Safety Office

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-1*H*-imidazolium Bis(tetraphenylborate) with Ketone, Aldehyde, and Nitrile as Guest Molecules

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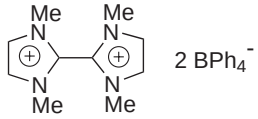
1,1',3,3'-Tetramethyl-2,2'-bi-1*H*-imidazolium bis(tetraphenylborate), an ion-association compound, afforded inclusion crystals with a variety of guest molecules, such as ketone, aldehyde, and nitrile. X-ray crystallographic analyses revealed intermolecular interactions between the biimidazolium dication 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 Macrocyclic and Acyclic Bis(2,5-diphenyl-1,3,4-oxadiazole)s with Electron-Transporting and Hole-Blocking Ability in Organic Electroluminescent Devices

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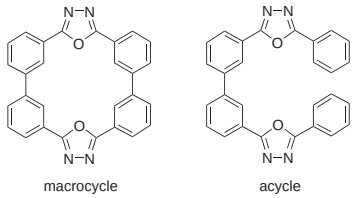
[*Macromol. Chem. Phys.* **206**, 1576–1582 (2005)]

Two types of bis(2,5-diphenyl-1,3,4-oxadiazole)s, macrocyclic and acyclic, were prepared and evaluated as electron-transporting and hole-blocking materials in phosphorescent EL devices. Maximum efficiencies of η_{ext} = 10.4% at J = 0.11 mA·cm^{-2} for the macrocycle and η_{ext} = 14.1% at J = 3.01 mA·cm^{-2} for the acycle were observed. X-ray crystallographic analysis and DSC measurements revealed a strong intermolecular interaction between the macrocycles and weaker intermolecular interactions between the acycles. The EL characteristics depend on the intermolecular interactions.



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

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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 dithiazolylbenzothiadiazole unit would be useful as a core for unique electron-accepting π-conjugated molecules.