unique atom arrangement and resultant asymmetry, chalcogen bonding can cause chirality in molecules or supramolecular assemblies. The VCD spectrum reveals this chirality as distinctive signals linked to the chalcogen bond. Researchers can learn more about the chirality and preferred conformation of chalcogen bonds by examining the VCD signals [30]. Think of a supramolecular structure with chiral chalcogen bonds as an illustration such as a self-assembly of 1,2-tellurazole 2-oxides into various supramolecular aggregates, the use of bis-(selenophene/tellurophene) derivatives as chelating systems toward anions or double chalcogen bonding interactions exhibited by benzo-1,3-chalcogenazoles or chalcogenadiazoles [31].

It is possible to use VCD spectroscopy to examine the chiral characteristics of the assembly. The distinctive signals of chalcogen bond will be visible in the VCD spectrum. These signals show that the interacting molecules within the assembly have a certain chiral configuration. The chirality and preferred conformation of the chalcogen bond may be inferred from the strength, shape, and location of the VCD signals. The study of chiral compounds or supramolecular systems, where chalcogen bonds are important, benefits greatly from the use of VCD spectroscopy. It provides precise chiral information that other spectroscopic methods lack, enabling researchers to better understand the structural and electrical characteristics of chalcogen bonding [32].

2.2.3. Thermodynamic measurements

The energetics of chalcogen bonding interactions, including enthalpy and entropic

contributions, is revealed through thermodynamic measurements as follow:

Calorimetry

To ascertain the enthalpic changes connected with chalcogen bonding, calorimetry methods such as differential scanning calorimetry (DSC) can be used [33]. Researchers can measure the intensity and durability of these connections by measuring the heat received or emitted during the creation or breakdown of chalcogen bonds. An exothermic heat change was seen during the production of a chalcogen bond between a selenium atom and a sulfur atom, for instance, as a result of calorimetry tests. The chalcogen bonding enthalpy measurements showed that the interaction had a sizable stabilizing energy. The enthalpic shifts related to chalcogen bonding can be determined using calorimetry methods like differential scanning calorimetry (DSC). The amount of heat absorbed or emitted when chalcogen bonds are formed or broken is assessed in DSC studies [34]. The strength and stability of these connections are quantified in this way. Calorimetry measurements show an exothermic heat change during the creation of a chalcogen bond, indicating the release of energy during bond formation. The amount of the interaction's stabilizing energy is reflected in the chalcogen bonding enthalpy measurement. In the case of the production of a chalcogen bond between a selenium atom and a sulfur atom, for instance, calorimetry measurements showed an exothermic heat change, indicating a substantial stabilizing energy involved in the interaction [35].

Isothermal titration calorimetry (ITC)

ITC is an effective method made especially for analyzing the thermodynamics of molecular interactions, such as chalcogen bonding. It calculates the transferred heat when a chalcogen-bonding partner is titrated into an electron donor or acceptor solution. Important thermodynamic variables, including the binding affinity (Kd) and the enthalpy change (H), related to the chalcogen bond, may be found by studying the heat changes as a concentration function. ITC research sheds important light on the robustness and durability of chalcogen bonding interactions. For instance, ITC tests showed that a tellurium atom and a nitrogen atom had a strong chalcogen connection. The two atoms appeared to interact strongly, as evidenced by the high binding affinity for chalcogen bonding that was observed [36]. Chalcogen bonding in tiny compounds will be studied via ITC and the processes are shown in **Figure 6**. For instance, a study examined the chalcogen bonds formed by Lewis bases like pyridine and ligands like selenourea that contain chalcogen. Titrating a pyridine solution into a selenourea solution allowed for ITC measurements. A favorable chalcogen bonding interaction was indicated by the obtained binding isotherms, which showed an exothermic heat change. The chalcogen bond's strength was quantified and confirmed by the binding constant derived by ITC, which also supplied information on the system's composition [37].

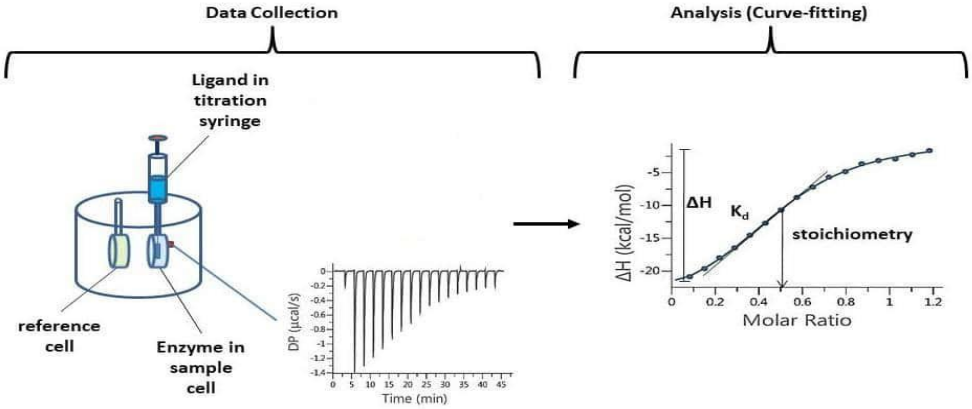

Figure 6. Isothermal titration calorimetry processes [37]

2.2.3.1. Quantum chemical calculations

Quantum chemical calculations are powerful computational tools widely employed for the characterization of chalcogen bonding. These calculations provide valuable insights into the electronic structure, bonding properties, and energetics of chalcogen-bonded systems. Two commonly used methods in quantum chemical calculations for studying chalcogen bonding are Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations.

Density Functional Theory (DFT)

DFT is a commonly utilized quantum mechanical technique that enables precise molecule property study and prediction. DFT simulations provide a thorough knowledge of the electronic structure and bonding interactions involved in chalcogen bonding. DFT sheds light on the distribution and behavior of electrons in chalcogen-bonded systems by resolving the electronic Schrödinger equation. It is capable of making precise predictions about the bond lengths, bond angles, and bond strengths of chalcogen bonds [38]. DFT studies also make it possible to evaluate the electronic characteristics of the chalcogen-bonded area, including electron density distribution and charge transport. By computing interaction energies and examining the molecular orbitals involved in the bonding, DFT simulations also make it easier to characterize the strength and directionality of chalcogen bonds. To compare various chalcogen bonding systems and investigate the effects of substituents, solvent effects, and conformational changes on the strength and stability of chalcogen bonds, calculations were performed [29]. DFT provides a number of benefits and has been effectively used to understand the type, power, and characteristics of these interactions. Some of the main DFT characteristics of chalcogen bonding are discussed below; the electronic structure of molecules involved in chalcogen bonding is thoroughly described by DFT. The distribution of electron densities, molecular orbitals, and energy levels involved in the bonding interaction are correctly predicted [40]. This knowledge aids in understanding the interactions between the Lewis base and the chalcogen atom and the modifications to the molecules' electrical structures that ensue. Characterizing chalcogen bonding involves a number of objectives, one of which is to ascertain the interaction's energy. The interaction energy between the chalcogen atom and the Lewis base can be precisely calculated using DFT. A key factor in determining the intensity of the chalcogen bonding and contrasting it with other non-covalent interactions is the interaction energy [41-45]. In addition, the ideal binding shape of chalcogen bonding complexes can be predicted by DFT simulations. Researchers can discover the most stable and energy-beneficial structures by investigating alternative binding configurations. Understanding the preferred spatial configuration of chalcogen bonding and how it affects the overall molecular structure is made easier by this [46-49]. DFT enables researchers to investigate the effects of substituents on the Lewis base or the chalcogen atom on the geometry and strength of chalcogen bonding. Researchers can clarify the effects of various functional groups on the interaction by methodically changing the chemical groups, which is essential for creating compounds with desirable chalcogen bonding properties. Chalcogen bonding interactions can be impacted by the solvent conditions of the environment [50]. The stability and energetics of chalcogen bonding can be studied using DFT calculations with implicit or explicit solvent models [51]. Understanding the behavior of chalcogen bonding in solution and living contexts requires the knowledge of this information. When other non-covalent interactions, such as hydrogen bonding or π-π stacking, coexist with or compete with chalcogen bonding, DFT can investigate these interactions. This aid in comprehending how various interactions interact in complex molecular systems [52-55].

Molecular Dynamics (MD) Simulations

In Molecular Dynamics simulations, the mobility and behavior of atoms and molecules over time are computationally modeled. They

enable the investigation of the structural and dynamic characteristics of chalcogen bonding interactions by presenting a dynamic image of those interactions [56-57]. The study of chalcogen bonds in a true-to-life molecular setting, accounting for solvent effects, temperature, and pressure, is made possible using MD simulations. MD simulations can correctly simulate the behavior of chalcogen-bonded systems and offer insights into their conformational preferences, flexibility, and stability using force fields and empirical potentials [58]. The examination of the conformational preferences of chalcogen-bonded complexes is possible using MD simulations. An example on tellurium and nitrogen chalcogen-bonded complexes, as depicted in Figure 7, MD simulations revealed several conformations and the dynamics of the chalcogen bond, revealing information on the bond's preferred orientations and flexibility (**Figure 7**) [59].

Chalcogen bonding-related intermolecular interactions can be captured using MD simulations. For instance, MD simulations clarified the stability of the chalcogen-bonded complex and the function of chalcogen bonding in the overall assembly structure in a supramolecular assembly with chalcogen bonds. MD simulations can take into account how solvents affect chalcogen bonding. Chalcogen-bonded systems were simulated in various solvent [60, 61].

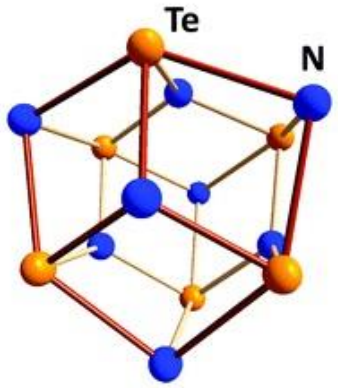

Figure 7. Tellurium and nitrogen complex [59]

4. Conclusion

Chalcogen bonding characterization is essential to understanding the distinctive characteristics and practical uses of these noncovalent interactions. Researchers have made tremendous progress in understanding the nature, strength, and directionality of chalcogen bonds using a number of experimental and computational methodologies. The investigation of intermolecular distances and angles in chalcogen-bonded complexes has been made possible by experimental techniques like X-ray crystallography, which have produced useful structural information. Spectroscopic techniques, including as infrared (IR) and NMR spectroscopy, have made it possible to identify the distinctive vibrational frequencies and chemical shifts connected with chalcogen bonds. Likewise, the chiral characteristics and conformational inclinations of chalcogen bonds have been better understood because of vibrational circular dichroism (VCD) spectroscopy. The energetics of chalcogen bonding has been studied using thermodynamic measures like calorimetry and isothermal titration calorimetry (ITC). These methods offer details on the thermodynamic stability, binding affinities, and enthalpic variations of chalcogen bonds. Chalcogen bonding may be characterized computationally using quantum chemistry computations, notably Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations. The electronic structures, bond strengths, and molecular characteristics of Chalcogen-bonded systems may all be predicted and analyzed using DFT computations.

On the other hand, MD simulations shed light on the preferred conformations, dynamic behavior, and solvent effects of chalcogen bonds. In general, these characterization methods have improved our comprehension of chalcogen bonding by illuminating its underlying ideas and possible uses. They have made it possible to develop new materials, catalysts, and medicinal compounds by supplying useful information on the geometry,

energetics, and electrical characteristics of chalcogen-bonded complexes.

Numerous branches of science and technology have advanced as a result of the characterization of chalcogen bonding, including molecular recognition, self-assembly, medication design, and materials engineering. The unique characteristics of chalcogen bonds may now be taken advantage, and their potential used in a variety of applications, with respect to the significant insights acquired through experimental and computational methodologies. Chalcogen bonding has been widely used in the realm of molecular recognition, for example. Chalcogen bonds are essential to molecular recognition processes because they allow for selective molecule binding and make it easier to create molecular receptors and sensors. Molecular recognition systems that are very specific and effective have been created by researchers by studying the structural and energetic characteristics of chalcogen bonding interactions.

The study of chalcogen bonding has also transformed the study of self-assembly. Using self-assembled structures based on chalcogen bonding, functional materials with specific features have been created and described. Researchers may manage the assembly of molecules and produce complex supramolecular structures, such as nanoscale devices, porous materials, and molecular switches, by varying the strength and directionality of chalcogen bonds. Thus, the capacity to describe and modify chalcogen bonding interactions has made it possible to create self-assembling systems with the appropriate functions and characteristics.

The study of chalcogen bonding is an area that is quickly developing, and new developments in experimental and computational methods are anticipated to increase our comprehension of the subtleties of these interactions. Continued study in this area will increase our understanding of chalcogen bonding, reveal new applications, and help create cutting-edge approaches in disciplines including supramolecular chemistry, materials science, and drug discovery. Understanding the structural, kinetic, and energetic features of chalcogen bonding using various experimental and computational approaches has been extremely beneficial. This understanding has paved the way for chalcogen bonding to be exploited in several branches of science and technology, advancing topics like molecular recognition and self-assembly as well as medication design and materials engineering.

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