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

Safety Office



TOMURA, Masaaki

Assistant Professor

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 ionradical 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. Construction of Molecular Networks Using Chloranilic Acid¹⁾

In the crystal structure of 4-cyanopyridinium hydrogen chloranilate, the centrosymmetric dimmers with $O-H\cdots O$ hydrogen bonds are linked by intermolecular $N-H\cdots O$ and $N\cdots Cl$ interactions to construct a two-dimensional large square grid molecular network (Figure 1).

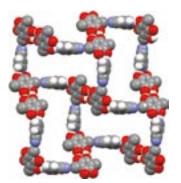
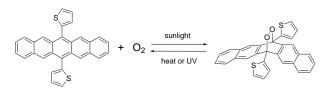


Figure 1. A two-dimensional large square grid molecular network.

2. Photooxidation and Reproduction of Pentacene Derivatives Substituted by Aromatic Groups²⁾

Pentacene derivatives substituted by aromatic groups at the

6,13-positions were prepared and investigated for their electronic properties and the photooxidation–deoxygenation.



3. X-Ray Crystallographic Analyses of Heterocyclic and Aromatic Compounds^{3–9)}

The X-ray crystallographic analyses of seven heterocyclic and aromatic compounds have revealed their interesting structural natures and unique molecular aggregations.

References

- 1) M. Tomura and Y. Yamashita, Anal. Sci. 24, x31-x32 (2008).
- 2) K. Ono, H. Totani, T. Hiei, A. Yoshino, K. Saito, K. Eguchi, M. Tomura, J. Nishida and Y. Yamashita, *Tetrahedron* 63, 9699–9704 (2007).
- 3) M. Tomura, K. Ono, M. Kaiden, K. Tsukamoto and K. Saito, *Acta Crystallogr., Sect. E* 63, 04568–04569 (2007).
- 4) K. Ono, M. Tomura and K. Saito, Acta Crystallogr., Sect. E 63, 04612–04612 (2007).
- 5) M. Tomura, Acta Crystallogr., Sect. E 64, 0170-0171 (2008).
- M. Tomura, H. Yamaguchi, K. Ono, M. Kaiden and K. Saito, Acta Crystallogr, Sect. E 64, 0172–0173 (2008).
- 7) K. Ono, M. Tomura and K. Saito, Acta Crystallogr., Sect. E 64, 0468–0468 (2008).
- M. Tomura and Y. Yamashita, Acta Crystallogr, Sect. E 64, 0545– 0545 (2008).
- K. Ono, K. Tsukamoto, M. Tomura and K. Saito, *Acta Crystallogr.*, Sect. E 64, 01069–01069 (2008).