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# Liên kết hydrogen không cổ điển $C_{sp2}$-H···O/Se/Te and O-H···Se/Te trong các hệ phức giữa acid formic acid và selenoformaldehyde, telluroformaldehydes

## Tóm tắt

Trong nghiên cứu này, độ bền các phức cũng như các liên kết hydrogen và đặc trưng của chúng trong các hệ giữa acid formic với các dẫn xuất aldehyde được khảo sát một cách đầy đủ. Nhìn chung, độ bền của các phức được tăng cường đáng kể đối với các nhóm thế cho hoặc nhận electron trong các dẫn xuất aldehyde. Các phức với sự thay thế Se được tìm thấy bền hơn so với các phức thế Te. Các phức đối với sự thế halogen được đánh giá kém bền hơn các phức của dẫn xuất thế -$CH_3$ và –$NH_2$. Các kết quả thu được chỉ ra độ bền đáng kể của liên kết O–H···Se/Te trong việc làm bền các phức so với C–H···O. Các kết quả tính toán cũng cho thấy rằng độ bền các liên kết hydrogen không cổ điển giảm theo thứ tự O–H···Se > O–H···Te ~ C–H···O > C–H···Se/Te. Sự chuyển dời xanh của liên kết C-H trong các phức khảo sát ở các liên kết hydrogen C–H···Se mạnh hơn so với C–H···Te. Phân tích NBO thấy rằng xu hướng chuyển dời xanh của tần số dao động liên kết $C_{sp2}$-H phụ thuộc chính vào sự giảm mật độ electron ở orbital phản liên kết σ*($C_{sp2}$–H) trong quá trình hình thành phức. Sự chuyển dời đỏ của tần số dao động liên kết O-H trong các liên kết hydrogen không cổ điển O-H···Se/Te được quyết định bởi sự tăng đáng kể mật độ electron tại orbital phản liên kết σ*(O–H) so với sự tăng cường đặc trưng s ở nguyên tử O trong quá trình tạo phức.

**Từ khóa:** *liên kết hydrogen không cổ điển O/$C_{sp2}$-H···O/Se/Te, Se/Te-aldehydes, acid formic.*

# The $C_{sp2}$-H···O/Se/Te and O-H···Se/Te nonconventional hydrogen bonds in the systems of formic acid with selenoformaldehydes and telluroformaldehydes

## ABSTRACT

In this study, a thorough investigation into the stability of complexes as well as the hydrogen bonds along with their characteristics in the systems between formic acid and chalcoaldehyde derivatives. Generally, the strength of complexes is enhanced irrespective of electron donating or withdrawing substitution in chalcoaldehyde derivatives. It is found that the complexes involving Se-substitution are slightly more stable than Te-one. The halogenated complexes are less stable than $CH_3$- and $NH_2$-substituted ones, in which the largest stability belongs to the complexes involving $NH_2$-substituted group. The obtained results show a dominant role of O–H···Se/Te compared to C–H···O in contributing to the stabilization of complexes. Calculated results indicate that the strength of nonconventional hydrogen bonds decreases in the order of O–H···Se > O–H···Te ~ C–H···O > C–H···Se/Te. The larger blue shift of C-H bond in the complexes investigated is observed in C–H···O compared to C–H···Se/Te. Following complexation, the magnitude of C-H blue shift is larger in the case of C–H···Se than in C–H···Te. NBO analysis shows that the blue-shifted stretching frequency of $C_{sp2}$–H depends mainly on a decrease of electron density at $\sigma^*(C_{sp2}–H)$ orbital. The redshift of O-H stretching frequency in O-H···Se/Te nonconventional hydrogen bonds in these systems is determined by a considerable increase of electron density at σ*(O–H) orbitals overcoming a s-character enhancement of O site upon complexation.

**Keywords:** *O/$C_{sp2}$-H···O/Se/Te nonconventional hydrogen bonds, Se/Te-aldehydes, formic acid.*

## 1. INTRODUCTION

Hydrogen bonds play an extremely important role because of their great properties in molecular information recognition, protein folding, structural rearrangement of nucleic acids, crystallization, polymerization, supramolecular chemistry, solvation, or in organic synthesis.[1,2] Many investigations were performed to understand the characteristics of hydrogen bonds as well as their importance in arrangement of molecules, reaction mechanism, as well as adsorption process, surface phenomena.[3-6] Noticeably, non-classical hydrogen bonds of the form C-H···O/N, C-H···π, C-H···X (X= F, Cl, Br) were detected in many molecular clusters, proteins, DNA, RNA, crystal structures of many materials, and surface reactions. Besides, organic synthesis methods based on the activation of C-H groups in intermediate complexes are one of the issues of current interest due to their importance in controlling the formation of desired products.[7,8] Experimental, Raman and theoretical findings of blue-shifted C-H bonds involved in C-H···O/N/halogen/π hydrogen bonds have been reported, of which the most abundant is the C-H···O/N form.[9-17] With these interesting findings on nonconventional hydrogen bonds, several models have been proposed to explain the nature of blue-shifted hydrogen bonding in individual systems, but none of them can be universally applied to other complex systems stabilized by hydrogen bonds.[9,16-20] Given the important role of hydrogen bonds in biological systems, the strength and properties of classical hydrogen bonds O-H···S, S-H···O/S have been studied and reported, for example, in some dimers of $H_2O$, $H_2S$, and $H_2O$···$H_2S$ system, by both theoretical and experimental methods.[21,22] Many nonconventional hydrogen bonds have been discovered recently and play important roles in proteins, catalysis... Indeed, the hydrogen bonds O/N-H···Se/Te were recently discovered experimentally.[23-25] However, systematic studies of the O-H···Se/Te hydrogen bond system to understand their strength and properties have not been reported. In addition, the influence of this O-H···Se/Te hydrogen bond on the strength and characteristics of the $C_{sp2}$–H···Se/Te hydrogen bond has not been considered and evaluated in literature.

In addition, the compounds having carbonyl group, including aldehydes, carboxylic acid, their halogenated and amides derivatives, are commonly found not only in the biologic structures such as proteins, lipid-membranes but also in other biologically active compounds like drugs. Theoretical studies on the dimers of carboxylic acids and amides indicated that the origin of stabilization in the studied complexes is charge-delocalization.[2,26] The experimental and theoretical investigations into O-H redshift and $C_{sp2}$-H blueshift in the hydrogen bonds in the complexes of formic acid, acetic acid, and acetaldehyde was reported.[27-29] Besides, strength and nature of blue- and redshifting hydrogen bonds were examined in mono- and di-hydrated complexes of the formamide, aldehydes and hydroxyl derivatives, carboxylic acids.[30-32] More recently, the $C_{sp2}$-H blue shift in the $C_{sp2}$–H···O hydrogen bonds have been reported for the complexes of aldehydes with formic acid, adding water into chalcogenoaldehydes, and in the binary systems of acetaldehyde and thioacetaldehyde with the substituted carboxylic and thiocarboxylic acids.[16,33,34]

Further, a theoretical study on the nature of hydrogen bonds for formamide and its heavy complexes ($NH_2CYH\cdots XH$; Y = O, S, Se, Te; X = F, HO, $NH_2$) was performed using density functional theory calculations and the quantum chemistry analyses.[35] Noticeably, the $C_{sp2}$-H···O/S/Se/Te hydrogen bonds were evaluated in the $XCHO\cdots nH_2Z$ and dimers of chalcogenoaldehyde derivatives systems.[36,37] However, the two hydrogen-bond systems between selenoformaldehyde or telluroformaldehyde and carboxylic acid along with their derivatives in consideration of the strength and the shifting of stretching frequency has not yet been observed clearly. In addition, the effects of various X substituents relating to the strength of nonconventional hydrogen bonds, which have essential role in stabilizing complexes as well as the shifts in $C_{sp2}$-H or O-H stretching frequency need to be addressed. Furthermore, the existence and role of various interactions following complexation such as O-H···Se/Te and $C_{sp2}$-H···O/Se/Te hydrogen bonds should be examined in the complexes of Se/Te derivatives to have insights into the nonconventional hydrogen bonds. In this work, the interaction complexes between aldehyde (XCHZ) and formic acid (HCOOH), with X = H, F, Cl, Br, $CH_3$, $NH_2$, and Z = Se, Te, are selected to have thorough insights into the effects of different X and Z on the polarity of $C_{sp2}$-H and the gas phase basicity of Z, as well as their role to the stability and characteristics of O-H···Se/Te, $C_{sp2}$-H···Se/Te nonconventional hydrogen bonds, and the complex strength.

## 2. COMPUTATIONAL METHODS

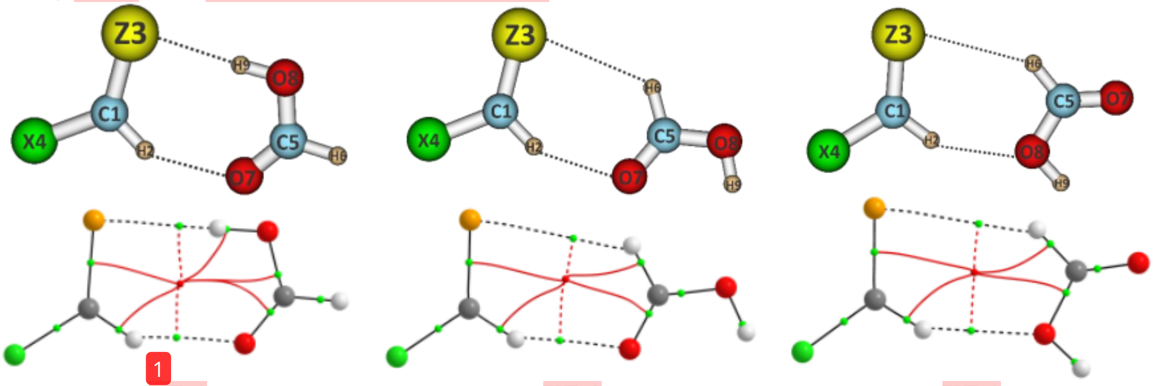
Geometry optimizations for all the structures considered, including the monomers and complexes, are carried out at the MP2/6-311++G(3df,2pd) level of theory. Harmonic vibrational frequencies are subsequently performed at the same level to identify the true equilibrium structures on the potential energy surface and to estimate their zero-point energies (ZPE). The interaction energy of each complex is calculated as the difference in the single-point energy of the complex and the correlated monomers and corrected for basis set superposition errors (BSSE) at the CCSD(T)/6-311++G(3df,2pd)//MP2/6-311++G(3df,2pd) level. Particularly, ΔE* is represented as the difference in total electronic energy between the complexes ($E_c$) and the sum of XCHZ and HCOOH optimized monomers ($E_{m1}$, $E_{m2}$) given by the expression: $\Delta E^* = E_c - (E_{m1} + E_{m2})$ (1). Moreover, deprotonation enthalpy (DPE) is defined as the enthalpy change for the deprotonation reactions: $XC(Z)H \rightarrow XCZ^- + H^+$ (2) and $HCOOH \rightarrow HCOO^- + H^+$ (3) and is considered as DPE of C-H and O-H bonds in both XCHZ and YCOOH monomers. Proton affinity (PA) is defined as the enthalpy change for the protonation reaction: $XC(Z)H + H^+ \rightarrow XC(ZH^+)H$ (4) and is considered as PA at the Se and Te sites in XCHZ monomers. All calculations mentioned above are carried out by employing the Gaussian 16 program.[38]

The Atoms-in-Molecules (AIM) analysis to search critical points and to estimate electron densities and Laplacians is performed at the MP2/6-311++G(3df,2pd) level using the AIMAll program.[39,40] The local electron energy density (H(r)) at the bond critical point (BCP) is computed by the equation: H(r) = G(r) + V(r) (5), in which V(r) and G(r) are the corresponding electron potential and kinetic energy density. The individual energy of each hydrogen bond ($E_{HB}$) is estimated using the formula $E_{HB} = 0.5V(r)$.[41] The natural bond orbital (NBO) analysis using NBO 5.G software with results of the intra- and intermolecular hyperconjugation energies and orbital occupancies was performed at the ωB97X-D/6-311++G(3df,2pd) level.[42,43] This range-separated hybrid functional (ωB97X-D) has been proved to be suitable for treating non-covalent interaction.[44] Besides, Symmetry Adapted Perturbation Theory (SAPT) calculations using the Psi4 program with the def2-TZVPD basis set are applied to unravel the different contributions of energy components to the stability of examined complexes.[45] The individual components of the interaction energy, including the electrostatic ($E_{elec}$), induction ($E_{ind}$), and dispersion ($E_{disp}$), are estimated particularly.

## 3. RESULTS AND DISCUSSION

### 3.1. Stable geometry and AIM analysis

The interaction of XCHZ with HCOOH induces 36 stable complexes, denoted by **XZ-n** (with X = H, F, Cl, Br, $CH_3$, $NH_2$; Z = Se, Te and n =1-3) with three geometries **XZ-n** displayed in Figure 1. The $sp^2$-hybridized carbon atom in XCHZ is labeled hereafter as $C_{sp2}$. Each complex contains a ring that is stabilized by two intermolecular contacts, including O–H···Se/Te and $C_{sp2}$–H···O in **XZ-1**, C–H···Se/Te and $C_{sp2}$–H···O in **XZ-2** and **XZ-3**. All H···O, H···Se and H···Te intermolecular distances (Table S1) are in the range of 2.18–2.45 Å, 2.33–3.20 Å and 2.65–3.33 Å, respectively, that in general are shorter or close to the sums of van der Waals radii of relevant atoms (being 2.72 Å for H···O, 3.00 Å for H···Se and 3.16 Å for H···Te). These results roughly suggest the presence of O–H···Se/Te and $C_{sp2}$–H···O/Se/Te nonconventional hydrogen bonds in the complexes. The presence of these intermolecular contacts through the bonding critical points (green points in Figure S1) is also confirmed by the values of electron density and Laplacian at BCPs (Table S1) and the values of local electron energy densities (H(r)) at BCPs.[40] Moreover, the H···Se/Te distances in $C_{sp2}$/O-H···Se/Te contacts are also close to those reported in literature for complexes between $NH_2CHSe$ and $NH_2CHTe$, with HF/$H_2O$/$NH_3$.[46] The intermolecular contact distances with the presence of chalcogen atoms (O, S, Se, Te) in hydrogen bonds were also reported in some studies.[16,33,35,47]



**XZ-1** **XZ-2** **XZ-3**

*Figure 1*: Optimized geometries and topological features of complexes upon interactions of XCHZ and HCOOH (X = H, F, Cl, Br, $CH_3$, $NH_2$ and Z = Se, Te) at MP2/6-311++G(3df,2pd)

As shown in Table S1, the decreasing tendency of strength for hydrogen bonds is in the sequence of O–H···Se to O–H···Te ~ C–H···O and then to C–H···Se/Te. Indeed, the $E_{HB}$ values indicate that the strength of C–H···O (-7.4 ÷ -15.6 $kJ.mol^{-1}$) is 2÷3 times as large as that of C–H···Se/Te (-3.3 ÷ -5.5 $kJ.mol^{-1}$) and the strength of O–H···Se (-16.8 ÷ -23.1 $kJ.mol^{-1}$) is 1.5 times as large as that of O–H···Te (-12.5 ÷ -13.8 $kJ.mol^{-1}$). Along with the results of individual hydrogen bond energies in literature by Khanh et al.[16], it is found that the stability of hydrogen bonds decrease in going from O–H···O >> O–H···S > O–H···Se > O–H···Te. These results are also supported by a previous investigation of hydrogen bonding complexes containing chalcogen atoms.[33] The second correlation of individual hydrogen bond energy ($E_{HB}$) vesus intermolecular distances R(C-H···O/Se/Te) is obtained according to expression $E_{HB} = -134.24 + 85.52R(C\text{-}H\cdots O/Se/Te) - 13.98R^2(C\text{-}H\cdots O/Se/Te)$ ($R^2 = 0.96$) as given in Figure 2. However, a highly linear correlation of individual bond energy ($E_{HB}$) with respect to intermolecular distances R(O-H···Se/Te) is observed as expression $E_{HB} = 29.205R(O\text{-}H\cdots Se/Te) - 78.638$ ($R^2 = 0.98$). The obtained results indicate that the shorter intermolecular distance is the stronger the nonconventional hydrogen bond is, and vice versa.

On the basis of individual hydrogen bond energy given in Table S1 of ESI, it can be suggested that the C–H···O hydrogen bonds play a main role in stabilizing **XZ-2** and **XZ-3** along with an additional role of the C–H···Se/Te ones. Nevertheless, for **XZ-1** complexes, the C–H···O hydrogen bonds serve as a supplementary factor along with a substantial importance of the O–H···Se/Te ones in complex stabilization. In order to clarify the relationship between the strength of nonconventional hydrogen bond and $r_{H\cdots O/Z}/\sum r_{vdW}$ ratio, the The $r_{H\cdots Z}/\sum r_{vdW}$ ratios are gathered and plotted in Table S2 and Figures S2, S3 of ESI. The results show that there is a good agreement between the $r_{H\cdots Z}/\sum r_{vdW}$ ratio and $E_{HB}$ of nonconventional hydrogen bonds in investigated complexes. Indeed, the $r_{H\cdots Z}/\sum r_{vdW}$ ratios of C-H···O hydrogen bonds in the **XSe/Te-1** are smaller than those in **XSe/Te-2**, and **XSe/Te-3**, being consistent with the larger strength of C-H···O hydrogen bonds in **XSe/Te-1** compared to **XSe/Te-2**, and **XSe/Te-3**. The $r_{H\cdots Z}/\sum r_{vdW}$ ratio of C-H···O in the complexes increases in the order of $NH_2 < Cl \sim Br < F < CH_3 < H$, along with the decrease in the strength of C-H···O hydrogen bonds in the sequence of $NH_2 > Cl \sim Br > F > CH_3 > H$ substituted derivatives. It is worth noted that the O-H···Se/Te hydrogen bonds are much more stronger than the $C_{sp2}$-H···Se/Te ones, which is proven by the much smaller $r_{H\cdots Z}/\sum r_{vdW}$ ratio of O-H···Se/Te that that of $C_{sp2}$-H···Se/Te hydrogen bonds. For **XZ-2** and **XZ-3**, the $r_{H\cdots Z}/\sum r_{vdW}$ ratios of C-H···Se/Te are larger than those of C-H···O, being in line with the weaker strength of the C-H···Se/Te than the C-H···O.

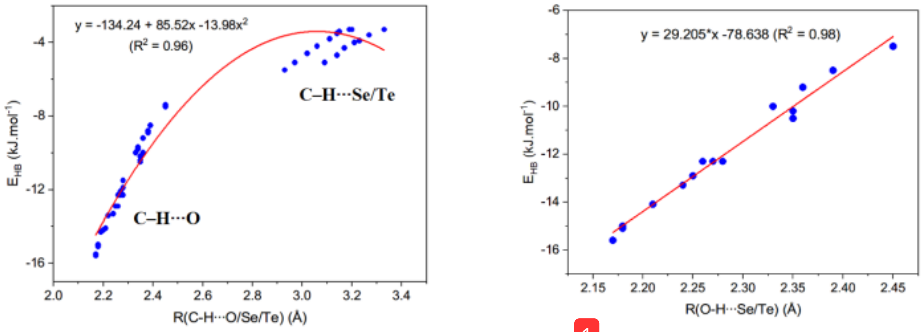


*Figure 2*: The relationships between $E_{HB}$ and R(C/O-H···O/Se/Te) in the complexes

*Table 1*: Deprotonation enthalpies of $C_{sp2}$–H (DPE) and proton affinities at Z sites (PA) at the CCSD(T)/6-311++G(3df,2pd) (in $kJ.mol^{-1}$)

| **Monomer** | **HCHSe** | **FCHSe** | **ClCHSe** | **BrCHSe** | **$CH_3CHSe$** | **$NH_2CHSe$** |
|---|---|---|---|---|---|---|
| PA(Se) | 775.0 | 737.9 | 766.3 | 773.0 | 811.7 | 860.0 |
| DPE($C_{sp2}$-H) | 1623.6 | 1567.2 | 1551.7 | 1539.0 | 1620.7 | 1595.6 |
| **Monomer** | **HCHTe** | **FCHTe** | **ClCHTe** | **BrCHTe** | **$CH_3CHTe$** | **$NH_2CHTe$** |
| PA(Te) | 812.2 | 780.7 | 802.7 | 807.9 | 841.0 | 884.6 |
| DPE($C_{sp2}$-H) | 1612.7 | 1561.0 | 1550.7 | 1540.8 | 1615.5 | 1582.3 |

In order to examine the effect of the proton-donor or proton-acceptor ability of the isolated monomers on the strength of intermolecular interactions, deprotonation enthalpies (DPE) of $C_{sp2}$–H and proton affinities (PA) at the Se/Te sites of XCHZ are calculated and given in Table 1. With the same Z in XCHZ, the strength of O-H···Z hydrogen bonds in **XZ-1** decreases in the order of $NH_2 > CH_3 > H >$ F/Cl/Br substitutions (*cf*. Table S1), which are in a good agreement with a decrease of gas-phase basicity (PA) at Se/Te site in XCHZ (*cf*. Table 1). However, a decrease of strength of C-H···O hydrogen bonds in **XZ-1** is in the order of $NH_2 >$ F/Cl/Br $> CH_3 >$ H substitutions, which differs from trend of the polarity of $C_{sp2}$-H bond in the isolated XCHZ. As a result, the strength of **XZ-1** is mainly proposed by the presence of O-H···Z. Similarly, a decrease in gas-phase basicity at Se/Te site in the sequence of $NH_2 > CH_3 > H >$ F/Cl/Br substitutions in XCHZ causes a reduction of strength of C-H···Z hydrogen bonds in **XZ-2, XZ-3** decrease in the same tendency. The strengthening trend of C-H···O hydrogen bonds in **XZ-2** and **XZ-3** is also suitable for an increase in the polarity of $C_{sp2}$-H bond in XCHZ in the order of $H < CH_3 < NH_2 <$ F/Cl/Br substitution (cf. Table S1). With the alike X in XCHZ, the stronger strength of O–H···Se hydrogen bonds compared to O–H···Te ones is observed in **XZ-1**. However, for the same X in the isolated XCHZ, proton affinity at Te site is larger than that at Se one (cf. Table 1), and accordingly these hydrogen bonds should be assigned by a larger electrostatic attraction of H and Se relative to H and Te.

### 3.2. Interaction energy and SAPT analysis

Interaction energies (ΔE*) of complexes, including both ZPE and BSSE correction at the CCSD(T)/6-311++G(3df,2pd)//MP2/6-311++G(3df,2pd) level are listed in Table 2, and their relationship is plotted in Figure 3. Generally, the interaction energies values in the range of -7.1 and -37.2 kJ.mol$^{-1}$ indicate that the obtained complexes are quite stable on the potential energy surface, in which the **XZ-1** complexes are 2÷3 times as stable as **XZ-2** and **XZ-3** complexes. The considerable strength of **XZ-1** is suggested by the presence of O-H···Z hydrogen bond with respective to the remaining nonconventional C-H···O/Z hydrogen bonds. The reason for the larger stability of **XZ-2** relative to **XZ-3** should be the larger gas phase basicity of O site of >C=O as compared to that of O site of –OH in formaldehyde acid. Both of them are stablized by the nonconventional hydrogen bonds including C-H···Z and C-H···O.

It is found that the most stable **XZ-1** of XCHZ···HCOOH in the present work have a comparable strength of XCHO···HCOOH complexes and slightly larger than that of XCHS···HCOOH.[16] The **XZ-1** complexes are more stable than the binary complexes of small aldehydes, and less stable than dimers of typical carboxlic acids. Indeed, the interaction energies of HCHO···HCHO, HCHO···HCHS, HCHS···HCHS are in turn -12.3, -11.7, -10.7 kJ.mol$^{-1}$ at CCSD(T)-F12/heavy-aug-cc-pVTZ level of theory.[48] The complexes of HCHO···HCHO and $CH_3CHO$···$CH_3CHO$ have interaction energies of -21.0 and -22.4 kJ.mol$^{-1}$ at MP2/aug-cc-pVTZ.[49] The very large interaction energies of $CH_3COOH$···$CH_3COOH$ and HCOOH···HCOOH at MP2/aug-cc-pVTZ are -60.7 kJ.mol$^{-1}$ and -56.9 kJ.mol$^{-1}$.[50]

*Table 2*: Interaction energy corrected by both ZPE and BSSE (ΔE*, kJ.mol$^{-1}$) of the complexes RCHZ···HCOOH at CCSD(T)/6-311++G(3df,2pd)//MP2/6-311++G(3df,2pd)

| Complex | ΔE* | Complex | ΔE* | Complex | ΔE* |
|---|---|---|---|---|---|
| **HSe-1** | -24.4 | **HSe-2** | -10.7 | **HSe-3** | -7.3 |
| **FSe-1** | -23.9 | **FSe-2** | -13.0 | **FSe-3** | -8.1 |
| **ClSe-1** | -24.9 | **ClSe-2** | -12.9 | **ClSe-3** | -8.4 |
| **BrSe-1** | -24.7 | **BrSe-2** | -12.9 | **BrSe-3** | -8.6 |
| **CH$_3$Se-1** | -28.4 | **CH$_3$Se-2** | -12.3 | **CH$_3$Se-3** | -8.9 |
| **NH$_2$Se-1** | -37.2 | **NH$_2$Se-2** | -16.6 | **NH$_2$Se-3** | -11.7 |
| **HTe-1** | -22.3 | **HTe-2** | -10.2 | **HTe-3** | -7.1 |
| **FTe-1** | -22.9 | **FTe-2** | -12.7 | **FTe-3** | -8.1 |
| **ClTe-1** | -23.6 | **ClTe-2** | -12.7 | **ClTe-3** | -8.3 |
| **BrTe-1** | -23.5 | **BrTe-2** | -12.6 | **BrTe-3** | -8.5 |
| **CH$_3$Te-1** | -25.8 | **CH$_3$Te-2** | -11.8 | **CH$_3$Te-3** | -8.4 |
| **NH$_2$Te-1** | -34.7 | **NH$_2$Te-2** | -16.6 | **NH$_2$Te-3** | -11.4 |

It is important to consider the substituent effects of X and Z in XCHZ monomers on the strength of interactions in the investigated complexes. The interaction energy of **XSe–n** is *ca.* 0.1–2.6 kJ.mol$^{-1}$ slightly more negative than that of **XTe–n**, about for the same X in XCHZ derivatives. This indicates a slightly less strength of **XTe–n** as compared to **XSe–n,** which should be resulting from stronger electrostatic force of Se and H atoms overcoming Te and H atoms.[33] Generally, the strength of **XZ-n** complexes is enhanced irrespective of electron donating or withdrawing X substitution (cf. Table 2 and Figure 3). For the alike Z, it is found that the halogenated complexes are less stable than $CH_3$- and $NH_2$-substituted ones, in which the largest stability belongs to the complexes **NH$_2$Z-n** with more negative values of 2.8-13.3 kJ.mol$^{-1}$. This implies a significant role of O–H···Se/Te and C–H···O/Se/Te nonconventional hydrogen bonds in contributing to the stability of **$NH_2Z$-n** compared to other complexes.

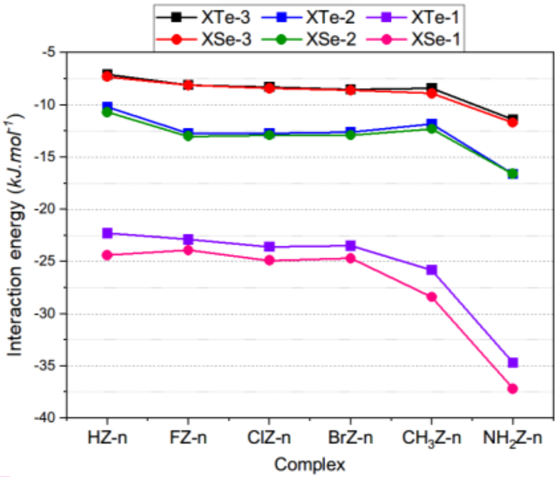


*Figure 3*: The relationship of the interaction energies and different X substitutions

As seen from Table 2, the interaction energy of complexes indeed increases in the substituting order: F < H < Br ~ Cl < $CH_3$ < $NH_2$ for **XSe-1** and H < F < Br ~ Cl < $CH_3$ < $NH_2$ for **XTe-1**. This result is suitable for the changing trend in the strength of O–H···Se/Te bonds in the complexes, affirming a main role of O–H···Se/Te bonds along with a an additional role of C–H···O hydrogen bonds in stabilizing **XZ-1**. The energetic components based on the SAPT2+ approach, which contribute to the stability of all complexes investigated, are shown in Table S2. The obtained results show that the stability of complexes are mainly contributed by three terms including electrostatic, dispersion, and induction with contributing percentages of *ca*. 8-53%, 7-46% and 7-63% respectively. The dominating role of electrostatic components contributing to the complex strength is also reported in the complexes of XCHO···HCOOH and XCHS···HCOOH.[16]

### 3.3. Characteristics of $C_{sp2}$-H···Se/Te and O-H···Se/Te hydrogen bonds

The formation of C–H···Z, C–H···O and O–H···Z interactions in the complexes are further clarified by the change in lengths (Δr, mÅ) and the stretching frequencies (Δν, $cm^{-1}$) of O–H and $C_{sp2}$–H bond participating in the considered hydrogen bonds. The results at MP2/6-311++G(3df,2pd) are gathered in Table 3.

Considering the nonconventional hydrogen bonds of C–H···Se/Te, the C–H length in **XZ-2** and **XZ-3** decreases slightly in the range of 0.07–0.93 mÅ, accompanied by an increase in their stretching frequency of 1.9–14.8 $cm^{-1}$ as compared to the corresponding values of isolated monomers. These changes show that C–H···Z interactions in the complexes belong to blue-shifting hydrogen bonds. Following complexation, the larger blue shift of C-H bond in the complexes investigated is observed in C–H···O compared to C–H···Se/Te, and has a much smaller magnitude than that in the complexes of XCHO···HCOOH. It was found that all C-H···Se/Te nonconventional hydrogen bonds in dimers of RCHZ (R=H, F, Cl, Br or $CH_3$, Z= Se, Te) are red-shifted.[16] In the present work, a small $C_{sp2}$-H elongation of 0.10–0.52 mÅ along with a decrease in stretching frequency of 0.2–6.5 $cm^{-1}$ is found in the case of **$NH_2$Se-3**, **BrTe-3**, **HTe-3**, **$CH_3$Te-3**, and **$NH_2$Te-3**, indicating red shifting hydrogen bonds. These values are quite close to a report of hydrogen bonded complexes between aldehydes and hydrogen chalcogenides.[36] The largest shortening of C-H bond length is observed for **FZ-2** and **FZ-3**, associated with the strongest electron-withdrawing group being F, whereas the smallest is observed in **$NH_2$Z-2** and **$NH_2$Z-3**. Besides, the blue shift of C–H6 bond in C5–H6···Z3 interaction in **XZ-2** and **XZ-3** decreases in the substituting order: F > Cl > Br > H > $CH_3$ > $NH_2$. This result is consistent with increased basicity at the Se/Te site in XCHZ (Table 1). The magnitude of the $C_{sp2}$-H blue shift with the Z same is more strongly affected by electron-withdrawing groups (F, Cl, Br) than by electron-donating groups ($CH_3$, $NH_2$). The magnitude of C5–H6 stretching frequency blueshifts are larger for C–H···Se than for C–H···Te, which is in an align with the increasing tendency of the proton affinity at Te relative to Se site (cf. Table 1). Furthermore, the larger blueshift of C–H bond in C–H···Z hydrogen bonds of **XZ-2** in comparison with that of **XZ-3** is observed, which relate to the more important role of C–H···O hydrogen bond in **XZ-2** compared to that in **XZ-3**, toward the blueshift of C–H stretching frequency.

*Table 3*: Changes in bond lengths (in mÅ) and their corresponding stretching frequencies (in cm$^{-1}$) at MP2/6-311++G(3df,2pd)

| **Complex** | **HSe-1** | **FSe-1** | **ClSe-1** | **BrSe-1** | **CH$_3$Se-1** | **NH$_2$Se-1** | **HTe-1** | **FTe-1** | **ClTe-1** | **BrTe-1** | **CH$_3$Te-1** | **NH$_2$Te-1** |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Δr(C1H2) | 0.42 | 0.76 | 1.54 | 1.77 | -0.37 | 0.22 | 1.09 | 0.51 | 1.37 | 1.55 | -0.08 | 0.69 |
| Δν(C1H2) | 8.4 | 3.8 | -4.5 | -6.8 | 18.9 | 8.1 | 0.3 | 7.2 | -2.4 | -4.6 | 14.3 | 1.6 |
| Δr(O8H9) | 15.32 | 12.49 | 13.24 | 13.17 | 16.80 | 21.18 | 13.97 | 12.20 | 12.78 | 12.69 | 15.09 | 19.24 |
| Δν(O8H9) | -326.2 | -266.6 | -284.0 | -282.5 | -355.5 | -439.4 | -299.5 | -261.9 | -274.6 | -273.1 | -322.1 | -402.6 |
| **Complex** | **HSe-2** | **FSe-2** | **ClSe-2** | **BrSe-2** | **CH$_3$Se-2** | **NH$_2$Se-2** | **HTe-2** | **FTe-2** | **ClTe-2** | **BrTe-2** | **CH$_3$Te-2** | **NH$_2$Te-2** |
| Δr(C1H2) | 0.17 | 0.21 | 0.76 | 0.92 | -0.34 | 0.18 | 0.84 | 0.04 | 0.72 | 0.89 | -0.20 | 0.53 |
| Δν(C1H2) | 7.8 | 7.8 | 3.0 | 1.2 | 15.6 | 6.9 | -0.3 | 10.0 | 3.3 | 1.0 | 12.8 | 1.3 |
| Δr(C5H6) | -0.73 | -0.93 | -0.79 | -0.76 | -0.47 | -0.30 | -0.52 | -0.78 | -0.65 | -0.60 | -0.28 | -0.07 |
| Δν(C5H6) | 11.8 | 14.8 | 13.0 | 12.5 | 8.7 | 6.5 | 7.3 | 11.2 | 9.5 | 8.8 | 4.3 | 1.9 |
| **Complex** | **HSe-3** | **FSe-3** | **ClSe-3** | **BrSe-3** | **CH$_3$Se-3** | **NH$_2$Se-3** | **HTe-3** | **FTe-3** | **ClTe-3** | **BrTe-3** | **CH$_3$Te-3** | **NH$_2$Te-3** |
| Δr(C1H2) | -0.07 | -0.33 | -0.17 | -0.07 | -0.48 | -0.21 | 0.51 | -0.36 | -0.09 | -0.04 | -0.43 | -0.05 |
| Δν(C1H2) | 10.1 | 13.4 | 13.6 | 12.6 | 16.7 | 12.5 | 3.5 | 13.6 | 12.5 | 11.8 | 15.2 | 9.9 |
| Δr(C5H6) | -0.07 | -0.43 | -0.20 | -0.17 | 0.09 | 0.24 | 0.18 | -0.16 | 0.06 | 0.10 | 0.38 | 0.52 |
| Δν(C5H6) | 3.2 | 8.5 | 5.4 | 4.9 | 1.1 | -1.0 | -1.8 | 3.3 | 0.3 | -0.2 | -4.4 | -6.5 |

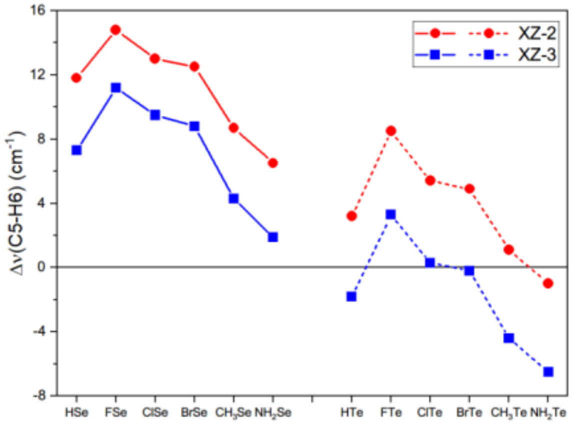


*Figure 4*: The relationship between the change in C-H stretching frequency and different X substitutions in **XZ-2** and **XZ-3**

For **XZ-3**, the C–H stretching frequency in C-H···O hydrogen bond displays a blueshift with a small contraction and an increase of stretching frequency (Δr = -0.04 ÷ -0.48 *m*Å and Δν = 9.9 ÷16.7 cm$^{-1}$), except for a small elongation in **HTe-3**.

Besides, the blueshift of the C-H bond observed in **XZ-2** is emphasized by a slight enhancement of in its bond length and corresponding stretching frequency (except for **HTe-2** with a slight redshift of C-H stretching frequency). The slight redshift is observed in **ClZ-1** and **BrZ-1**, while most **XZ-1** structures indicate a blue shift of C-H stretching frequency in C–H···O hydrogen bonds. The redshift for **ClZ-1** and **BrZ-1** should be designated to the largest polarity of the $C_{sp2}$-H bonds in ClCHZ and BrCHZ monomers (Z = Se, Te).[16] As shown in Table 3, a C-H bond contraction and an increase in its stretching frequency in **XSe-n** are larger than those in **XTe-n**. This observation is induced by the larger polarity of the C-H bond in **XCHTe** than in **XCHSe**. Meanwhile, with the same Z in **XZ-3**, the larger blueshift in **$CH_3Z$-3** in comparison with **F/Cl/BrZ-3** comes from the smaller polarity of the C-H bond in **$CH_3Z$-3**. A very small blue shift of $C_{Sp2}$-H in C–H···O in XCHZ···HCOOH (Z=Se, Te) as compared to the considerable blue shift of that in XCHO···HCOOH (up to 100 $cm^{-1}$) was attained.[16] This shows that a profound role of O-H···O relative to O-H···Se/Te in increasing the very considerable blue shift of $C_{sp2}$-H stretching frequency. In the other words, it implies a noticeable role of O compared to S, Se and Te atom in determining a significant blue shift of C-H stretching frequency following complexation.

On the other hand, for O–H···Se/Te hydrogen bonds in **XZ-1** form, the bond elongation of 12.5–21.2 mÅ for O–H···Se and 12.2–19.2 mÅ and O–H···Te is observed which is accompanied by a remarkable decrease of 266.6–439.4 $cm^{-1}$ and 261.9–402.6 $cm^{-1}$ in their stretching frequency, respectively (cf. Table 3). These changes show the redshift of O-H stretching frequencies involved in the O–H···Se/Te nonconventional hydrogen bonds. Particularly, with the same X in XCHZ, the redshift phenomenon in the O–H···Se hydrogen bonds is larger than the O–H···Te ones. In the case of the same Z, the redshift of O–H···Z hydrogen bonds is found in the increasing order of F/Cl/Br < H < $CH_3$ < $NH_2$ substitutions, which is in good agreement with the enhancement of proton affinity of chalcogen atom in the XCHZ (Table 1). The obtained result of O-H stretching frequency red shift in the hydrogen bond is similar to previous reports in complexes of chalcogen derivatives and formic acid.[16,33]

### 3.4. NBO analysis

In order to clarify the strength and characteristics of hydrogen bonds and complexes investigated, the NBO analysis is carried out at ωB97X-D/6-311++G(3df,2pd) as presented in Table 4. The positive values of electron density transfer (EDT) for most of complexes (0.0003–0.0587 e) imply that the electron density is transferred mainly from XCHZ to HCOOH. This tendency is caused by the very large second-order perturbative energy of electron transfer n(Z3)→σ*(C5–H6) (7.02-20.57 $kJ.mol^{-1}$) and n(Z3)→σ*(O8–H9) (65.42-109.35 $kJ.mol^{-1}$) in comparison to n(O7/O8)→σ*(C1–H2) (2.88-14.59 $kJ.mol^{-1}$), except for **FSe-2**, **ClSe-2** and **BrSe-2** with the negative values of EDT. Hence, the interactions of n(Z3)→σ*(C5–H6) and n(Z3)→σ*(O8–H9) electron density transfers play a dominant role in stabilizing most of complexes as compared to those of the n(O7/O8)→σ*(C–H) transfers, except for a larger role of n(O7)→σ*(C1-H2) (10.58-11.41 $kJ.mol^{-1}$) compared to n(Z3)→σ*(C5–H6) (7.02-7.48 $kJ.mol^{-1}$) interaction found in **FSe-2**, **ClSe-2** and **BrSe-2** (cf. Table 4). This should be due to the larger polarity of C-H bond in XCHSe (with X=F, Cl, Br), leading to the larger ability of electron acceptance of σ*(C1–H2) orbital.

The very large $E_{inter}$ values of n(Z3)→σ*(O8–H9) in **XZ-1** compared to n(Z3)→σ*(C5–H6) in **XZ-2** and **XZ-3** indicate that the much stronger electron density transfers from lone pair of electrons from Z3 to σ*(O8–H9) orbitals are much more stronger than from Z3 to σ*(C5–H6) ones. Moreover, $E_{inter}$[n(O7/O8)→σ*(C1–H2)] is larger for **XZ-1** than **XZ-2** and **XZ-3**, implying a stronger electron density transfer in **XZ-1**. These obtained results of $E_{inter}$ are in good consistency with the trend in stability of hydrogen bond as analyzed in AIM part above.

For changing X in XCHZ, $E_{inter}$[n(Z3)→σ*(C5–H6)] in **XZ-2**, **XZ-3** and $E_{inter}$[n(Z3) → σ*(O8–H9)] in **XZ-1** increase in the order of F/Cl/Br < H < $CH_3$ < $NH_2$ substituents, which is in good agreement with the increasing trend of the proton affinity at Z3 site (Table 1). In other words, the intermolecular charge density transfers from XCHZ to HCOOH are rised by the presence of electron-donating groups such as $CH_3$ and $NH_2$, and are diminished by electron-withdrawing substituents. It is noted that the increase in values of $E_{inter}$[n(O7/O8)→σ*(C1–H2)] is attained by the substitution of electron-donating or electron-withdrawing groups.

*Table 4*: Electron density transfer (EDT), hyperconjugation interaction energies ($E_{inter}$, in $kJ.mol^{-1}$), and changes of electron density (Δσ*, in electron) and s-character percentage of atom involving hydrogen bond (Δ%s, in %)

| **Complex** | **HSe-1** | **FSe-1** | **ClSe-1** | **BrSe-1** | **$CH_3$Se-1** | **$NH_2$Se-1** | **HTe-1** | **FTe-1** | **ClTe-1** | **BrTe-1** | **$CH_3$Te-1** | **$NH_2$Te-1** |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| EDT | 0.051 | 0.036 | 0.039 | 0.038 | 0.052 | 0.059 | 0.050 | 0.039 | 0.041 | 0.040 | 0.050 | 0.056 |
| $E_{inter}[n(O7)\rightarrow\sigma^*(C1\text{-}H2)]$ | 9.28 | 12.54 | 13.21 | 12.25 | 9.91 | 14.59 | 7.36 | 9.99 | 10.83 | 10.03 | 8.23 | 13.54 |
| $E_{inter}[n(Z3)\rightarrow\sigma^*(O8\text{-}H9)]$ | 84.06 | 68.05 | 70.77 | 68.76 | 90.54 | 109.35 | 75.32 | 65.42 | 67.51 | 66.00 | 77.16 | 95.35 |
| $\Delta\sigma^*(C1\text{-}H2)$ | -0.002 | -0.002 | -0.002 | -0.002 | -0.002 | -0.002 | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 |
| $\Delta\%s(C1)$ | 1.51 | 1.68 | 1.71 | 1.71 | 1.52 | 1.74 | 1.43 | 1.66 | 1.72 | 1.74 | 1.43 | 1.71 |
| $\Delta\sigma^*(O8\text{-}H9)$ | 0.052 | 0.042 | 0.045 | 0.045 | 0.055 | 0.064 | 0.051 | 0.044 | 0.046 | 0.046 | 0.053 | 0.061 |
| $\Delta\%s(O8)$ | 3.37 | 2.97 | 3.07 | 3.03 | 3.57 | 4.07 | 3.05 | 2.78 | 2.85 | 2.83 | 3.23 | 3.70 |
| **Complex** | **HSe-2** | **FSe-2** | **ClSe-2** | **BrSe-2** | **$CH_3$Se-2** | **$NH_2$Se-2** | **HTe-2** | **FTe-2** | **ClTe-2** | **BrTe-2** | **$CH_3$Te-2** | **$NH_2$Te-2** |
| EDT | 0.003 | -0.002 | -0.002 | -0.002 | 0.003 | 0.003 | 0.005 | 0.001 | 0.001 | 0.001 | 0.004 | 0.004 |
| $E_{inter}[n(O7)\rightarrow\sigma^*(C1\text{-}H2)]$ | 7.61 | 10.58 | 11.41 | 10.78 | 7.61 | 10.45 | 6.65 | 8.69 | 9.78 | 9.32 | 6.98 | 10.7 |
| $E_{inter}[n(Z3)\rightarrow\sigma^*(C5\text{-}H6)]$ | 9.41 | 7.02 | 7.48 | 7.48 | 11.37 | 14.59 | 10.91 | 9.03 | 9.28 | 9.28 | 12.79 | 16.39 |
| $\Delta\sigma^*(C1\text{-}H2)$ | -0.001 | -0.002 | -0.002 | -0.002 | -0.002 | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 |
| $\Delta\%s(C1)$ | 1.13 | 1.3 | 1.44 | 1.5 | 1.1 | 1.21 | 1.12 | 1.31 | 1.46 | 1.52 | 1.11 | 1.26 |
| $\Delta\sigma^*(C5\text{-}H6)$ | 0.001 | -0.001 | -0.001 | -0.001 | 0.001 | -0.001 | 0.003 | 0.002 | 0.002 | 0.002 | 0.003 | 0.002 |
| $\Delta\%s(C5)$ | 0.50 | 0.38 | 0.39 | 0.38 | 0.61 | 0.86 | 0.45 | 0.37 | 0.37 | 0.37 | 0.55 | 0.80 |
| **Complex** | **HSe-3** | **FSe-3** | **ClSe-3** | **BrSe-3** | **$CH_3$Se-3** | **$NH_2$Se-3** | **HTe-3** | **FTe-3** | **ClTe-3** | **BrTe-3** | **$CH_3$Te-3** | **$NH_2$Te-3** |
| EDT | 0.007 | 0.002 | 0.002 | 0.002 | 0.006 | 0.007 | 0.009 | 0.005 | 0.005 | 0.005 | 0.008 | 0.010 |
| $E_{inter}[n(O8)\rightarrow\sigma^*(C1\text{-}H2)]$ | 3.51 | 5.68 | 5.89 | 5.39 | 3.64 | 4.85 | 2.88 | 4.39 | 4.93 | 4.51 | 2.97 | 4.47 |
| $E_{inter}[n(Z3)\rightarrow\sigma^*(C5\text{-}H6)]$ | 12.5 | 9.45 | 10.03 | 9.82 | 14.3 | 18.22 | 14.71 | 12.46 | 12.79 | 12.58 | 16.59 | 20.57 |
| $\Delta\sigma^*(C1\text{-}H2)$ | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 | -0.001 | 0.001 |
| $\Delta\%s(C1)$ | 0.72 | 0.84 | 0.94 | 0.97 | 0.68 | 0.76 | 0.72 | 0.85 | 0.96 | 1.00 | 0.68 | 0.80 |
| $\Delta\sigma^*(C5\text{-}H6)$ | 0.003 | 0.001 | 0.002 | 0.002 | 0.003 | 0.002 | 0.005 | 0.004 | 0.004 | 0.004 | 0.005 | 0.005 |
| $\Delta\%s(C5)$ | 0.72 | 0.64 | 0.64 | 0.63 | 0.83 | 1.15 | 0.66 | 0.62 | 0.61 | 0.60 | 0.75 | 1.09 |

*(EDT, $E_{inter}$ at ωB97X-D/6-311++G(3df,2pd); Δσ*, Δ%s at MP2/6-311++G(3df,2pd))*

The C1-H2 stretching frequency blueshift in C1–H2···O7/O8 is caused by a small decrease of electron density at σ*(C1–H2) orbital from 0.001e to 0.002e (excepting for a very slight increase of σ*($C_{sp2}$–H) occupation in **$NH_2$Te-3**). Generally, the blueshift of C5-H6 stretching frequency in the complexes is emphasized by a slight increase in electron density at σ*(C5–H6) from -0.001e to 0.005e. The O8-H9 stretching frequency redshift is induced by a large increase in electron density at σ*(O8-H9) orbital from 0.042e to 0.064e. The larger blueshift of C5-H6 stretching frequency is observed in **XSe-n** compared to **XTe-n.** Indeed, the electron density of the σ*(C5–H6) orbital gets a larger increase when Se is replaced by Te, and s–character percentage of C5 is smaller for C5–H6···Te3 than C5–H6···Se3. The larger blueshift of C5-H6···Se3 bonds, which relates directly to the smaller values of Δσ*(C5-H6), is found in **XZ-2** in comparison to **XZ-3**. Moreover, the substitution of the H atom in HCHZ by electron-donating groups ($CH_3$, $NH_2$) leads to an enhancement of $C_{sp2}$–H stretching frequency involving $C_{sp2}$–H···Z hydrogen bonds. At the same time, the corresponding diminishment is caused by the presence of electron-withdrawing groups (F, Cl, Br). Consequently, it can be underlined that the larger contraction of the $C_{sp2}$-H bond and its stretching frequency blueshift is identified by a decrease in the population of electron density at σ*(C5–H6) orbitals and an increase in the percentage of s-character of $C_{sp2}$ atom. This observation is similar to results obtained in complexes of aldehydes and carboxylic acids.[16,33,36]

For C1-H2···O7/O8 hydrogen bonds, the stronger blueshift of C1-H2 stretching frequency in **XSe-n** compared to that in **XTe-n** relates to a larger decrease of electron density in σ*(C1–H2) orbital. The larger redshift phenomenon in the O8–H9···Se hydrogen bonds compared to the O8–H9···Te ones (cf. Table 4) arises from a significant enhancement in occupation of $\sigma^*$(O8–H9) orbital. For the X substitution in XCHZ, the increase in electron density of $\sigma^*$(O8–H9) orbital and s-character percentage of the O8 site is smaller for halogenated derivatives than for $CH_3$ and $NH_2$ substitutions. Consequently, it can be suggested that the increasing occupation of $\sigma^*$(O8–H9) orbital is the main factor in determining red-shifting hydrogen bonds in all examined complexes.

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