International Journal of New Chemistry, 2017, 4 (3), 86- 92.
.
Published online January 2017 in http://www.ijnc.ir/.
Original Article

Online ISSN 2383-188X
Open Access

Investigation of Thermochemistry of 3-Butadiene Monomeric Derivatives with Nanoparticles of Fullerenes, Nanotubes and Nano Cones at Room Temperature by DFT Method

***Duddukuru Kupta**

.Department of Chemistry, Sri Krishnadevaraya University, Anantapur 515003, Andhra Pradesh, India

Corresponding Author e-mail Address: D.kupta@gmail.com*

Received 10 September 2017; Accepted 28 October 2017; Published 2 November 2017

Abstract

Abstract

In this study, trans-3-butadiene monomer derivatives with different carbon nanoparticles of the same mass (mass mass) under different temperature conditions were studied using density functional theory. 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.

.

Keywords: Monomer, Trans-3, Butadiene, Nanoparticles of the same carbon, Fullerene, Functional density theory

1. Introduction

Polybutadiene is one of the first elastomers or tires that were invented. A high percentage of polybutadiene is used to make rubber and tire, and a smaller percentage of it is added as an additive to other tires to improve their mechanical strength. Polybutadiene is polymerized by three different methods, in which case three isomers of Cis, Trans, and Vinyl are obtained. The properties of polybutadiene vary depending on the percentage of these three isomers. For example: Polybutadiene with high isomeric cysts is called High Cis Polybutadiene and it has a high and very popular elasticity whereas polybutadienes with a high percentage of trans-isomer are called High Trans Polybutadiene and have crystalline and Without any useful use. The annual production of this polymer in 2001 was more than 2.1 million tons, which is ranked second in terms of the amount of consumption among tires after STR butadiene rubber (SBR) or (Styrene Butadiene Rubber). Due to the large use of cis type, in this study only the derivatives of this structure are investigated with nanosized nanostructures with the same carbon content of the fullerene type, nanotubes and nano cones. Other names of this structure are Cisco E4-PolyBotadan, DNA, Ameripol, Taktene, Europrene Cis and Buna CB [1-6].

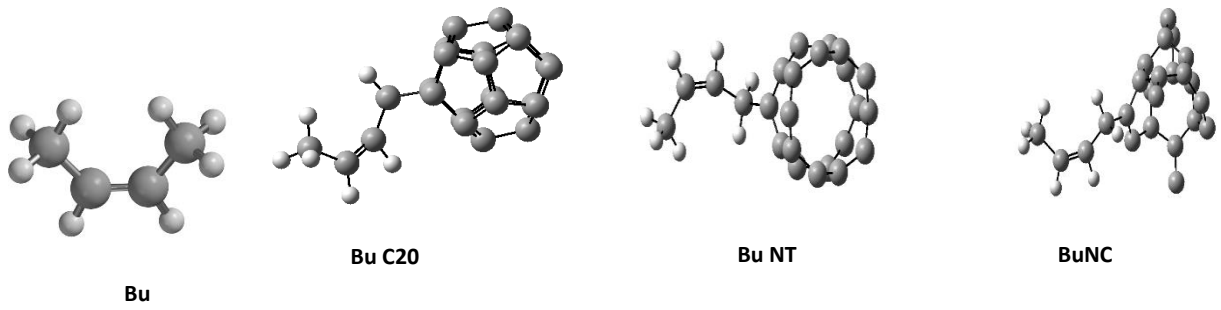

Fig 1. cis-butadiene monomer and its derivatives with fullerene carbon nanotubes, nanotubes and nano cones

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [7]. 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 its 3-Butadiene Monomeric Derivatives with Nanoparticles of Fullerenes, Nanotubes 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 [8-11] .

3. Results

The computational analysis of the monomer cis from its 4-butadiene-increasing additive reaction and its derivatives with fullerene carbon nanotubes, nanotubes and nano cones was studied using density functional theory. This operation was performed using Gaussian 98 and Gossive software. . The compounds were first optimized by density functional theory in the base series (6-31g). Then, IR studies were performed to calculate the thermodynamic parameters related to the process. All calculations were carried out at B3lyp / 6-31g, at a temperature of 297 ° K and a pressure of one The atmosphere has been done. The results of the calculations showed that by increasing the molecular volume and molecular surface in the hair of the nanomaterials that are masses, the increase in the reaction of cis-3-butadiene and its derivatives with fullerene carbon nanotubes, nanotubes and nano-cones of a special heat capacity increase and, of course, internal energy will also be reduced (Figure 2-4) [12-15].

Table 1. Some chemical properties calculated at B3lyp / 6-31g for monomeric cis-3-butadiene and its derivatives with fullerene carbon nanotubes, nanotubes and nano cones

	Temperature=298.15K , pressure=1 atm			
	Bu	Bu C20	Bu NT	BuNC
	C_4H_8	C24H7	C24H7	C24H7
ENERGY(au)	-154.240838	-900.769899	۳۴۹۳۵۵-899.	-899.245465
E HOMO(eV)	-7.79	-10.23	9.48-	-9.39

E LUMO (eV)	-8.76	-3.39	-3.75	-2.19
Dipole Moment (Debye)	0.13	2.27	4.12	2.38
Weight(amu)	56.108	295.320	295.320	295.320
Volume(A^3)	84.22	289.98	346.45	339.04
Area (A^2)	106.53	261.03	311.34	325.58
Polarizibility	44.34	63.28	68.12	67.18
ZPE (KJ/mol)	339.27	659.14	494.56	536.50
H° (au)	-154.106034	-900.507755	-899.141550	-899.022812
CV (J/mol)	63.88	204.73	350.97	328.04
S° (J/mol)	285.02	420.19	556.01	539.17
G° (au)	-154.138401	-900.555472	-899.204690	-899.084040

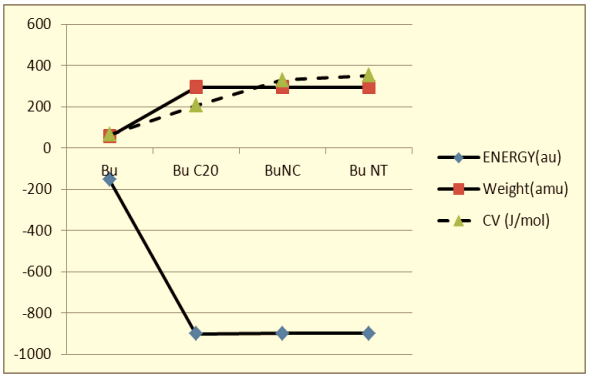

Fig 2 The comparison of molecular mass, internal energy and specific heat capacity of monomeric cysteine 3 butadiene and its derivatives with fullerene carbon nanotubes, nanotubes and nano cones

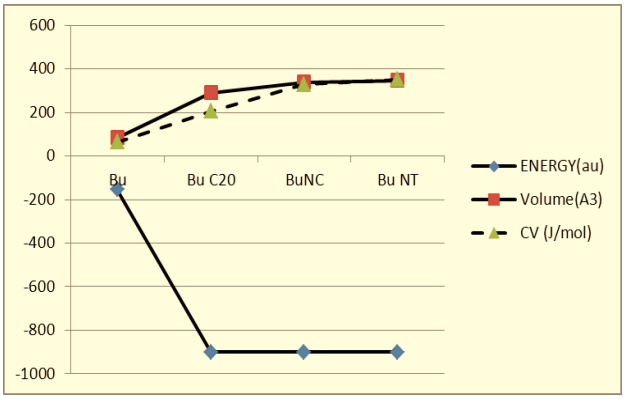

Figure 3: Comparison of molecular volume, internal energy and specific heat capacity of monomeric cis-3-butadiene and its derivatives with fullerene carbon nanotubes, nanotubes and nano cones

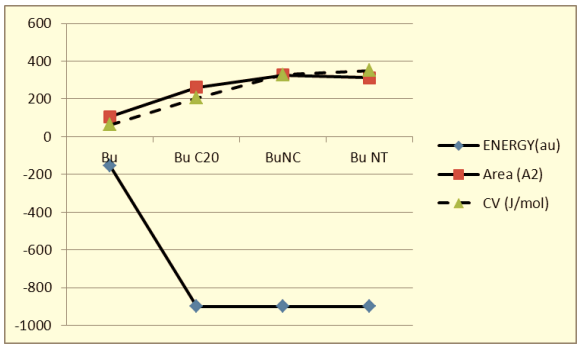

Fig 4: Comparison of molecular level, internal energy and specific heat capacity of monomeric cis-3-butadiene and its derivatives with fullerene carbon nanotubes, nanotubes and nano-cones

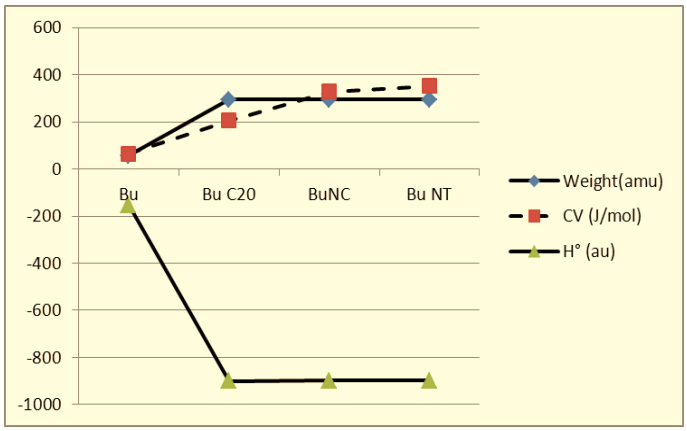

Fig. 5 Comparison of molecular enthalpy, molecular mass and specific heat capacity of monomeric cis-3-butadiene and its derivatives with fullerene carbon nanotubes, nanotubes and nano cones

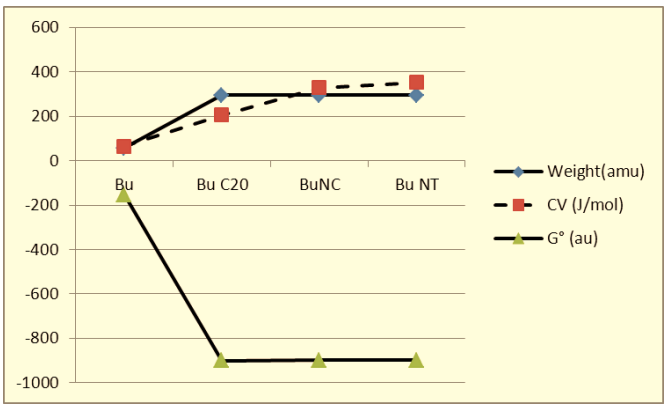

Fig. 6 Graph of Molybdenum Free Energy Gravity, Molecular Mass, and Special Heat Capacity of Monomeric System 3, Butadiene and its Derivatives with Nanostructures

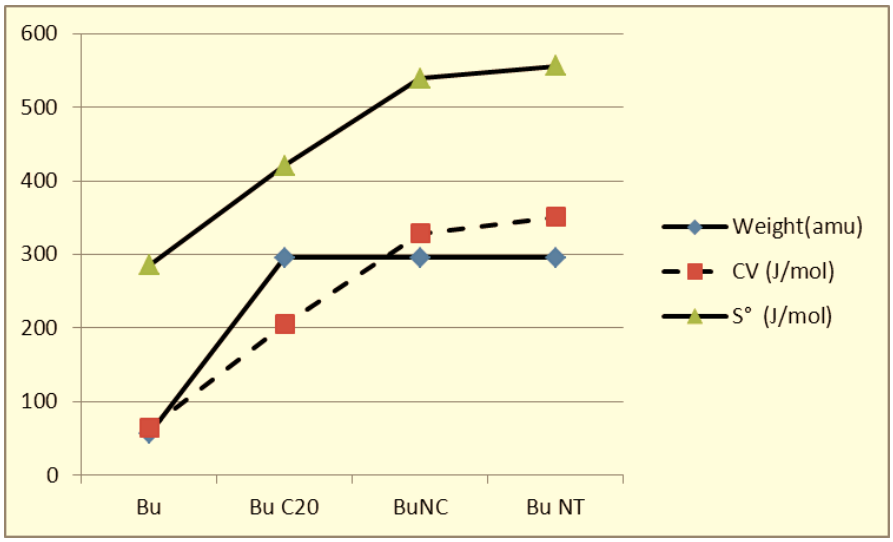

Fig. 7. Characteristic of the molecular entropy, molecular mass and specific heat capacity of monomer cis-3-butadiene and its derivatives with fullerene carbon nanotubes, nanotubes and nano cones

Also, the results of the calculations showed that by increasing the volume and molecular level, from its cis-3-butadiene monomer to its derivatives with fullerene carbon nanotubes, nano-tubes and nano-cones, the specific heat capacity increased, but with increasing molecular mass , The molten enthalpy and the free energy of the molybdenum Gibbs decreases (Fig. 5-6). Also, the study of molar entropy showed that with increasing molecular volume and the surface of the molecule, entropy also increases (Fig. 7)

4. Conclusion:

The results of the calculations show that its 3-butadiene monomer to its derivatives with fullerene carbon nanotubes, nano tubes, and nano cones increases the thermal capacity of the resulting derivatives. Since the number of carbon in the nanostructures of the case The use in this study is considered to be the same, so the molecular mass of the resulting derivatives is equal, and according to the shape of each of the nanostructures, the volume and surface of the molecules of the derivatives of the nanostructures are also different, on the one hand, changes in the volume and level of the derivatives molecules Different nanoscale structures with similar carbon numbers and capacity changes The following particular trend shows the following same.

Reference

[1] V. Iliev, D. Tomova, S. Rakovsky,*Desalination*, 26, 101 (2010).

[2] Y. Ma, J. Zhang, B. Tian, F. Chen, L.Wang, *J. Hazard. Mater.*, 182, 386 (2010).

[3] L. Zhang, F. Lv, W. Zhang, R. Li, H.Zhong, Y. Zhao, Y. Zhang, X. Wang, *J. Hazard. Mater.*, 171, 294 (2009) .

[4] Q. Shen, H. Yang, Q. Xu, Y. Zhu, R. Hao,*Mater. Lett.* ,64, 442 (2010) .

[5] M. Grätzel, *J. Photochem. Photobiol. C*,41, 45 (2003).

[6] S.E. Shaheen, C.J. Brabec, F. Padinger,T. Fromherz, J.C. Hummelen, N.S. Sariciftci,*Appl. Phys. Lett*., 78, 841 (2001) .

[7] F. Wang, S. Min, Y. Han, L. F eng,*Superlattice Microstruct*., 48, 170 (2010).

[8] Z. Zhang, Y. Yuan, L. Liang, Y. Cheng,H. Xu, G. Shi, L. Jin, *Thin Solid Films*, 516, 8663 (2008).

[9] J.C. Thiéblemont, A. Brun, J. Marty, M.F. Planche, *Polymer*, 361, 605 (1995).

[10] A. Alumaa, A. Hallik, V. Sammelselg, J.Tamm, *Synth. Met*., 157, 485 (2007) .

[11] D. Chowdhury, A. Paul, A. Chattopadhyay,*Langmuir* 214, 123 (2005) .

[12] K. Inumaru, M. Murashima, T. Kasahara,S. Yamanaka, *Appl. Catal. B*, 52, 275 (2004).

[13] B.D. Cullity, Elements of X-ray Diffraction, third ed., Addison- Wesley,Reading, MA, 102, 284 (1978).

[14] K. Nagaveni , G. Sivalingam , M.S. Hegde , Giridhar Madras, *Solar Applied Catalysis B Environmental*, 48, 83 (2004).

[15] B. Wang, Ch. Li, J. Pang, X. Qing, J.Zhai, Q. Li, *Applied Surface Science*, 258, 9989 (2012).