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A density functional theory study on the effect of size on the ionization potential of different carbon fullerenes

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ABSTRACT

Theoretical investigations were performed to study the structures and properties of different carbon nanoclusters. The computed properties were compared with those of the fullerene. The study systems included carbon fullerenes C_{20}, C_{26}, C_{28} and ionization potential of studied fullerenes are reported and compared to those of the fullerenes. It was found that the computed electronic properties are significantly influenced by the shape and size of different carbon nanoclusters.

1. Introduction

Fullerenes which can be regarded as one of the synthetic deformations of the carbon element are obtained from the heat of graphite.[1-3] Like many important scientific discoveries, buckyball was also accidentally discovered and created a major explosive crash in various sciences, especially chemistry.[4-6] The novelty and ideality of this newly discovered product has made scientists interested in many experiments on fullerenes. Different calculations, as well as laboratory experiments, bring fullerenes to the point where, in the near future, they will certainly be used in many sciences and fields including medicine.[7-10]

2. Results and discussion

The ion potential of the least energy is necessary to separate the far away electron. From the core this energy is related to loss of the most outer electrons. It is, therefore, evident that there is a direct relationship between the ionization potential and the orbital energy from which the electrons are detached. In addition, it depends on the energy of the cationic regeneration of the electrons resulting from the reduction of the coefficient coverage, the loss of an electron and the change in the interaction between the electrons. Besides, the second factor has a small effect on the ionization potential.

Therefore, knowing the orbital external energy of the electron can obtain an appropriate approximation of the ionization potential. The results of the calculations are presented in the **Table 1**. The maximum ionization potential is related to C_{30} with a value of 7.41ev, and the lowers ionization potential associated with C_{26} is to consider some of the reasons why C_{30} has the greatest potential for ionization, that in neutral mole C_{30} has the same dipole of 0/15D while with the loss of its same dipole electron, it changes to l.173D, and this mans fullerene C_{30}, by turning this electron into an asymmetric and unstable molecule (**Fig. 1**). In the case of C_{26}, the same dipole in neutral state, 0/29D, and in a positive state at one, it improves to 0/26, indicating that the molecule is symmetrical.

Table 1 Results of ionization potential.

Carbon nanoparticles	Neutral Fullerene energy	Fullerene energy 1^+	Energy difference	Ionization potential
C_{20}	-761/44	-761/200	0/239	6/64
C_{26}	-990/05	-989/8	0/232	6/33
C_{28}	-1066/33	-1066/02	0/267	7/27
C_{30}	-1142/55	-1142/27	0/272	7/41

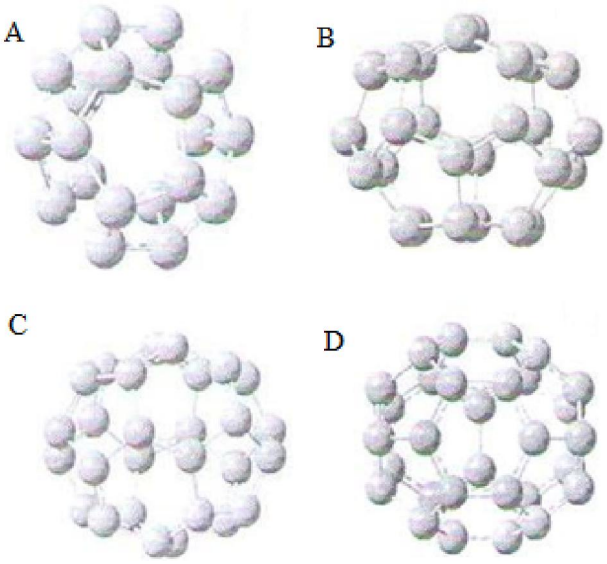

Fig 1. (a) C_{20}, (b) C_{26}, (c) C_{28}, (d) C_{30}.

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3. Conclusion

Our study shows the importance of the effect of the fullerene size on the ionization potential as it has obtained ionization energy by neutral and charged carbon fullerenes (20-30) systems. According to these calculations, with the increase in the size of fullerene, the potential of the juncture increases affecting the stability and symmetry of fullerene. In this sense, the factors depend on the torsion angle. In C_{30}, the ionization potential is 7.41ev, in comparison to other fullerenes, a lot of energy is needed to separate an electron from it so it has the most stability.

4. Materials and methods

In this paper, investigations were performed to study the density of citizenship on the effect of the size of the molecule on the potential of ionization of the fluorine 20-30 nanoparticles. All of the optimal–structures in this article have been evaluated by Gaussian software. Gaussian software is an efficient program for performing various calculations in a semi–experimental way. It's also possible to perform calculations both in the gas phase and in the soluble phase in the base or excited state. We have obtained from the energy outlet, the same bipolar, molecular loads and ionization potential, which gives us an overview of the molecular behavior that we will discuss below.

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