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Thermodynamic study of derivatives of PVC monomer with nanoparticles of fullerene, nanotube and nano cones at room temperature, using DFT method

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Abstract

In this study, the thermodynamic properties of polyvinyl chloride monomer derivatives, PVC with nanoparticles of fullerene, nanotubes and nano cones at room temperature, were studied by DFT method. For this purpose, the materials were first geometric optimized, then the thermodynamic parameters were calculated for all of them. Then, the process of changing the energy-dependent parameters such as specific heat capacity, enthalpy, entropy and Gibbs free energy relative to molecular mass, molecular volume and measured level in this study at a given temperature, were evaluated against each other.

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Keywords: PVC, carbon-containing fullerenes, density functional theory

1. Introduction

Polyvinyl chloride is formed by the polymerization of monomer vinyl chloride, and its commercial production is often by suspended polymerization, as well as less massive and emulsion polymerization and sometimes soluble polymerization. The polyvinyl chloride crystallinity is low but due to the high polymer volume chains resulting from the high chlorine dissolution, it has a lot of hardness and hardiness. Polyvinyl chloride or PVC is actually a very popular plastic and is considered to be the most valuable petrochemical

product. Usually most human PVC is used in building, because PVC is cheap and easily bonded. Recently PVC has been used in many areas instead of materials used in buildings such as wood, cement and pottery. Despite the advent of an ideal material for building, there is still concern about the cost of PVC for the natural environment and human health. (1-9).

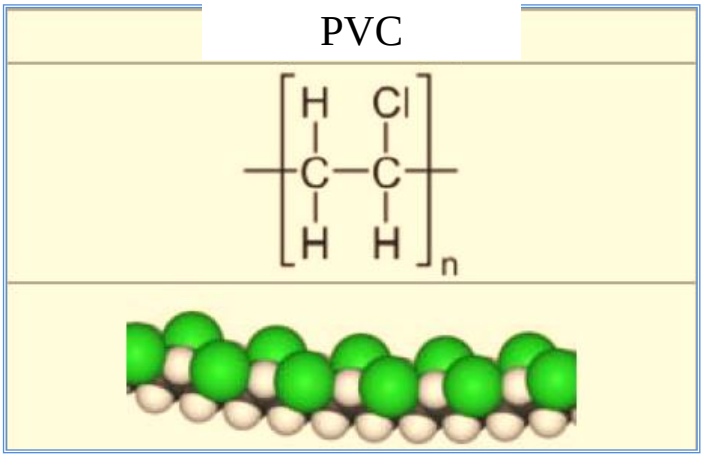

Fig 1 PVC Polyvinyl Chloride

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [10]. Geometries for all compounds are computed by means of the density functional theory (DFT) with Becke's three-parameter functional (B3) plus Lee, Yang, and Parr (LYP) correlation functional. For all atoms, the standard 6-31G basis set is utilized. The structures of PVC monomer with nanoparticles of fullerene, nanotube and nano cones were designed primarily using of Gauss View 5.0.8 and nanotube modeler 1.3.0.3 soft wares. The interaction **effects** of Fluoxetine on Fullerene were investigated [11-16].

3. Results

In this study, the substance of monomer vinyl chloride, or VC, and its derivatives with nanosized mass structures of fullerene, nanotubes and nano cones at room temperature, have been studied using density functional theory.

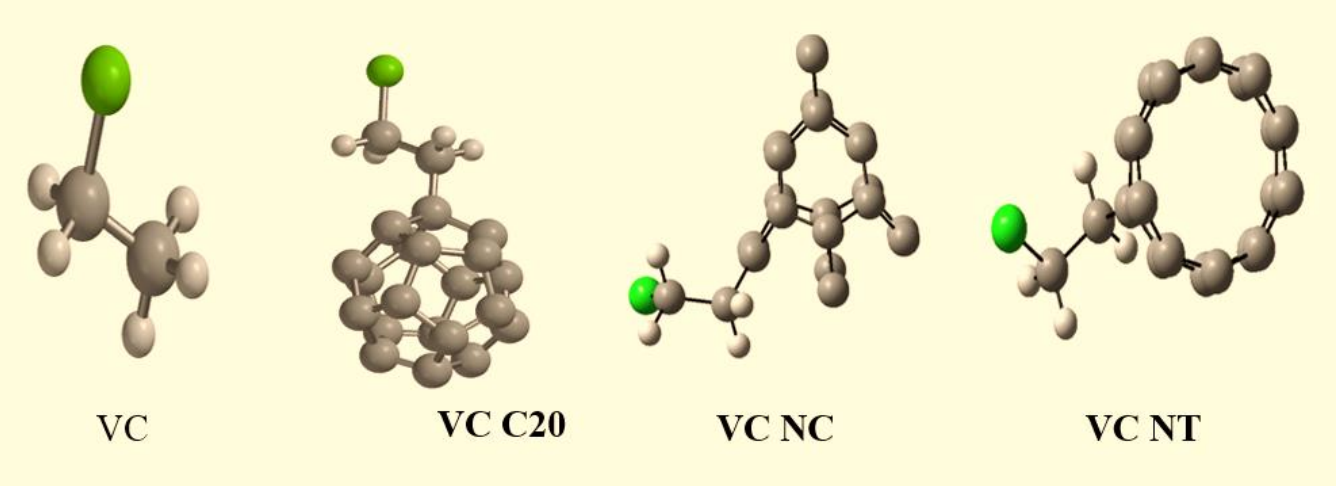

Fig 2 Vinyl chloride monomer or VC and its derivatives with nanoparticles of fullerene, nano tubes and nano cones at room temperature, by DFT method

Table 1. Some chemical properties calculated at B3lyp / 6-31g levels for monomer vinyl chloride or VC and its derivatives with nanoparticles of fullerene, nanotube and nano cones at room temperature, by DFT method

	Temperature=298.15K , pressure=1 atm			
	VC	VC C20	VC NT	VC NC
	C_2H_5Cl	$C_{22}H_4Cl$	$C_{22}H_4Cl$	$C_{22}H_4Cl$
ENERGY(au)	-532.304635	-1278.82223	-1277.43291	-1277.84827
E HOMO(eV)	-10.20	-10.54	-9.35	-9.65
E LUMO (eV)	10.32	-3.70	-5.01	-3.57
Dipole Moment (Debye)	2.41	5.73	4.72	4.55
Weight(amu)	64.515	303.727	303.727	303.727
Volume(A^3)	65.44	270.88	314.89	325.07
Area (A^2)	87.92	241.79	269.88	305.91
Polarizibility	41.91	61.73	65.89	66.31
ZPE (KJ/mol)	209.22	528.90	378.61	436.93
H° (au)	-532.220372	-1278.61048	-1277.27033	1277.66671
CV (J/mol)	44.24	186.18	325.88	270.97
S° (J/mol)	268.72	410.24	540.70	484.23
G° (au)	-532.250888	-1278.65707	-1277.33174	-1277.72170

Calculations and results:

Computational analysis of vinyl chloride monomer or VC and its derivatives with nanosized nanomaterials of fullerene, nanotubes and nano cones at room temperature was investigated using functional density theory. This operation was performed using Gaussian 98 and Gossive software. The compounds were initially optimized by density functional theory method in the

base series (6-31g). Then, IR studies were carried out to calculate the thermodynamic parameters related to the process. All calculations at the B3lyp / 6-31g level at 297 K and atmospheric pressure done . The results of the calculations showed that by increasing the volume and molecular level of the primary monomer, derivatives with different nanostructures with the same carbon content increase the specific heat capacity, and, of course, the internal energy also decreases (Fig. 3-5)

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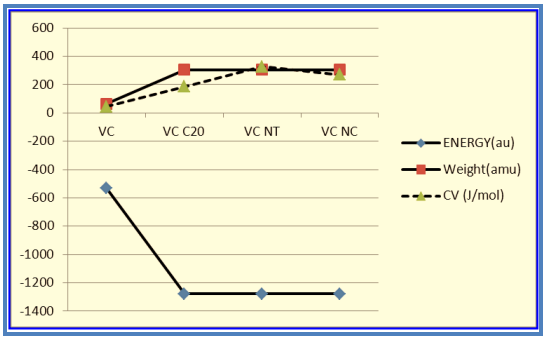

Fig 3. Comparison of the molecular mass, internal energy and specific heat capacity of the vinyl chloride monomer or VC and its derivatives with nanoparticles of fullerene, nanotubes and nano cones at room temperature, using the DFT method

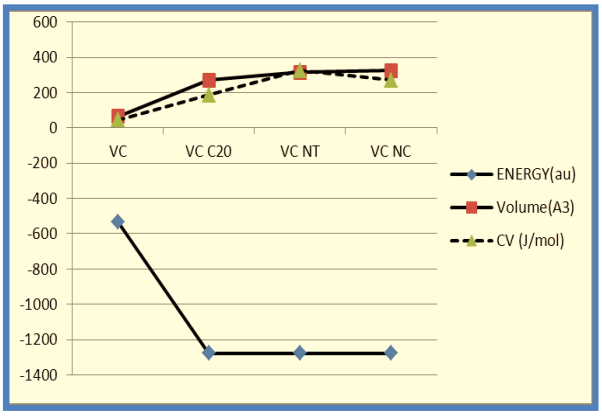

Fig 4. Comparison of molecular volume, internal energy and specific heat capacity of vinyl chloride monomer or VC and its derivatives with nanoparticles of fullerene, nanotubes and nano cones at room temperature, by DFT method

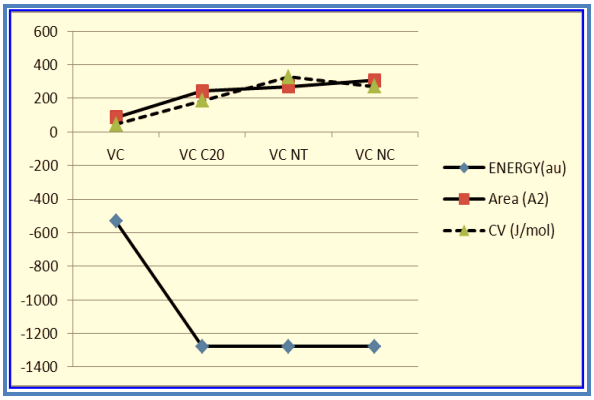

Fig 5. Comparison of molecular level, internal energy and specific heat capacity of vinyl chloride monomer or VC and its derivatives with nanoparticles of fullerene, nanotube and nano cones at room temperature, by DFT method

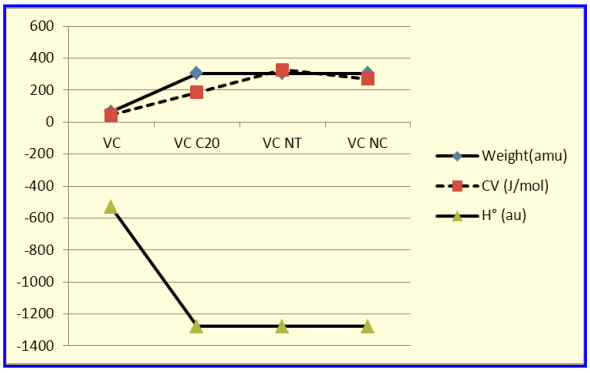

Fig. 6 Comparison of molecular enthalpy, molecular mass and specific heat capacity of vinyl chloride monomer or VC and its derivatives with nanoparticles of fullerene, nanotubes and nano cones at room temperature by DFT method

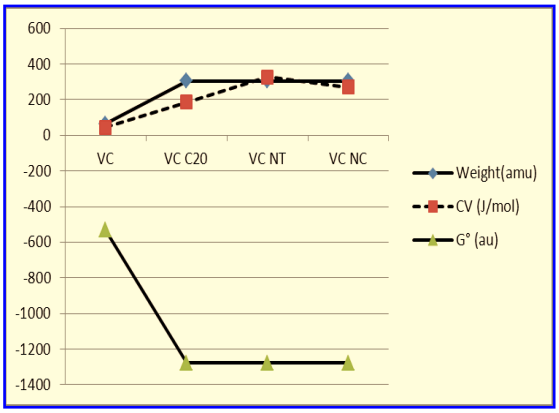

Fig. 7 Characteristic of the Gibbs Molybdenum Free Energy Relation, molecular mass and specific heat capacity of the vinyl chloride monomer or VC and its derivatives with nanomechanical structures of fullerene, nanotube and nano cones at room temperature, using DFT method

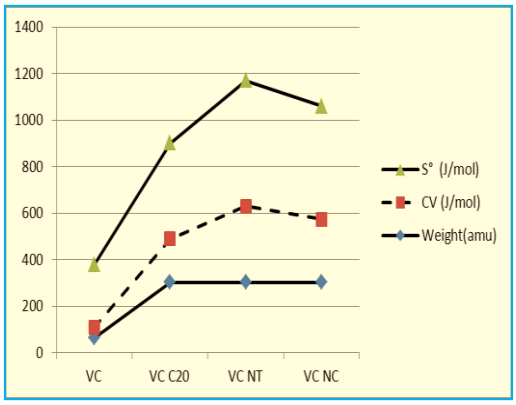

Fig 8: Comparison of molecular entropy, molecular mass and specific heat capacity of vinyl chloride monomer or VC and its derivatives with nanosized nanocrystals of fullerene, nanotubes and nano cones at room temperature by DFT method

Also, the results of the calculations showed that increasing the molecular mass from the initial monomer to its derivatives with similar carbon nanostructures increases the specific heat capacity, but with increasing

molecular mass, the molar enthalpy and the free energy of the molybdenum Gibbs decreases. (5-6). Also, the study of molar entropy showed that with increasing molecular mass, molecular volume and molecular surface from the primary monomer to its derivatives with similar carbon nanostructures increases (Fig. 7.)

3. Discussion and Conclusion

The results of the calculations show that vinyl chloride monomer or VC after adding the same carbon nanoparticles to that of the specific heat capacity of the derivatives due to increasing the volume and surface of the resulting molecule increases. On the other hand, various derivatives with increasing amounts Their specific heat capacity at different temperatures shows the following trend:

$$Cv_{VC\ NT} > Cv_{VC\ NC} > Cv_{VC\ C20} > Cv_{VC}$$

Since the number of carbon in the nanostructures used in this study is considered to be the same, the molecular mass of the resulting derivatives is equal, and according to the shape of each of the nanostructures, the volume and level of the molecules of the derivatives of the nanostructures are different. , On the other hand, changes in the volume of the molecules of derivatives of different nanostructures with the same carbon number as shown below:

$$V_{VC\ NC} > V_{VC\ NT} > V_{VC\ C20} > V_{VC}$$

Also, the comparison of the level of the molecules of various nanostructure derivatives with the number of carbon is similar to the following:

$$A_{VC\ NC} > A_{VC\ NT} > A_{VC\ C20} > A_{VC}$$

Comparison of the incremental trend of the specific heat capacity, the volume and surface of the molecules of the derivatives of different nanostructures with the same number of carbon and their coordination shows that under different conditions, with increasing, volume and level of the molecule, the specific heat capacity of the molecule is also increased. We know that the specific heat capacity of a CV is the amount of heat that is given to a mole of matter to rise to a temperature of one degree, it is evident that the more energy the material is, the less the specific heat of its CV. Therefore, it is concluded that the molecules of derivatives of different nanosized nanostructures with different carbon numbers of TEX explosives have molecular mass,

volume and surface area. The product is less energy efficient. Table 1. Comparison of the values of other thermodynamic parameters studied in this study confirms the results.

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