Social Contribution from the Fundamental Research

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In recent years, the well-defined thiophene(Th)-based oligomers and polymers have been demonstrated and their electronic properties have been widely examined to develop the new organic materials such as opto-electronic devices and electric conductors. In relation with such intensive researches, dihexyl-2,2'-bithiophene (DHBTh) derivatives of the three types were designed and were synthesized to figure out their fundamental properties as the function unit in the materials, as follows.

1) the donor-acceptor DHBTh system
2) the DHBTh quinonone system
3) the highly extended DHBTh conjugation system with various pai-electronic components

Their structure-property relationships were studied, proving that orientations (head-to-head, head-to-tail, and tail-to-tail) of the DHBTh constituents in the systems regularly affected not only their chemical reactions but also their physicochemical behaviors such as electrochemical and opto-electronic properties. In particular, the tetracyanothienoquinonoid system, a good electron acceptor similar to tetracyanoquinodimethane (TCNQ), was found to show organic semi-conductive features depending on the orientation modes of DHBTh and to exhibit a highly self-assembling behavior as well. Furthermore, based on the structure-property relationships, the orientation effect of DHBTh in the extended conjugation systems was first tried to parameterize quantitatively, with which the transition energies of their electronic absorption maxima can be reproduced within errors of less than 0.4 kcal/mol.

From the viewpoint of fundamental researches and applicable devices, several recent topics of the DHBTh derivatives will be presented.