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An investigation using density functional theory into how various carbon fullerenes' ionization potentials change with size

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ABSTRACT

Through theoretical analyses, the structures and properties of many carbon nanoclusters were investigated. We compared the estimated fullerene properties to the actual ones. The ionization potentials of the carbon fullerenes C20, C26, and C28 that were evaluated in our study setups are presented and compared. It was found that the computed electrical properties were significantly impacted by the shape and size of the carbon nanoclusters.

Keywords: Fullerenes Ionization Ionization potential 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 [4-6]

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

Table 1 Results of ionization potential.

It improves to 0/26 in a positive state at one from 0/29D, proving that the molecule is symmetrical. deterioration in chemicals and associated disciplines. The distinctiveness and ideality of fullerenes have sparked the attention of scientists, leading to several inquiries into the substance. A number of calculations and lab studies have placed fullerenes in a position where they will almost certainly find uses in a wide variety of scientific and medical fields in the near future. eight to ten

2. Results and discussion

In order to free the farthest electron, the lowest energy ion potential is needed. The release of the outermost electrons is related to this energy, which comes from the core. It follows that the energy of the electron's detached orbit has a direct correlation with the ionization potential. Additionally, it is sensitive to the cationic regeneration energy of the electrons, which changes when their connection with one other changes, when their coefficient coverage decreases, or when an electron loses its charge. The ionization potential is little affected by the second component. So, knowing the electron's orbital external energy allows one to predict the ionization potential quite well. The calculated results are shown in Table 1. If you look at Fig. 1, you can see that C30 has a dipole of 0/15D in a neutral mole, but when an electron is lost, it changes to l.173D, creating fullerene C30. This makes the molecule very unstable and asymmetrical, which is why it has the highest potential for ionization. Contrast this with C26, whose ionization potential is 7.41 eV lower. Concerning C26, the neutral form of the same dipole,

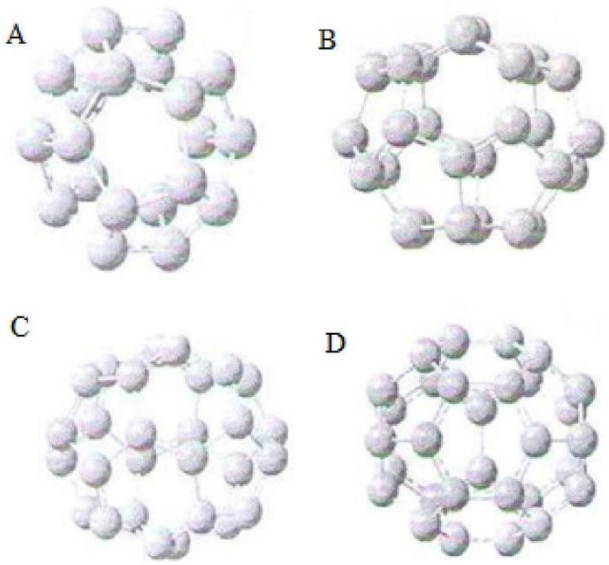

Fig 1. (a) C_{20}, (b) C_{26}, (c) C_{28}, (d) C_{30}.

Conclusion

Based on the ionization energy derived from neutral and charged carbon fullerenes (20-30) systems, our work demonstrates that the influence of fullerene size on the ionization potential is important. As the fullerene size rises, the calculations show that the junction potential increases as well, which impacts fullerene stability and symmetry. Here, the torsion angle determines the components. C30 is the most stable fullerene because its ionization potential is 7.41 eV, which is much higher than that of other fullerenes.

1. Materials and methods

The potential for ionization of fluorine 20-30 nanoparticles was investigated in this work by studying the impact of molecule size on citizenship density. This article presents only optimum structures that have been tested using Gaussian software. An effective program for doing a variety of computations in a semi-experimental fashion is Gaussian software. It's also feasible to conduct calculations in the excited or base state while in the soluble phase, as well as in the gas phase. We have successfully extracted the same bipolar molecular loads and isolating potential, which provides a synopsis of the molecular behavior that will be addressed later on.

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