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DFT INVESTIGATION OF GEOMETRICAL STRUCTURE, IR AND RAMAN SPECTRA OF VINYL HALIDES CH_2=CH–X (X IS F, Cl AND Br)

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ABSTRACT: The geometrical structure and conformational energy stability of vinyl halides CH_2=CH–X (X = F, Cl, and Br) were examined by using Density Functional Theory calculations (B3LYP method in combination with 6-311G* basis sets). The values of HOMO-LUMO gap (ΔE) for vinyl halides (fluoride, chloride and bromide) were 7.68 (eV), 7.10 (eV) and 6.55 (eV) respectively. The calculated geometrical parameters were in good agreement with the previously observed results. Both HOMO-LUMO gap and geometrical parameters were found to account for the stability of the molecules. Electron distribution in HOMO-LUMO Frontier molecular orbitals was investigated to show the charge transfer within the molecules. The atomic charges and molecular electrostatic potential were interpreted together to demonstrate the electrophilic -nucleophilic reactivity. The vibrational frequencies were computed, the comparison between the three halides revealed that vinyl chloride and vinyl bromide have strong C-X stretching vibrations bands, but for vinyl fluoride the bands are weaker, the intensity characterization increasing from F to Br respectively.

INTRODUCTION: Vinyl halides have a halogen bonded to a carbon atom that is double-bonded to another carbon, similar to phenyl halides in which a halogen is attached to a benzene ring. Both vinyl and phenyl halides belong to a group known as organic halides. In hydrocarbon, one hydrogen atom is replaced by halogen atom to produce vinyl halides.

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In the presence of heat or light, hydrocarbon undergoes in successive chlorination reactions when treated with Cl_2 or Br_2 to form a mixture of vinyl halides. This reaction involves free radical intermediates, as a first step halogen molecules absorb energy from the heat or light and dissociate into halogen atoms.

After the halogen radical is formed, it reacts with a type of hydrocarbons, and a chain reaction continues [1]. Most vinyl halides are natural products that are liquids at room temperature and insoluble in water. These classes of organic groups have considerable interest in industrial applications, solvents for the non-polar compounds and they used in the synthesis of wide range of organic compounds as starting materials. Vinyl bromides are used as substrates for cross-coupling reactions. Vinyl chloride is mostly used in manufacturing polyvinyl chloride (PVC) plastic and vinyl products. Vinyl fluoride is a common theme in the synthesis of analogs of biologically active compounds [2-4]. Nucleophilic substitution (SN_2) reaction at a vinylic sp^2 carbon is considered one of the most fundamental reactions in organic chemistry [5]. A nucleophile is a species containing an unshared electron pair (lone-pair electrons), incorporating an alkyl halide by replacing the halogen substituent (leaving group). In nucleophilic reactions, the C–X bond of the substrate undergoes heterolysis, and a new bond to the carbon atom is formed by the lone-pair electrons of the nucleophile [6].

The substituent in a good leaving group must leave as a relatively stable, weakly basic molecule or ion. The halogen substituent is the leading group in alkyl halides, which leaves as a halide ion. Therefore, halide ion good leaving groups because they are relatively stable and very weak bases. Several studies investigated the substitution reactions of vinyl halides where the effect of vinyl halides bearing other organic compounds was described. The adsorption of vinyl fluoride and vinyl chloride on TiO_2 [7], the polymerization of isobutyl vinyl ether with $C_2H_5AlCl_2$ [8], the structural behaviour and stability of vinyl sulfonyl halides $CH_2=CH–SO_2X$ [9] and the formation of selenium derivatives $CH_2=CH–SeO_2X$ (X=F and Cl) [10], were the different conformational stabilities have been produced as a result of the coupling effects between the vinyl C=C moiety and the two S=O (or Se=O) bonds, in which the planar cis and trans are constituted and non-planar gauche form that may be stabilized.

Although, these comprehensive studies discussed vinyl halides reactions with natural products and compounds, there is a lack in the study of the substitution effect of the halides molecules on the vinyl group itself, except for a set of Ab initio studies including Density functional theory (DFT) descriptors for structure units of vinyl polymers [11, 12]. In the present study, a molecular structure and spectroscopic studies of $CH_2=CH–X$ (X is F, Cl and Br will be introduced. DFT energy optimization for all different structures of the simpler molecules $CH_2=CH–X$ (X=F, Cl and Br) will be carried out and the relative conformational stability will be determined. Additionally, calculation of the vibrational frequencies was performed on the basis of the optimized structures, and hence, the vibrational data were used to make plots for the vibrational IR and Raman spectra of the molecules.

MATERIALS AND METHODS: Density functional theory is considered as one of the most significant methods outside ab initio calculations. It's a powerful tool for the investigation of molecular properties along with quantum chemical computations. In the frame of DFT, the Becke's three-parameter hybrid function combined with the Lee–Yang–Parr correlation function (B3LYP) [13] with the standard 6-311G* basis sets were used in estimating all molecular geometry and IR, Raman frequencies embedded in this work. The calculations were implemented by using Gamess quantum chemistry package [14]. Firstly, the most stable geometrical configurations have been optimized for all the proposed kinds of Vinyl halide and then the basis of optimized geometry has been taken to calculate the infrared and Raman shift spectra. The vibrational frequencies related to the fundamental modes were computed, and the results included no imaginary frequencies. This is remarkable confirmation that the calculations provide maximum stability associated with minimum potential energy for the optimized structures. All the results were visualized using Chemcraft - graphical software [15] and Avogadro, an open-source molecular builder and visualization tool [16].

RESULTS AND DISCUSSION:

Molecular Geometry: The ascertained bond lengths, the numbering of the vinyl halides atoms and bond angles are represented alongside in **Fig. 1** and **Table 1**. The calculated optimized structures of the title molecules were in good agreement with the previous experimental results [17-19]. No significant variation in the geometrical parameters due to the exchange of halogen atom in hydrocarbon group except for the C-X bond, the bond length increases, and at the same time, the strength of C-X bonds decreases with the size of the halide atom. The lengths 1.348, 1.752 and 1.914 Å were determined for C-F, C-Cl, and C-Br bonds respectively in high correspondence with other researchers [20-22]. The augmented geometrical parameters make for a great close estimation and serve as the base upon that the vibrational frequencies were calculated.

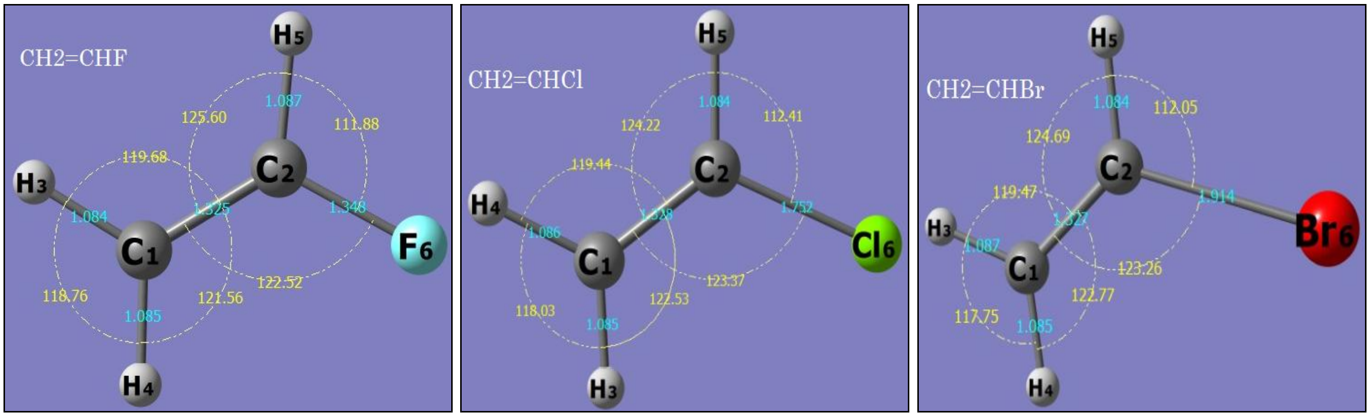

FIG. 1: OPTIMIZED GEOMETRICAL PARAMETERS (BOND LENGTH / Å, BOND ANGLE / O) OF CH_2=CHX (X = F, Cl, Br)

TABLE 1: MOLECULAR STRUCTURES OF CH_2=CH–F, Cl AND Br

	CH_2=CH-F		CH_2=CH-Cl		CH_2=CH-Br	
	Experiment	This work	Experiment	This work	Experiment	This work
C_1-C_2	1.332	1.325	1.332	1.328	1.332	1.327
C_2-X	1.348	1.348	1.726	1.752	1.884	1.914
C_2-H_5	1.073	1.087	1.079	1.084	1.080	1.084
C_1-H_3	1.080	1.084	1.078	1.085	1.080	1.087
C_1-H_4	1.080	1.085	1.079	1.086	1.088	1.085
$\angle C_1C_2X$	120.80	122.52	122.30	123.37	122.6	123.26
$\angle C_1C_2H_5$	124.93	125.60	123.80	124.22	123.7	124.96
$\angle C_2C_1H_3$	119.30	119.86	119.50	119.44	119.5	119.47
$\angle C_2C_1H_4$	121.20	121.56	121.00	122.53	121.3	122.77

The LUMO (lower unoccupied molecular orbital) and the HOMO (higher occupied molecular orbital) are called FMOs (Frontier molecular orbitals). FMOs play an effective role in electric and optical properties. LUMO represents the competency for acceptance of an electron, whereas HOMO represents the capability for donation an electron. The frontier orbital gap serves to illustrate the chemical hardness and softness, chemical reactivity and optical polarizability of a molecule. The molecule, either hard or soft can detect from the HOMO-LUMO gap (ΔE).

More voluminous ΔE is corresponding to the harder molecule and diminutive one, indicating to the softer molecule [23, 24]. As shown in **Table 2**, the values of the HOMO-LUMO gap (ΔE) for vinyl halides (fluoride, chloride, and bromide) are 7.68 eV, 7.10 eV and 6.55eV respectively.

Among vinyl halides, we can conclude that vinyl fluoride is the hardest while vinyl bromide is the softest. This result is interpreting the large value of C-Br bond length rather than C-F and C-Cl.

TABLE 2: ENERGIES VALUES OF HOMO AND LUMO. ΔEG (HOMO–LUMO), ATOMIC CHARGES FOR THE PROPOSED VINYL HALIDE CH_2=CHX (X = F, Cl, Br)

Parameter	CH_2=CH-F	CH_2=CH-Cl	CH_2=CH-Br
EHOMO (eV)	-6.99	-7.05	-6.93
ELUMO(eV)	0.69	0.054	-0.38
Δ Eg (eV)	7.68	7.10	6.55
Atomic charges			
C 1	-0.3775	-0.3775	-0.3028
C 2	0.1919	-0.2067	-0.1642
H 3	0.1549	0.1716	0.1648
H 4	0.1605	0.1636	0.1748
H 5	0.1397	0.1900	0.1890
X 6	F, -0.2696	Cl, -0.0286	Br, -0.0617

The HOMO-LUMO atomic orbital composition is shown in **Fig. 2**. It is clear that HOMO is distributed on the whole C_1=C_2 bonds for the three conjugated Vinyl halides. LUMO is delocalized over the C_2–H_5 bonds and $H_3C_1H_4$ group. Then, the transfer of electron density of HOMO–LUMO orbitals takes place from the C_1=C_2 direct to C_2–H5 bonds, $H_3C_1H_4$ group.

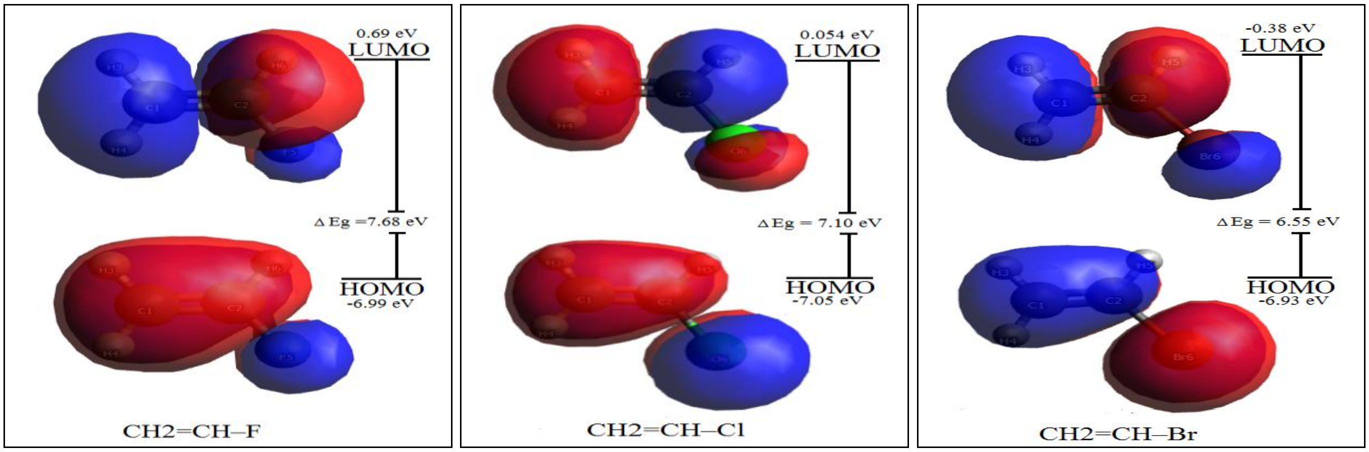

FIG. 2: FRONTIER MOLECULAR ORBITALS FOR THE HOMO AND LUMO ENERGIES OF CH_2=CH–F, Cl AND Br

Based on the analysis of both Molecular electrostatic potential MEP **Fig. 3** and atomic charge distribution **Table 2**, the negative atomic charge on C_1 (-0.3028) and C_2 (-0.1642) in Vinyl bromide and C_1 (-0.2899), C_2 (-0.2067) in Vinyl chloride produces an electronegative surface (red colours) on C_1=C_2 region, electropositive regions (blue colours) which are localized on H_3 (0.1648), H_4 (0.1748), H_5(0.1890) in Vinyl bromide and on H_3 (0.1716), H_4(0.1636), H_5(0.1900) in Vinyl chloride. A small negative charge shows up an intermediate potential (white colors) on Br (-0.0617), C_l (-0.0286) atoms. Although the positive charges on H_3 (0.1549) and H_5 (0.1397) in vinyl fluoride are less than in Vinyl bromide and Vinyl chloride, the electropositive regions become more denser (more blue in colour) on H_3 and H_5 in vinyl fluoride due to the interaction between negative charge on C_1 (-0.3775) and positive charge on C_2 (0.1919), which leads to an intermediate potential on C_1=C_2 region, the high negative charge on F atom (-0.2696) indicating a maximum electro-negative region (more red in colour). The electrophilic and nucleophilic reactivity is established on the grounds of positive (blue) and negative (red) regions indicated by MEP. The electrophilic reagents attacking the positive regions and nucleophilic reagents are reaction partner to negative regions. From these results, the H atoms contained in the three types of vinyl halides are exposed to electrophilic reaction, while nucleophilic reagents are directed to C_1=C_2. The most notable is that F atom in vinyl fluoride (the most negative (red) regions) is strongly attractive to nucleophilic reactivity rather than vinyl chloride and vinyl bromide.

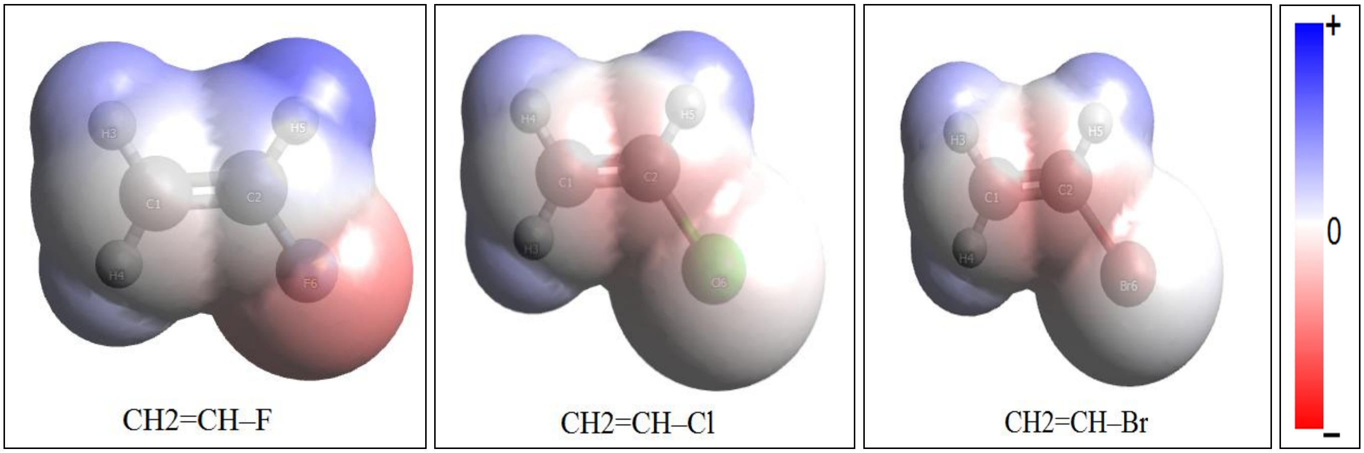

FIG. 3: MOLECULAR ELECTROSTATIC POTENTIAL SURFACES MEP FOR CH_2=CH–F, Cl AND Br

Vibrational Analysis: Due to the C-X stretching vibration, strong characteristic absorptions are observed. The position of the band is influenced by neighboring atoms or groups, the minor the halide atom, the more influence of the neighbor. Diverse rotational isomers might often be distinguished since, in general, the tran-form absorbs toward higher frequencies over the gauche-form. Bands of weak-to-medium intensity would also be watched because of the overtones of the C-X stretching vibration. In Raman spectra, the C-X stretching vibrations bring about vigorous bands for X=CI and Br, but for fluorine the bands are weaker, the intensity incrementing from F to Br. Mono haloalkanes (omitting fluorine as the atom may be excessively awful minute) often shows more than one C-X stretching band because of the distinctive could be allow the rotational isomeric configurations accessible. The population of a provided isomer is cleary, determined by energy considerations and this has a bearing on the observed intensity of the C-X stretching bands. In other words, the more stable the isomer, the more preponderant the intensity of the C-X stretching band connected to it.

Infra-red Spectra and Raman Spectra: On the recorded FT-IR and Raman spectra, these vibrational assignments have been utilized, based on the theoretically determined wave numbers by B3LYP with 6-311G* **Fig. 4** and **5**. All the calculated wavenumbers are positive, which means that the evident stability of the optimized structure.

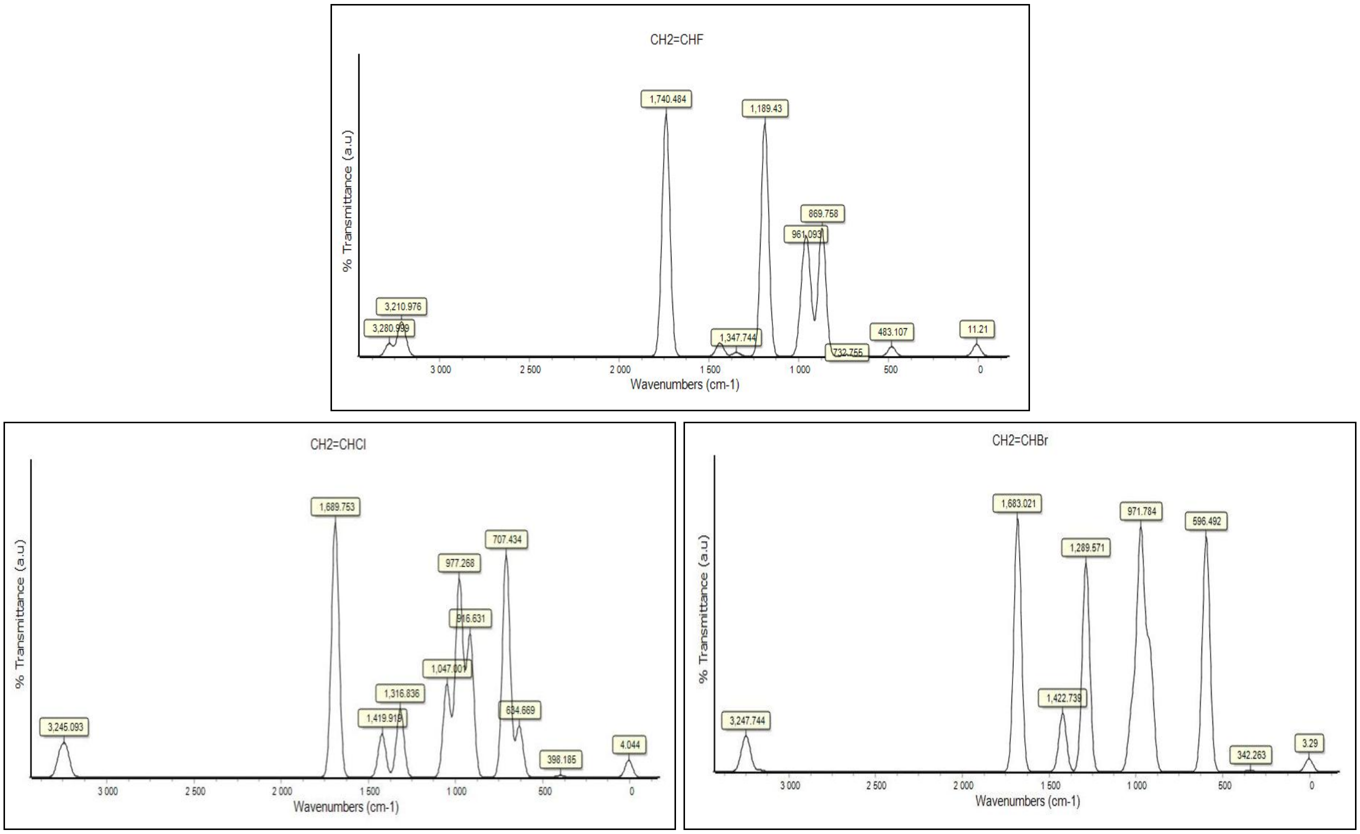

FIG. 4: INFRARED SPECTRA FOR CH_2=CHX (X = F, Cl, Br)

C-H Vibrations Raman: A fingerprint of vinyl halide molecules is the C-H stretching vibrations because its identification with peaks usually occurs in the region between 3100-2900 cm^{-1}. For vinyl fluoride, vinyl chloride, and vinyl bromide, the B3LYP/6-311G* method generated C-H stretching frequencies between 3189 and 3169 cm^{-1}, which matched the experimental values of (3180, 3172 and 3154 cm^{-1}) [25] respectively. The obtained values may have reasonably great concurrence for the experimental values.

C=C Vibrations IR: Vinyl halides exhibit bands at 1348 cm^{-1}, 1420 cm$^{-1,}$ and 1423 cm^{-1} in the theoretical FT-IR spectra for vinyl fluoride, vinyl chloride, and vinyl bromide respectively. A preponderance of these bands is of a sensibly great concurrence for the experimentally observed peaks of medium strength 1390 cm^{-1}, 1440 $cm^{-1,}$ and 1450 cm^{-1}. Shifting the C=C stretching vibration to higher frequencies is due to that the fluorine atoms directly attached to carbon double bonds.

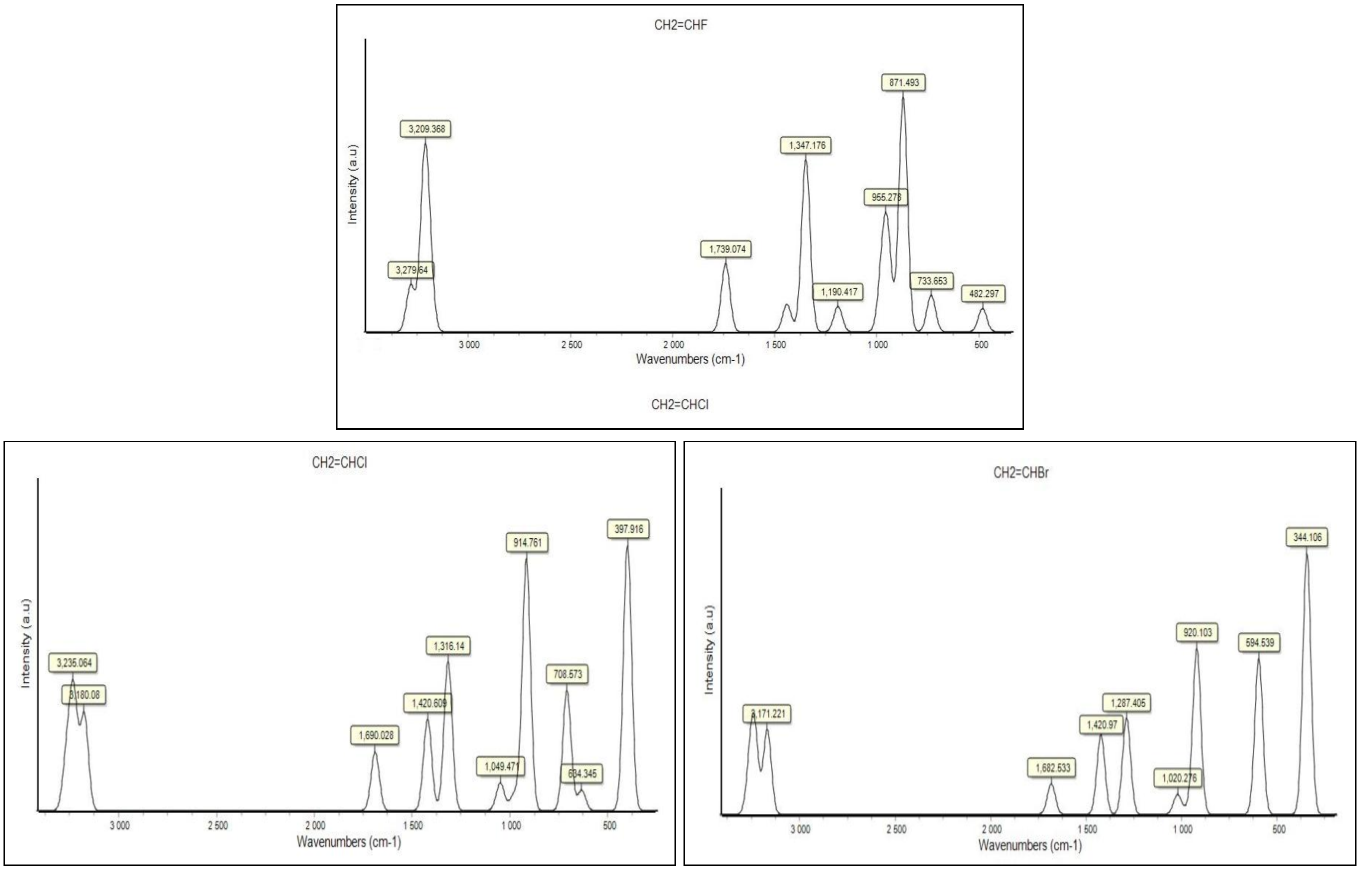

FIG. 5: RAMAN SPECTRA FOR CH_2=CHX (X = F, Cl, Br)

C-X Vibrations: The experimentally obtained C-X bands were located at 955 cm^{-1}, 715 $cm^{-1,}$ and 601 cm^{-1} while at the same time the hypothetical calculations predicted values of 949 cm^{-1}, 708 cm^{-1} and 596 cm^{-1} which were quite close for vinyl fluoride, vinyl chloride and vinyl bromide respectively. There were so numerous more that were forecast and detected in the experimental FT-IR spectra, in addition to this band. The vibration is easily influenced by adjacent atoms or groups, therefore the band due to the C-F stretching vibration may be found over a wide frequency range, 1360-1000 cm^{-1} [26-35]. The C-Cl stretching vibrations give generally strong bands in the region 760-505 cm^{-1} [36-43]. Due to the C-Br stretching vibrations, bromine compound is absorbed strongly in the region 650-485 cm^{-1}.

CONCLUSION: In the present work, the geometrical structure and Infra-red, Raman spectra of the molecules CH_2=CH–X (X=F and Cl) were carried out by using DFT investigation. From the determined data, the values of HOMO-LUMO gap (ΔE) are descending, starting from vinyl fluoride to vinyl chloride then vinyl bromide, while the bond length variations are ascending for the same previous order. We can conclude that vinyl fluoride is the hardest (more stable) while vinyl bromide is the softest (less stable). Frontier molecular orbital analysis shows that the charge transfer occurs from C_1=C_2 to C_2–H_5 bonds, $H_3C_1H_4$ group.

Also, the delocalization of electron charge density indicated by the atomic charges distribution and molecular electrostatic potential interpretation inferred that vinyl fluoride has a huge possibility for nucleophilic attack rather than vinyl chloride and vinyl bromide.

Remarkable good agreements were found between the experimental frequencies to those calculated. Also, the comparison between the three halides demonstrated that the C-X stretching vibrations result in strong bands for X=Cl and Br, but for fluorine the bands are weaker, the intensity increases from F to Br.

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CONFLICTS OF INTEREST: Nil

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