Novel structure of water-soluble C_{60} Synthesized by ozonization

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Discovery and mass production of C_{60}[1, 2] drew the attention of many scientists from various disciplines due to its unique structure and property. Utilizing the unique properties of C_{60}, research on the application of C_{60} in super conductor, sensor, solar cells, diode and so on is intensively carried out. In case of bio-applications, water-soluble fullerenes and endohedral fullerenes are expected to be an anti-HIV reagent, anti-cancer reagent, MRI imaging reagent, DNA cutter[3-5]. We have synthesized the water-soluble C_{60} using two oxidation processes. In the synthesis of water-soluble C_{60}, the starting materials are fullerene oxides, and derivatives obtained from the nucleophilic addition are available. The fullerene oxides have been synthesized by two kinds of oxidation processes. In the first method[6], fullerene is reacted with O_2 gas and UV irradiation. In the other method, fullerene is reacted with ozone gas. The water-soluble C_{60} are synthesized by boiling the obtained fullerene oxides in NaOH aqueous solution. When the products synthesized by the above two methods are compared, the yield of the product with ozone was about 80% and it is higher than that obtained from the other method. The solubility of fullerene obtained from the two methods is due to the bonding of a number of oxygen/hydroxyl to the surface of fullerene. The synthesized water-soluble C_{60} were analyzed by using mass analysis, FT-IR, UV-Vis, ^{13}C-NMR and ^{1}H-NMR. The structure of the water-soluble fullerene was considered as follows:

(1) The parts of 6-6 bonds of C_{60} are broken.
(2) The functional groups such as proton (-H) and hydroxyl (-OH) ion are attached to the carbon atom in C_{60}.
(3) The C_{60} derivatives have the composition of $C_{60}H_{2n}(OH)_{2n}$.

In the mass analysis, however, only the C_{60} peak was observed. Therefore, the determination of the number of functional groups in a fullerene is not possible. Here, we investigated a stable structure of water-soluble C_{60} using ab initio calculation to predict the orientation of the functional group. From the results of this calculation, the structure with hydroxyls attached to symmetrically opposite position was found to be the most stable. It is considered that each hydroxyl forms a hydrogen bond, and concurrently Coulomb force, Stereo force and three-dimensional factor closing fullerene cage equilibrate. The fullerene derivative with the above unique structure has not been reported yet. In this presentation, we report the detail of a novel structure of water-soluble C_{60}, and its reaction mechanism.

Acknowledgements
This work was supported by Grant-in-Aid for Basic Research #(S) 14103016, and #(S) 13852016 from the Ministry of Education, Science, Culture and Sport of Japan and #H14-nano-021 from the Ministry of Health, Labor and Welfare.

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