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**หมายเหตุ:**

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Theoretical Study on the Hole-Transport Property of Fullerene Hydrides C_{60}H_{2} and C_{60}H_{4}

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Abstract
Hole-transport property of C_{60}H_{2} [1] and C_{60}H_{4} [2] is discussed from the viewpoint of reorganization energy $\lambda$ and hole-transfer rate constant $k_{ht}$, comparing with that of C_{60}. All synthesized isomers [3] of C_{60}H_{2} and C_{60}H_{4} have better hole-transport property than C_{60}. It is also revealed that the hole-transport property is closely related to the delocalization of HOMO.

Introduction
Organic materials, which have lightness, flexibility, and are environmentally-friendly, are expected as essential parts of organic light-emitting devices (OLEDs) and organic field-effect transistors (OFETs). In these organic devices, hole mobility in the organic hole-transport material is one of the most important properties in the performance, therefore, the development of new material with good hole-transport property are matters of great urgency.

In the present study, we focus on the hole-transport property of fullerene hydrides C_{60}H_{2} [1] and C_{60}H_{4} [2], comparing with that of C_{60}. Hydrogenation has much influence on the hole-transport property of the C_{60} material because it removes electronic degeneracy of C_{60}⁺. Potential utility of C_{60}H_{2} and C_{60}H_{4} as hole-transport material is discussed from the viewpoint of reorganization energy $\lambda$ and hole-transfer rate constant $k_{ht}$.

Computational Method
In Marcus theory, $k_{ht}$ of a hole-transfer reaction between two equivalent molecules M(A) and M(B) is represented as

$$k_{ht} = \frac{4\pi^2}{h} \frac{H_{AB}^2}{\sqrt{4\pi \lambda k_B T}} e^{-\lambda/4k_B T}.$$

Thus, $k_{ht}$ is mainly dependent on $\lambda$ and the electronic coupling $H_{AB}$. Assuming that $H_{AB}$ is the same for all molecules, smaller $\lambda$ simply results in the larger $k_{ht}$. The calculation of $\lambda$ and $k_{ht}$ is performed by the density functional theory (B3LYP/6-311G(d)) using Gaussian 03.

Results and Discussions
For selected 11 isomers of C_{60}H_{2} and 9 isomers of C_{60}H_{4} shown in Fig. 1, $\lambda$ and $k_{ht}$ were calculated on the assumption that $H_{AB}$ is the same for all molecules.
(See Fig. 2). $C_{60}H_2$ isomers overall tend to have good hole-transport property than $C_{60}$. Synthesized isomers $[3] \ a$ and $2a$ of $C_{60}H_2$ have 20% smaller $\lambda$ than $C_{60}$, and $k_{ht}$ of these are about 1.5 times as large as that of $C_{60}$. Also, isomer $1$ of $C_{60}H_4$, which is the major product of the synthesis, has 50% smaller $\lambda$, and its $k_{ht}$ is about 3.3 times. These results indicate that some isomers of $C_{60}H_2$ and $C_{60}H_4$ have potential utility as hole-transport material.

Figure 3(a) shows HOMO of $C_{60}H_4$ isomer $1$ with the largest $k_{ht}$ and that of $2$ with the smallest $k_{ht}$. It is found that $1$ with more delocalized HOMO has larger $k_{ht}$ than $2$. This result coincides with the intuitive picture of the hole hopping illustrated in Fig. 3(b).

Conclusions We studied the hole-transport property of $C_{60}H_2$ and $C_{60}H_4$ in terms of $\lambda$ and $k_{ht}$. The major findings are as follows: i) the synthesized isomers of $C_{60}H_2$ and $C_{60}H_4$ have great potential as hole-transport material, ii) $\lambda$ and $k_{ht}$ are closely related to the delocalization of HOMO.

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