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

Heterocycles containing sulfur and/or nitrogen atoms are useful as components of functional materials since heteroatoms in their rings are helpful to stabilize ions or ion-radical species, and extended π-conjugation decreases Coulombic repulsion. In addition intermolecular interactions caused by heteroatom contacts can be expected to form novel molecular assemblies. In this project new electron acceptors, donors, and donor-acceptor compounds based on heterocycles such as 1,2,5-thiadiazole and 1,3-dithiole were synthesized and their properties including those of the charge-transfer complexes or ion-radical salts were investigated. Unique crystal structures were constructed by using weak intermolecular interactions such as hydrogen bonding or heteroatom contacts.

IX-Z-1 Molecular Arrangement in the Cocrystals of 1,1’,3,3’-Tetramethyl-2,2’-bi-1H-imidazolium Bis(tetraphenylborate) with Ketone, Aldehyde, and Nitrile as Guest Molecules

ONO, Katsuhiko¹; IWAO, Takeshi¹; UCHIUMI, Hideki¹; SUZUKI, Takahisa¹; TOMURA, Masaaki; OHKITA, Masakazu¹; SAITO, Katsuhiro¹

¹Nagoya Inst. Tech.)

[1,1’,3,3’-Tetramethyl-2,2’-bi-1H-imidazolium bis(tetraphenylborate), an ion-association compound, afforded inclusion crystals with a variety of guest molecules, such as ketone, aldehyde, and nitrile. X-ray crystallographic analyses revealed intermolecular interactions between the biimidazolium dication and the guest molecules in the inclusion crystals. Their contact modes depended on the molecular structures of the guest molecules, resulting in various molecular arrangements.]

IX-Z-2 Macro cyclic and Acyclic Bis(2,5-diphenyl-1,3,4-oxadiazole)s with Electron-Transporting and Hole-Blocking Ability in Organic Electroluminescent Devices

ONO, Katsuhiko¹; EZAKA, Seichi¹; HIGASHIBATA, Akinori¹; HOSOKAWA, Ryohei¹; OHKITA, Masakazu¹; SAITO, Katsuhiro¹; SUTO, Michitaka²; TOMURA, Masaaki; MATSUSHITA, Yosuke³; NAKA, Shigeki³; OKADA, Hiroyuki³; ONNAGAWA, Hiroyoshi³

¹Nagoya Inst. Tech.; ²Dow Corning Asia Ltd.; ³Toyama Univ.)

[1,1’,3,3’-Tetramethyl-2,2’-bi-1H-imidazolium bis(tetraphenylborate), an ion-association compound, afforded inclusion crystals with a variety of guest molecules, such as ketone, aldehyde, and nitrile. X-ray crystallographic analyses revealed intermolecular interactions between the biimidazolium dication and the guest molecules in the inclusion crystals. Their contact modes depended on the molecular structures of the guest molecules, resulting in various molecular arrangements.]

IX-Z-3 Synthesis, Characterization and FET Properties of Novel Dithiazolylbenzothiadiazole Derivatives

AKHTARUZZAMAN, Md.¹; KAMATA, Naoto¹; NISHIDA, Jun-ichi¹; ANDO, Shinji¹; TADA, Hirokazu²; TOMURA, Masaaki; YAMASHITA, Yoshio³

¹Tokyo Inst. Tech.; ²IMS and Osaka Univ.; ³IMS and Tokyo Inst. Tech.)

[Novel dithiazolylbenzothiadiazole derivatives easily obtained show efficient fluorescence with high electron affinity. The FET device of a trifluoromethylphenyl derivative exhibited a good n-type performance with high electron mobility. Since substituents can be easily introduced to the α-position of thiazole, the dithiazolyl-benzothiadiazole unit would be useful as a core for unique electron-accepting π-conjugated molecules.]

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

Heterocycles containing sulfur and/or nitrogen atoms are useful as components of functional materials since heteroatoms in their rings are helpful to stabilize ions or ion-radical species, and extended π-conjugation decreases Coulombic repulsion. In addition intermolecular interactions caused by heteroatom contacts can be expected to form novel molecular assemblies. In this project new electron acceptors, donors, and donor-acceptor compounds based on heterocycles such as 1,2,5-thiadiazole and 1,3-dithiole were synthesized and their properties including those of the charge-transfer complexes or ion-radical salts were investigated. Unique crystal structures were constructed by using weak intermolecular interactions such as hydrogen bonding or heteroatom contacts.