Development of Novel Heterocyclic Compounds and Their Molecular Assemblies for Advanced Materials

Safety Office

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Heterocycles containing sulfur and/or nitrogen atoms are useful as components of functional organic materials since heteroatoms in their rings are helpful to stabilize ions or ion-radical species. In addition, intermolecular interactions caused by heteroatom contacts can be expected to form unique molecular assemblies. In this project, novel functional organic materials based on various heterocycles were synthesized and their physical and structural properties were investigated.

1. X-Ray Crystallographic Analyses of Heterocyclic and Aromatic Compounds

The X-ray crystallographic analyses of five heterocyclic and aromatic compounds have revealed their interesting structural natures and unique molecular aggregations. A large number of short intermolecular S···S and S···N contacts are observed in the crystal structures of [1,3]dithiolo[4,5-*c*][1,2,5]thiadiazole-5-thione, 2-thioxo-[1,3]dithiolo[4,5-*b*]pyrazine-5,6-dicarbonitrile and dimethyl 2-([1,3]dithiolo[4,5-*c*][1,2,5]thiadiazol-5-ylidene)-1,3-dithiole-4,5-dicarboxylate. In the bis(tetra-*n*-butylammonium) bis(5,6-dicyanopyrazine-2,3-dithiolato-κ^2S,S')nickel(II) complex, the centrosymmetric dianion is planar, with an r.m.s. deviation of 0.031(1) Å. We have also found a novel hydrate isomer of cyananilic acid, dihydrate derivative. The cyananilate dianion molecule is planar with an r.m.s. deviation of 0.011(2) Å and is located on an inversion center. The cyananilate molecules are linked via the oxonium ions with intermolecular O–H···O and O–H···N interactions.

Multifunction Integrated Macromolecules for Molecular-Scale Electronics

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Recently a single electron tunnel device (**SET**) has attracted much attention as an ultra-low-power device. In this project, to establish an innovative fabrication process for **SET** systems, we have been developing step-wise synthetic protocols for mono-molecular single-electron tunnel devices and their integrated circuits (**MOSET IC**).

1. Synthesis of 10 nm-Long Molecular Linkers for Supramolecular Architecture

We have already established the synthetic process for a series of "single-nanometer scale" devices. In the current study, we have synthesized long molecular linkers for supramolecular approaches, which are one of the key parts for the integration of nanosize devices to "deca~hecto-nanometer scale" electronic circuits. Figure 1 shows the examples.

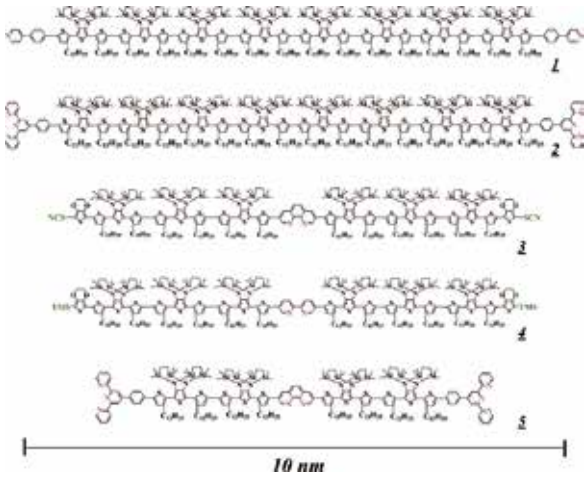

Figure 1. Examples of long molecular linkers with coordination sites.