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An analysis of the size dependence of the ionization potential of several carbon fullerenes using density functional theory

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ABSTRACT

A variety of carbon nanoclusters were studied in terms of their architectures and characteristics via theoretical examinations. The fullerene's characteristics were compared to the calculated ones. We present and compare the ionization potentials of the fullerenes that were tested, which comprised carbon fullerenes C20, C26, and C28, in our research systems. The calculated electrical characteristics were discovered to be strongly affected by the size and form 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

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.

decline in chemistry and other related fields. The freshness
Fullerenes have piqued the curiosity of scientists, who have conducted several research on the newly found substance because to its ideality. Thanks to several computations and laboratory investigations, fullerenes are already at a stage where they will almost surely find applications in numerous scientific and medical domains in the not-too-distant future. seven to ten

2. Results and discussion

To disentangle the distant electron, the ion potential with the lowest energy is required. This energy originates from the core and is associated with the expulsion of the outermost electrons. The ionization potential is directly proportional to the energy of the electron's detached orbit, as is thus clearly shown. Furthermore, it is dependent on the energy of the electrons' cationic regeneration as a consequence of a decrease in coefficient coverage, an electron's loss, or a change in their interaction with one another. The second component does affect the ionization potential, but only slightly. Thus, one may derive a good estimate of the ionization potential by knowing the electron's orbital external energy. You can see the computed results in Table 1. Consider some of the reasons why C30 has the greatest potential for ionization—in a neutral mole, it has a dipole of 0/15D, but when an electron is lost, it changes to 1.173D, resulting in fullerene C30—by transforming this electron into an asymmetric and unstable molecule (Fig. 1). This is in contrast to C26, which has a lower ionization potential of 7.41ev. When it comes to C26, the same dipole in its neutral form,

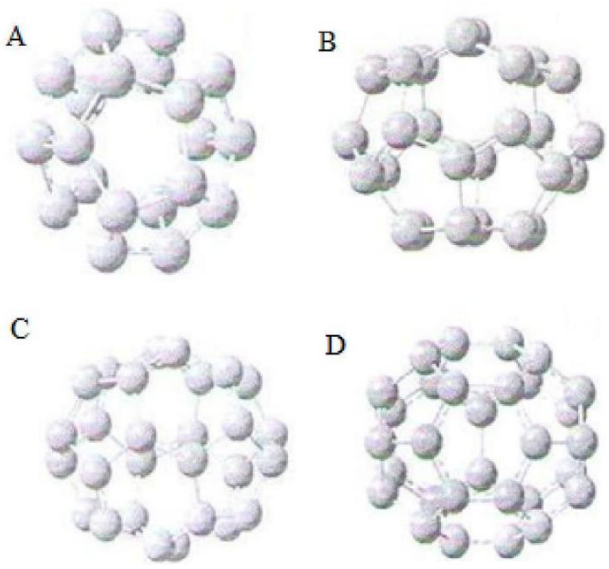

Fig 1. (a) C_{20}, (b) C_{26}, (c) C_{28}, (d) C_{30}.

3. 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.

4. 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 do computations 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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