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. A Two-Dimensional Ladder-Type Network in the 2:1 Co-Crystal of 1,2,5-Thiadiazole-3,4-dicarboxylic Acid and 4,4'-Bipyridine[1)]

The crystal structure of the 2:1 co-crystal of 1,2,5-thiadiazole-3,4-dicarboxylic acid and 4,4'-bipyridine has been determined by X-ray diffraction. Two intramolecular O–H···N [2.730(7) Å] and O–H···O [2.433(6) Å] hydrogen bonds are observed in the thiadiazole molecule. In the crystal structure, the molecules form a unique two-dimensional ladder-type network linked by intermolecular O–H···N [2.704(4) Å] hydrogen bonds and S···O [3.100(5) Å] heteroatom interactions.

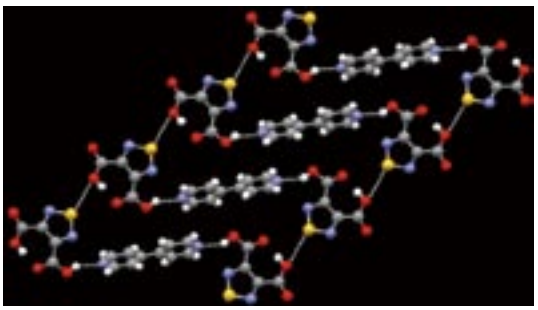
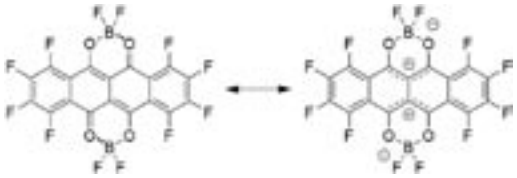


Figure 1. A unique two-dimensional ladder-type network.

2. A BF_2 Complex of a Dihydroxydione with a Perfluorotetracene Skeleton[2)]

A BF_2 complex containing an octafluorotetracene moiety was synthesized as a new type of electron acceptor. This compound exhibits a long-wavelength absorption based on the perfluorotetracene skeleton and high electron affinity due to its quadrupolar structure enhanced by fluorination. The BF_2 complex exhibited n-type semiconducting behavior.



3. Photovoltaic Properties of (*E*)-2-Cyano-3-[4-(diphenylamino)phenyl]acrylic Acid Substituted by *tert*-Butyl Groups[3)]

The title dye and its related compounds were synthesized. The *tert*-butyl substituents decreased molecular stacking in the crystals, thus affecting the photovoltaic properties of the dyes. A solar cell using the dye exhibited higher performance than that for the analog without *tert*-butyl group substitution.

References

1) M. Tomura and Y. Yamashita, *Struct. Chem.* **21**, 107–111 (2010).
2) K. Ono, J. Hashizume, H. Yamaguchi, M. Tomura, J. Nishida and Y. Yamashita, *Org. Lett.* **11**, 4326–4329 (2009).
3) K. Ono, T. Yamaguchi and M. Tomura, *Chem. Lett.* **39**, 864–866 (2010).