

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

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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. Molecular and Crystal Structure of Cyananilic Acid Dihydrate

Cyananilic acid shows both electron accepting and proton

donating properties. Supramolecular synthons formed with cyananilic acid have been used for constructing a variety of molecular networks. A molecular and crystal structure of cyananilic acid was reported as its hexahydrate derivative in 1975.¹⁾ We have found a novel hydrate isomer of cyananilic acid, dihydrate derivative. Cyananilic acid dihydrate crystallizes in the triclinic $P\bar{1}$ space group with one molecule in the unit cell. Cell parameters are $a = 4.940(6)$ Å, $b = 7.064(8)$ Å, $c = 7.404(8)$ Å, $\alpha = 109.20(2)^\circ$, $\beta = 94.73(1)^\circ$, $\gamma = 102.27(1)^\circ$ and $V = 235.2(5)$ Å³. 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.

Reference

1) E. K. Anderson and I. G. K. Anderson, *Acta Crystallogr., Sect. B* **31**, 379–383 (1975).

Multifunction Integrated Macromolecules for Molecular-Scale Electronics

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

different reactivity for metal-catalyzed coupling reactions. Thus, a selective and stepwise cross coupling will lead to more complicated macromolecular systems. Now we have been developing the synthetic protocols for mono-molecular integrated circuits such as single electron memory and counter, using these building blocks **1-16** (Figure 1(b)).

1. Upgrade of Building Blocks toward Higher Integration of Single-Electron Tunnel Devices

We have developed a generally applicable stepwise synthetic protocol for basic mono-molecular single-electron tunnel devices starting with our versatile building blocks (**1-4**) (Figure 1(a-b)). In order to advance to the next stage of nanofabrication, we have prepared a new set of molecular building blocks (**5-16**) in view of recent progress in cross coupling reactions of C–Cl and C–H bonds of heterocycles. The end points of these molecular blocks have significantly

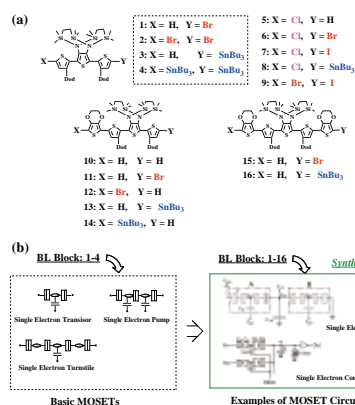


Figure 1. (a) Molecular structure of building blocks. (b) A strategy for mono-molecular MOSETs integration.