Synthesis of π-Extended Helicenes: Helically Twisted Wire Molecules with Large Effective Conjugation Length

NAKAKUKI, Yusuke[1], HIROSE Takashi[2], LI, Ruiji[1], MATSUDA, Kenji[1]

[1] *Grad. Sch. of Eng., Kyoto Univ. Katsura, Nishikyo-ku, Kyoto 615-8510, Japan*

[2] *ICR, Kyoto Univ. Gokasho, Uji, Kyoto 611−0011, Japan*

Email: nakakuki.yusuke.22n@st.kyoto-u.ac.jp

Helical graphenes are promising candidates for the nanometer-sized molecular inductors and molecular spring materials that respond to microscopic forces. However, because of the difficulties in synthesis, their properties remain unknown. In our previous work, we synthesized hexa-*peri*-hexabenzo[7]helicene (**2**),[1] which represents a primary substructure of the helical graphenes. In this work, we synthesized tetra-*peri*-tetrabenzo[5]helicene (**1**) and octa-*peri*-octabenzo[9]helicene (**3**). π-Extended helicenes **1**–**3** showed the lowest-energy absorption bands at 500−1100 nm. Isolated enantiomers of π-extended helicenes exhibited Cotton effects around their characteristic absorption bands with large dissymmetry factors of absorption (Figure 1). According to DFT calculations, the difference in g_{CD} of π-extended helicenes is likely attributed to the difference in $\theta_{\mu,m}$ values.

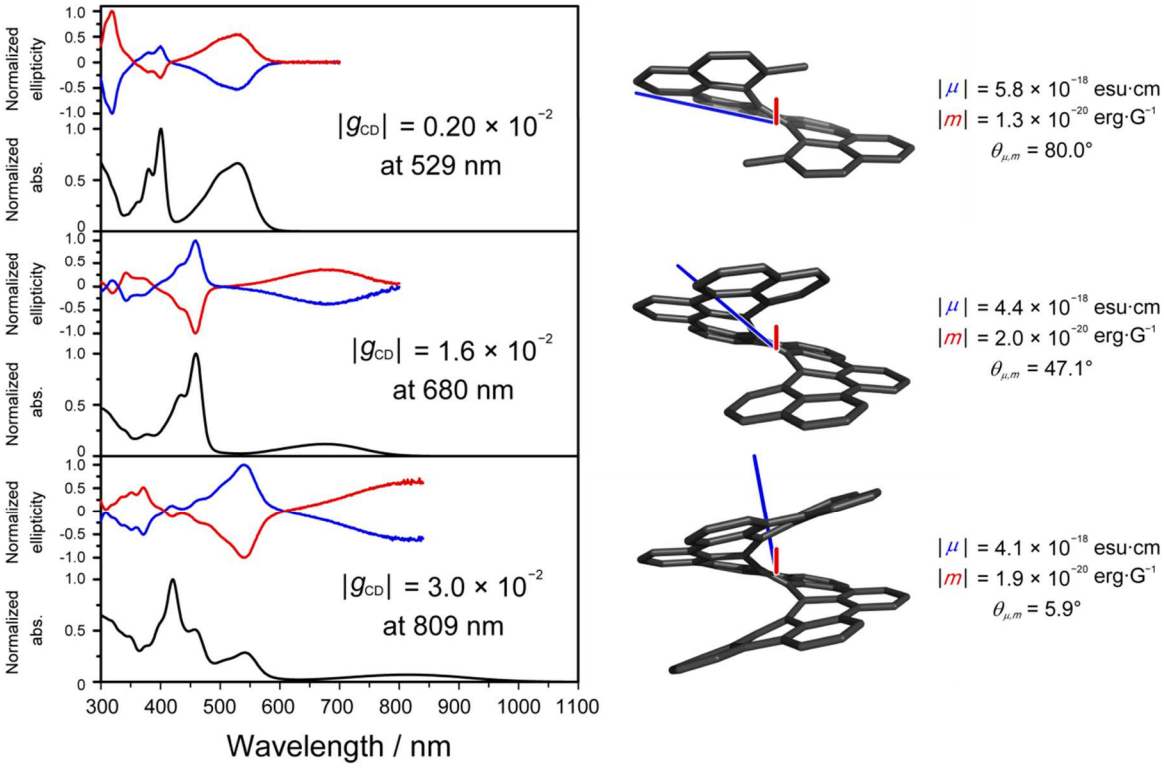

Figure 1. a) UV-vis-NIR absorption and circular dichroism spectra of π-extended helicenes in toluene at 25 °C for their (*P*)-isomer (red) and (*M*)-isomer (blue). (b) Transition dipole moments of π-extended helicenes for the $S_0 \rightarrow S_1$ transition. The directions of transition electric dipole moments (μ) and transition magnetic dipole moments (m) were shown in blue and red lines, respectively.

[1] Y. Nakakuki, T. Hirose, H. Sotome, H. Miyasaka, K. Matsuda, *J. Am. Chem. Soc*. **2018**, *140*, 4317.