



Original Research Article

Theoretical investigations on the vibronic coupling effect and NBO Studies of Stability on the GeX_2 ($\text{X}=\text{F}$, Cl , and Br) molecules

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ABSTRACT

The contemporary paper refers back to the instability of linear in GeX_2 ($\text{X}=\text{F}$, Cl & Br) molecules because of the vibronic coupling effect. Optimization and the following frequency calculations in those molecules found out that every one of those molecules were unstable in high symmetry linear (with $D_{\infty h}$ symmetry) geometry and their systems have been bent to lower C_{2v} symmetry geometry. On this work, we've used, TD-DFT (B3LYP/6-31G (d) calculations to gain the strength curves of the ground and excited in the bending directions Q (π_u) of compounds 1–3. The vibronic coupling interaction between $^1\Sigma_g^+$ ground and the first $^1\pi_u$ excited states in the Q (π_u) direction via $(^1\Sigma_g^+ + ^1\pi_u) \otimes \pi_u$ PJTE problem was the reason for the symmetry breaking phenomenon. Additionally, changing atoms with different elements together with the electronegative exchange and the degree of overlap at once have an effect on the pattern of molecular orbitals. The NBO calculations were carried out to define a stability measure through the stabilization energy, E^2 parameter. According to the consequences received from the vibronic principle of PJT, the bent shape of those analogs is the result of $\text{LP}(3) \text{X} \rightarrow \text{LP}^*(2)\text{Ge}1$ electron delocalization. The PJT stabilization strength decreases from compound 1 to compound three. Moreover, by the decrease of the energy gaps between reference states (Δ) the primary force constant of the ground state in the Q (π_u) direction (K_0) could decrease from compound 1 to compound 3.

Keywords: Vibronic coupling; Symmetry breaking; pseudo Jahn–Teller effect (PJTE), Natural bond orbital (NBO) analysis; Stabilization energies $E^{(2)}$

Introduction

All properties of a chemical compound are as a characteristic of its molecular coordinates. In keeping with the principle of electron structure, a chemical compound can take many forms. But it is obvious that real molecules in nature have the least energy in their most stable state. In truth, the most excellent structure is mathematically dependent to be on the minimum ability strength level (PES), that's transferring from an risky configuration of excessive symmetry to a stable configuration of low symmetry, and that is the concept of symmetry failure [1-3]. on other words, the total energy of a molecule is directly related to its structural shape. According to Mullikan's idea, whilst one shape transforms into any other structure, the energy undergoes a change as well. Most molecules are deformed because of the deviation of bond lengths and bond angles caused by rotational and stretching processes within the molecule. Clearly, the lowest energy geometry is the maximum thermodynamically strong structure. But from the molecular orbital (MO) factor of view, the power of a molecule is same to the sum of the occupied orbitals. The physical interpretation of this principle is possible primarily based at the powerful overlap of orbitals (Fij). Overlap between orbitals that have a bonding interaction lowers the molecular energy.

In the studied structures, the instability of configuring high symmetry from $D_{\infty h}$ to C_{2v} due to the vibronic connection of the presence of two ground and excited electronic states that interact with sufficient nuclear displacement and cause linear instability. Change of configuration from linear state to bent geometry is defined as symmetry failure system (SBS) [4]. System symmetry breaking is an old concept in physics that is defined based on energy considerations: a symmetric system can lose its symmetry and reach a lower energy configuration [5]. The initial symmetric state can be unstable or quasi-stable. In the latter case, an energy barrier must occur before symmetry breaking, which must be overcome. In fact, vibronic coupling is introduced as a disorder factor. Among the vibronic coupling effects of the Jan-Teller effect is the pseudo-Jan-Teller effect (PJT) [6-9]. The effects that arise from the vibronic combination of two or more asymmetric electronic states with nuclear displacements are called "pseudo Jahn-Teller effect". In other words, the mixing effect of two or more non-equivalent vibronic electronic states, under nuclear displacement, this concept is due to the strong coupling of ground and excited states, which leads to instability of the ground state, and in many ways similar to the instability of the ion effect. in this study, the Mulliken approximation and Natural Bond Orbital (NBO) were

employed for the description, respectively, the effects of substituent atoms on the partial atomic charges and some of the significant donor-acceptor interactions, their stabilization energies $E^{(2)}$. Natural bond orbital (NBO) analysis used to determine the stability of the compounds. Natural bonding orbital analysis is a useful method of providing information about the interaction of both orbital spaces filled and virtual. This can increase the anticipation of inter-molecular interactions and interactions [10-12].

Computational Details

Structural properties of GeX_2 molecules ($\text{X}=\text{F}, \text{Cl}, \text{Br}$) were studied by B3LYP/ 6-31G (d). First, for the structure of these combinations, the Z-Matrix input of Gaussian 09 [13] software turned into written. Optimization calculations and vibrational frequency evaluation of those systems were achieved by means of Gaussian application with hybrid density practical concept with 6-31G (d) foundation series. These compounds in the ground state have ($^1\Sigma_g^+$) (SGG) symmetry, the lowest energy level of which corresponds to $(\pi_u)^2 (^1\Sigma_g^+)^2$. The symmetry obtained from the calculations for these molecules is $D_{\infty h}$ with two virtual frequencies PIU (π_u), and the effects received are mentioned in the table below for these compounds. The zero-point (ZPE) and total electronic (Eel) energies ($E_0 = E_{el} + \text{ZPE}$) acquired from geometry optimization of the linear ($D_{\infty h}$ symmetry) and bent (C_{2v} symmetry) systems of compounds calculated on the B3LYP/ 6-31G (d) degree of idea, are given in table 1. Values are in Hartree.

Table 1

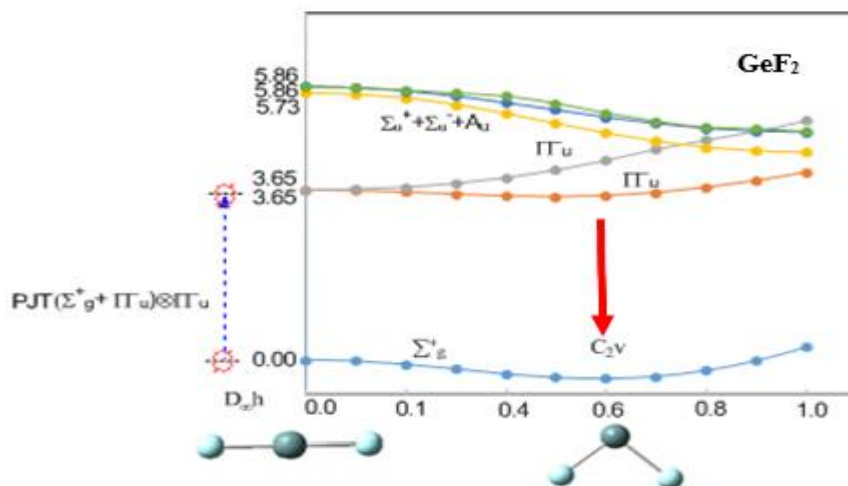
The results of optimization and frequency analysis of linear GeX_2 compounds ($\text{X}=\text{F}, \text{Cl}, \text{Br}$) at the computational level B3LYP /6-31G (d)

Molecule	GeBr_2	GeCl_2	GeF_2
Grand state	SGG ($^1\Sigma_g^+$)	SGG ($^1\Sigma_g^+$)	SGG ($^1\Sigma_g^+$)
kind of virtual frequency	PIU (π_u)	PIU (π_u)	PIU (π_u)
Values of virtual frequency	-239.96	-144.38	-111.49
Force Constant(linear)	0.8620	0.5774	0.5525
Zero point energy(linear)	0.002722	0.001344	0.000997
Zero point energy(bent)	0.003767	0.002026	0.001484
total energy $E_0=E_{el}+ \text{ZPE}$	-2274.670	-2995.407	-7218.443

(linear, $D_{\infty h}$)			
total energy			
$E_0 = E_{el} + ZPE$	-2274.737	-2995.461	-7218.491
(bent, C_{2v})			
$\Delta E(E_{PJT})$	0.067	0.054	0.048

As a result of applying $Q\pi_u$ on the core configuration in the ground electronic state, a bent structure with C_{2v} symmetry was obtained, which is the result of the mixing of ($^1\Sigma_g^+$ and (π_u)) orbitals, and is displayed as follows: $\Gamma\Sigma_g^+ \times \Gamma\pi_u = \Gamma\pi_u$

The result of this is the creation of a pseudo-Jahn-Teller effect, i.e. $(\Sigma_g^+ + \pi_u) \otimes \pi_u$ of these three combinations. It's far obvious that the energies of the ground state and the excited state change along the bending coordinates. The look at of chemical structures is primarily based on nuclear separation and electron motion. That fixing the Schrödinger equation for the electrons in the potential due to the nucleus in that particular arrangement leads to a "potential energy level". A potential energy level represents the strength of a molecule as a characteristic of its geometry. The concept of potential energy levels is the heart of computational chemistry. Each electronic state has its own potential energy level and the separation between these levels leads to electron spectra. Each point in the PES represents a molecular compound with its own structure and energy (strength).



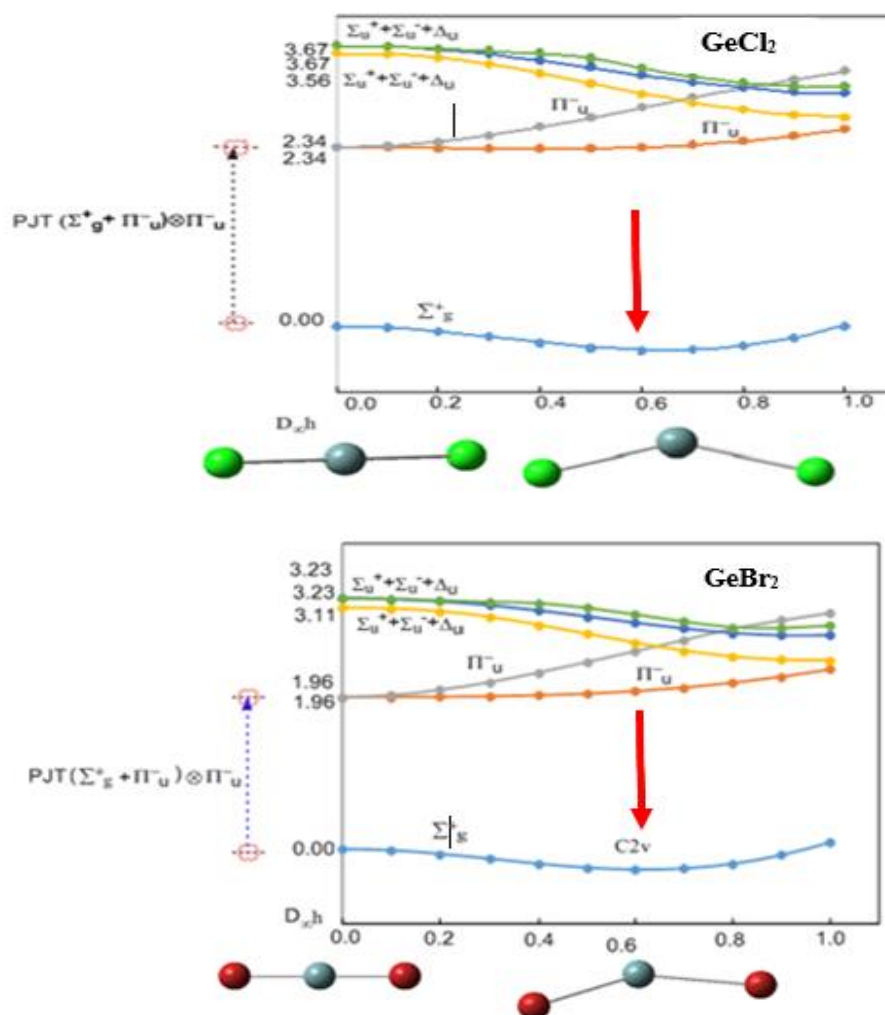


Figure 1- Energy curves (in electron volts) - along the $Q\pi_u$ bend

The high symmetry structure inside the absence of a distortion mode on the ground state has the primary force constant

$$K_0 = \langle \Sigma_g | H_{Q_T}^2 | \Sigma_g \rangle$$

When the normal coordinate (twist mode) $Q\pi_u$ is applied, the energy of the electronic configuration of the ground state is reduced and the energy of the electronic configuration of the excited state with Π_u symmetry is added. The combination of the ground and excited state adds the vibronic coupling constant k_v to the initial force constant, which:

$$K = K_0 + K_v$$

$$F = \left\langle \Sigma_g \left| \frac{\partial H}{\partial Q_{\pi u}} \right| \Pi_u \right\rangle$$

According to the equation below:

$$K_v = 2 \frac{\left\langle \Sigma_g \left| \frac{\partial H}{\partial Q_{\pi u}} \right| \Pi_u \right\rangle^2}{E_{\Sigma_g} - E_{\Pi_u}}$$

The numerator of the fraction is positive and the denominator of the fraction becomes negative due to the fact that the energy of the excited state is greater than that of the ground state. Therefore, the expression below K becomes negative.

When $K(v) < 0$, the instability of $K(<0)$ may lead to $K(0 > 0)$ or $|K_v| > K_0$. The graphs with the computational level B3LYP/6-31G(d) show that the curvature of the curve in the ground state is negative, according to the relation $K = K_0 - \frac{F^2}{\Delta}$ for any polyatomic system in the high symmetry configuration, the values of K_0 It is positive [4].

- Structural parameters

Structural parameters related to compounds 1 to 3 in $D_{\infty h}$ and C_{2v} configurations are presented in Table 2.

Table 2. Results from the analysis of structural parameters of GeX_2 compounds ($X = F, Cl, Br$) with computing level B3LYP/ 6-31G(d).

Compound	1 (GeF ₂)		2 (GeCl ₂)		3 (GeBr ₂)	
geometry	D _{∞h}	C _{2v}	D _{∞h}	C _{2v}	D _{∞h}	C _{2v}
Bond lengths (Å)						
r _{M-X}	1.835	1.758	2.353	2.219	2.485	2.363
Δ[r _{M-M} (D _{∞h})- r _{M-M} (C _{2v})]	0.07758		0.13435		0.12207	
Bond angles (°)						
θ _{X-M-X}	180.0	97.3	180.0	100.8	180.0	102.3

$\Delta[\theta_{M-M}(D_{\infty h}) - \theta_{M-M}(C_{2v})]$	82.7	79.2	77.7
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NBO calculations in compounds GeX_2 ($X=F, Cl, Br$) with $B_3LYP/6-31G(d)$ computational level

NBO analysis is used to study stability energies resulting from electron delocalization.

Table 3 lists the highest stabilization energies E^2 of donors and acceptors for these compounds. The interaction between donor and acceptor of electrons is larger when the E^2 value increases. The delocalization of electronic density between Lewis-type NBO orbitals (donor) and non-Lewis NBO orbitals (acceptor) corresponds to one stabilizing donor-acceptor interaction [14]. According to the results obtained from the vibronic theory of PJT, the bent structure of these analogues is the result of $LP(3) X \rightarrow LP^*(2)$ Ge1 electron delocalization. Intramolecular NBO interactions show that the origin of intramolecular interactions between acceptor and donor belongs to different fragments of the same molecule. The amount of partial charge transferred between an electron donor and acceptor (donor \rightarrow acceptor) was calculated by the occupation numbers (population) from NBO data to evaluate the orbital interaction energy $\Delta E^{(2)}$ is between the HOMO and LUMO of the donor-acceptor system. On other words, In these case, the NBO analysis is useful to determine relevant interactions between Lewis-type NBO orbitals (donor) and non-Lewis NBO orbitals (acceptor), and to define electronic density delocalization

$$\Delta E^2 = 2 \frac{(\psi^* | \hat{F} | \psi)^2}{\epsilon_{acc} - \epsilon_{donor}}$$

Table 3. Natural bond orbital analysis of the second-order E^2 (kcal/mol) interaction energies calculated between the electron donor acceptor orbital in stable structures of these compounds

Donor Lewis-type NBOs	Occupancy(i)	Hybrid	Acceptor NBO (j)	Occupancy (j)	F(i,j) a.u	E^2 (kcal mol ⁻¹)
<i>GeF₂</i>						
BD (1)Ge 1 - F 2	1.99547	Sp ^{12.37}	BD*(1)Ge 1 - F 3	0.03994	0.037	2.14
BD (1)Ge 1 - F 3	1.99547	Sp ^{12.37}	BD*(1)Ge 1 - F 2	0.03994	0.037	2.14
LP (2) F 2	1.95620	p ^{1.00}	BD*(1)Ge 1 - F 3	0.03994	0.058	8.51
LP (3) F 2	1.90198	p ^{1.00}	LP*(2)Ge 1	0.18861	0.071	21.58
LP (2) F 3	1.95620	p ^{1.00}	BD*(1)Ge 1 - F 2	0.03994	0.058	8.51
LP (3) F 3	1.90198	p ^{1.00}	LP*(2)Ge 1	0.18861	0.071	21.58
$\Delta q_{i,j}=1.71337$						ΣE^2 64.46

<i>GeCl₂</i>							
BD (1)Ge 1 - Cl 2	1.99566	Sp ^{15.51}	BD*(1)Ge 1 -Cl 3	0.04001	0.022	0.99	
BD (1)Ge 1 - Cl 3	1.99566	Sp ^{15.51}	BD*(1)Ge 1 -Cl 2	0.04001	0.022	0.99	
LP (2) Cl 2	1.95787	Sp ^{84.77}	BD*(1)Ge 1 -Cl 3	0.04001	0.043	6.44	
LP (3) Cl 2	1.87684	p ^{1.00}	LP*(2)Ge 1	0.24142	0.055	19.63	
LP (2) Cl 3	1.95787	p ^{1.00}	BD*(1)Ge 1 -Cl 2	0.04001	0.043	6.44	
LP (3) Cl 3	1.87684	p ^{1.00}	LP*(2)Ge 1	0.24142	0.055	19.63	
				$\Delta q=1.63542$	$\Sigma E2$	54.12	
<i>GeBr₂</i>							
BD (1)Ge 1 - Br 2	1.99604	Sp ^{17.74}	BD*(1)Ge 1 -Br 3	0.04571	0.016	0.59	
LP (2) Br 2	1.95172	Sp ^{62.86}	BD*(1)Ge 1 -Br 3	0.04571	0.042	6.96	
LP (3) Br 2	1.85158	p ^{1.00}	LP*(2)Ge 1	0.29222	0.054	21.46	
LP (2) Br 3	1.95172	p ^{1.00}	BD*(1)Ge 1 -Br 2	0.04571	0.042	6.96	
LP (3) Br 3	1.85158	p ^{1.00}	LP*(2)Ge 1	0.29222	0.054	21.46	
				$\Delta q=1.55936$	$\Sigma E2$	57.43	

- CMO analysis results

Interpretation of COM output (contribution of HOMO LUMO orbitals) and electron destabilization

Quantitative details of the linear combination of orbitals (orbital contributions) in electron destabilization (CT) were investigated with NBO software, which includes the unstable focal molecular orbital (CMO) analysis program. The interpretation of the CMO output of the obtained wave functions for the HOMO and LUMO orbitals confirms the pseudo Jahn Teller effect and the related transitions.

- In GeX₂ composition, the contribution of these orbitals is calculated as LCNBO-MO linear combination of natural orbital.

$$\Psi_{HOMO-1} = 0.705(LP(3)F2(lp) - 0.688(BD(2)Ge1 - F3)$$

$$\Psi_{LUMO+1} = 0.949(BD*(2)Ge1 - F3) - 0.227(LP(3)F2(lp)$$

$$\Psi_{HOMO-2} = -0.706(LP(3)Cl3(lp) + 0.683(BD(1)Ge1 - Cl2)$$

$$\Psi_{LUMO+1} = 0.956(BD*(2)Ge1 - Cl2) - 0.254(LP(3)Cl3(lp)$$

$$\Psi_{HOMO-2} = -0.706(LP(3)Br3(lp) + 0.677(BD(1)Ge1 - Br2)$$

$$\Psi_{LUMO+1} = 0.950(BD*(2)Ge1 - Br2) - 0.281(LP(3)Br3(lp)$$

- *Evaluation of electronegativity changes and hardness*

The strength gap ΔE (LUMO-HOMO) and the hardness of the total index of chemical reactivity become $\chi = -\mu$. The energies of the highest filled orbital, HOMO, and the lowest empty orbital, LUMO, had been calculated for the linear and bent states at the B3LYP/6-31G(d) computational level. Some other essential belongings of chemical bonds is polarity. Electronegativity of a primary agent this is transferred to practical organizations. Ionization energy I , electron-withdrawing energy A , hardness η , electronegativity X for compounds 1- three are shown in Table 4. A numerical criterion is stated for polarizability. Issue is described as follows:

$$\eta = 0.5(I - A)$$

Considering the validity of Koopman's theorem, we have:

$$IP = -\epsilon_{HOMO} (eV)$$

$$EA = -\epsilon_{LUMO} (eV)$$

$$\eta = 0.5(\epsilon_{LUMO} - \epsilon_{HOMO})$$

These data, as well as the energy, were obtained from the Gaussian output file in Hartree and converted to kJ/mol (1 Hartree = 2625.50 kJ/mol).

Table 4 - Electronic calculations of linear and bent structures in compounds) GeX_2 ($\text{X}=\text{F}$, Cl , and Br) at the computational level B3LYP/ 6-31G (d)

	ϵ_{HOMO}	ϵ_{LUMO}	$\epsilon_{LUMO} - \epsilon_{HOMO}$	I	A	η	χ	$\Delta[\eta(C_{2v}) - \eta(D_{\infty h})]$	$\Delta[\chi(C_{2v}) - \chi(D_{\infty h})]$
Symmetry									
1- C_{2v}	-0.31018	-0.09653	0.21365	0.31018	0.09653	0.106825	-0.1018	0.026405 (16.57) ^a	0.0857 (53.78.) ^a
1- $D_{\infty h}$	-0.26792	-0.10708	0.16084	0.26792	0.10708	0.08042	-0.1875	0.00	0.00
2- C_{2v}	-0.29327	-0.12573	0.16754	0.29327	0.12573	0.08377	-0.12573	0.02483 (15.58) ^a	0.07994 (50.16) ^a
2- $D_{\infty h}$	-0.26461	-0.14674	0.11787	0.26461	0.14674	0.05894	-0.20567	0.00	0.00
3- C_{2v}	-0.26570	-0.14856	0.11714	0.26570	0.14856	0.058570	-0.20713	0.006815 (4.28) ^a	-0.01515 (-9.51) ^a
3- $D_{\infty h}$	-0.24373	-0.14022	0.10351	0.24373	0.14022	0.051755	-0.19198	0.00	0.00

^a Numbers in parenthesis are in kcal mol⁻¹.

The energy gap between orbitals is one of the parameters of controlling the transfer of pure charge in the interacting to the receiver. As well as, known that molecules with larger HOMO-LUMO gap have kinetic stability and lower chemical reactivity. Therefore, symmetry breaking plays a crucial role in the physical properties of molecules

Results and discussion

The beginning of the structural distinction in isoelectronic compounds affects the structural home extra. Investigations display that the most effective motive for the structural distinction in compounds with high symmetry is the pseudo-Jahn Teller effect. With proper reasons from the structural and active factor of view, the investigation of electron destabilization transitions has to offer a proper justification for the instability of the shape with high symmetry because of the pseudo-Jahn-Teller effect.

1- Examination in terms of structural parameters

The information in Tables 1 and 2 of the results show that:

- The order of Ge-X bond for compounds has increased from 1 to 3, which was calculated using NBO results and the Wiberg WBI bond index method, (0.9824, 0.8719, 0.6194) and this is a self-confirmation that the length of Ge-X bond in bent structures is compared to Linear structures are reduced. Table 4 shows that the stronger the bond order, the lower the energy level of the bonding molecular orbital and the higher the energy level of the anti-bonding molecular orbital.
- Zero-point energy, ZPE, which is obtained from quantum mechanics calculations; Reduced from 1 to 3. Zero-point energy depends on intramolecular parameters (bond stretching and angular bending). According to Table 1, the reduction of virtual vibration frequencies from 1 to 3 is in good agreement with the constant reduction of bond tensile force in these linear compounds.
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2- Examination from the energetic point of view

- The energy difference between the reference states in the configurations decreases from 1 to 3. In other words, the stability energy of Jahn Teller (EPJT) decreases, the reasons for which are checked by examining the following parameters:

- Checking the hardness and electronegativity of the structure

The calculations in Table 4 show that the hardness of molecules for compounds decreases from 1 to 3, which corresponds to the decrease in energy separation between HOMO-LUMO. Soft molecules have a smaller separation and this is an emphasis on the softness of the structure. Also, the separation between the energy states involved in the pseudo-Jahn-Teller effect in the unbent configurations decreases from 1 to 3, which is consistent with the decrease in electronegativity and hardness.

- From the point of view of the interaction of instability with the energy of the second order disorder $E^{(2)}$ (NBO analysis)

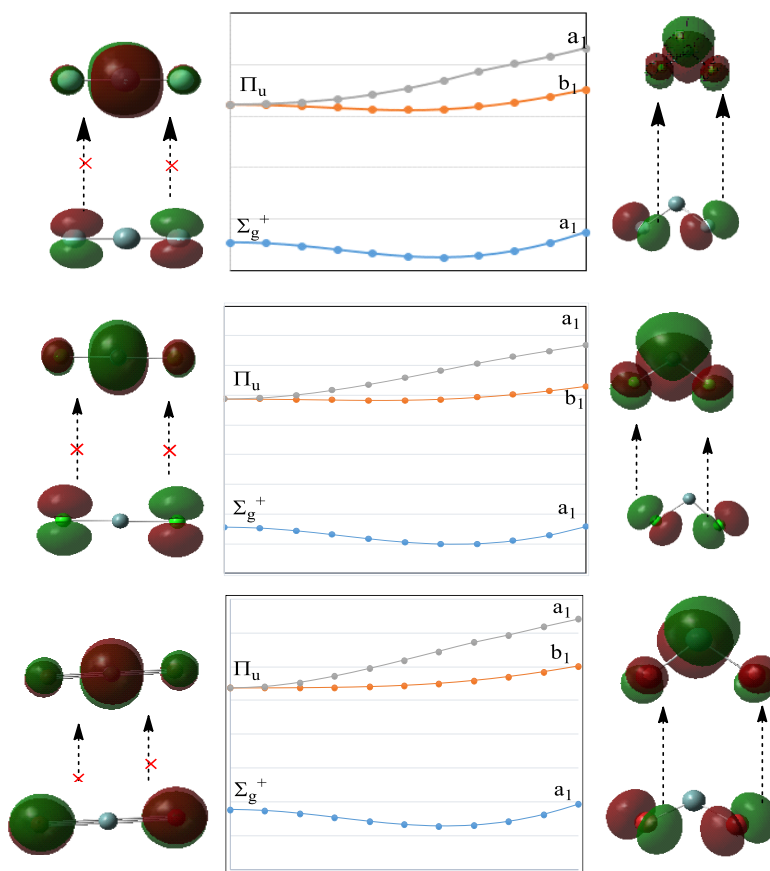
- Based on the results obtained from pseudo- Jahn–Teller effect (PJTE) in bent structures with C_{2v} symmetry, the highest second-order disorder energy $E^{(2)}$ for GeX_2 compounds ($X=F, Cl, Br$) in the electron delocalization interaction $Lp(3) X \rightarrow LP^*(2) Ge$ was observed.

The disorder energy $E^{(2)}$ depends on $F_{(ij)}$ and $\Delta(\mathcal{E}_{accepter} - \mathcal{E}_{donor})$ which is completely consistent with the decrease of $F_{(ij)}$ parameter value (0.058, 0.045 and 0.042) in Table 3.

On the other hand, the quantitative value $E^{(2)}$ is responsible for the weak bonding orbital interaction and the larger $\Delta E^{(2)}$ is the effect of strong charge transfer (CT) in the orbital interaction, and the reduction of $\Delta(\mathcal{E}_{accepter} - \mathcal{E}_{donor})$ in compounds 1 to 3 include 1.71337, 1.63542, 1.55936, show the stability of the bent structure in comparison with the linear structure and confirms the reduction of electron destabilization and the reduction of the pseudo- Jahn–Teller effect (PJTE) in compounds 1 to 3.

- Comparing the overlap of orbitals in linear and bent state

π_u orbitals are decomposed into two orbitals a_1 and b_1 in linear mode. In the bent state, the two orbitals $1a_1$ (ground) and $2a_1$ (excited) because of the same symmetry and purpose interference and keep away from crossing each other according to the perturbation regulation (avoid crossing) [15-16]. In the studies, it is the basis of the HOMO energy because in the bent state, the energy increases compared to the linear state. So the bent molecule is more stable than the linear molecule. All of the obtained consequences are consistent with the bent shape of the molecule (in step with Table four).



Conclusion

In the present study, the instability of the linear structures of GeX_2 analogs ($\text{X}=\text{F}, \text{Cl}, \text{Br}$) was investigated at the B3LYP/DFT computational level with 6-31G (d) basis series.

- In this study, the reduction of symmetry has caused the stability of the structures.

- The vibronic coupling of the interaction between the ground and excited state along the Q_{π_u} coordinate is the only reason for the symmetry breaking through the Jan Teller pseudo-problem. $(^1\Sigma_g^+ + ^1\Pi_u) \otimes \pi_u$
- The values show that decreasing symmetry is associated with decreasing electronegativity and hardness.
- The output of Gaussian software shows both parameters root-mean-square deviation (RMSD) and root mean square fluctuation (RMSF) define as a difference between two structures for a specific set of atoms and the Fluctuation around an average, respectively. The RMSF value is used to measure the flexibility of a structure (parameters of the system) and these values for the $D_{\infty h}$ structures are less in comparison with the C_{2v} structures.

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