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Computational Study on Molecular Structures of C20, C60, C240, C540, C960, C2160 and C3840 Fullerene Nano Molecules under Synchrotron Radiations Using Fuzzy Logic

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Introduction

The theory of fuzzy sets enables representation end processing of vague propositions and uncertain information. In contrast to the probability theory, fuzzy theory is a possibility approach. For instance, it is based on possibility theory. The concept of fuzzy sets extends this crisp assignment by allowing membership values between zero and one. These fuzzy sets are normalized to the interval (0, 1). Verbal fuzzy expressions are described by fuzzy theory and by means of linguistic variables. For example, the solubility of a substance in water can be characterized by the fuzzy terms "high" and "low", if the linguistic variables are further to be distinguished, so–called modifiers are applied. Fuzzy set operations are derived from classical soft theory. In addition, there exist theories for calculating with fuzzy numbers, functions, relations, measures or integrals. Furthermore, fuzzy theory can be used either for data analysis for dealing with fuzzy logic. In this editorial, typical applications in analytics are pattern recognition based on unsupervised and supervised learning, multicriteria optimization, comparisons of spectra, chromatograms or depth profiles on the basis of fuzzy functions, fuzzy modeling, fuzzy logic for fuzzy control and approximate reasoning was described for molecular structures of C20, C60, C240, C540, C960, C2160, and C3840 fullerene Nano molecules under synchrotron radiations.

On the other hand, in this editorial, C20, C60, C240, C540, C960, C2160, and C3840 fullerene Nano molecules were studied by means of their bond lengths, energies and molecular structures are optimized by performing HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP levels of theory using the standard 31G, 6–31G*, 6–31+G*, 6–31G(3df, 3pd), 6–311G, 6–311G* and 6–311+G* basis sets of the Gaussian 09 under synchrotron radiations. Moreover, calculations are carried out on the molecular structures of these fullerene Nano molecules using Hartree–Fock (HF) calculations and also Density Functional Theory (DFT) methods by performing HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP levels of theory using the standard 31G, 6–31G*, 6–31+G*, 6–31G(3df, 3pd), 6–311G, 6–311G* and 6–311+G* basis sets of the Gaussian 09 under synchrotron radiations. Besides in this method of investigation, bond lengths between five membered–six membered rings and also six membered–six membered rings, encapsulating energies and bond lengths in C20, C60, C240, C540, C960, C2160, and C3840 fullerene Nano molecules in free states are determined under synchrotron radiations.

Fullerene Nano molecules are characterized with presence of 12 five–membered rings and varying number of six–membered rings in their molecular structures [1–16]. Fullerene Nano molecules (Cn) with sizes n=3840, 3838, 3836,…, 24, 22, 20, have been observed in Buckminsterfullerenes (Buckyballs) collisions with fast highly charged atomic ions, electrons and laser pulses [17–21]. The knowledge of the molecular structure properties, binding energies, charge distribution and aromatic properties of these fullerenes Nano molecules are essential to understand the fragmentation trends and, in particular, why fullerene Nano molecules with a certain number of Carbon atoms appear more frequently than others. In present editorial, C20, C60, C240, C540, C960, C2160, and C3840 and their $C20^{+}$, $C20^{2+}$, $C20^{3+}$, $C20^{-}$, $C20^{2-}$, $C20^{3-}$, $C60^{+}$, $C60^{2+}$, $C60^{3+}$, $C60^{-}$, $C60^{2-}$, $C60^{3-}$, $C240^{+}$, $C240^{2+}$, $C240^{3+}$, $C240^{-}$, $C240^{2-}$, $C240^{3-}$, $C540^{+}$, $C540^{2+}$, $C540^{3+}$, $C540^{-}$, $C540^{2-}$, $C540^{3-}$, $C960^{+}$, $C960^{2+}$, $C960^{3+}$, $C960^{-}$, $C960^{2-}$, $C960^{3-}$, $C2160^{+}$, $C2160^{2+}$, $C2160^{3+}$, $C2160^{-}$, $C2160^{2-}$, $C2160^{3-}$, $C3840^{+}$, $C3840^{2+}$, $C3840^{3+}$, $C3840^{-}$, $C3840^{2-}$ and $C3840^{3-}$ charged forms have been considered for *ab initio* calculations under synchrotron radiations. The geometries of all neutral species considered in this editorial were fully optimized at HF/6–311+G*. Then, geometries were re–optimized in the frame work of the Density Functional Theory (DFT) under synchrotron radiations. For the charged species, geometry optimizations were performed at the B3LYP/6–311+G* basis sets. Two different spin multiplicities were considered in the case of charged species under synchrotron radiations. Nucleus–Independent Chemical Shifts (NICS) values were taken form GIAO–SCF/3–31G and GIAO–B3LYP/6–311+G* levels using optimized B3LYP/6–311+G* geometries. It should be noted that in these calculations, only closed–shell singlet states were considered under synchrotron radiations.

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