

Safety Office

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

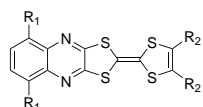
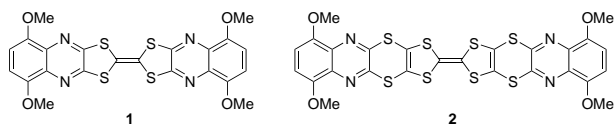
Heterocycles containing sulfur and/or nitrogen atoms are useful as components of functional materials since heteroatoms in their rings are helpful to stabilize ions or ion-radical species, and extended π -conjugation decreases Coulombic repulsion. In addition intermolecular interactions caused by heteroatom 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-U-1 TTF Derivatives Containing Fused-Pyrazine Rings for Novel Donor-Acceptor Systems

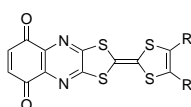
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In this work, novel π -extended tetrathiafulvalen (TTF) derivatives **1-10** fused with electron-accepting pyrazine rings are described. We have succeeded in preparing two kinds of TTF derivatives **1** and **2** containing two pyrazine rings. Furthermore, we have prepared asymmetrical TTF derivatives **3-6** containing one pyrazine ring to increase the electron-donating properties. In some cases, hydroxyl groups were introduced to intermolecular hydrogen bonds. Oxidation of hydroquinone derivatives afforded a new type of donor-acceptor compounds **7-10** with quinone units, which showed both oxidation and reduction potentials. The electrical conductivity of the donor-acceptor compound was about 10^{-8} S/cm as single component. We have also prepared several CT complexes based on the new TTF derivatives and investigated the structures and properties.



- 3:** R₁ = OMe; R₂ = SMe
4: R₁ = OMe; R₂, R₂ = SCH₂CH₂S
5: R₁ = OH; R₂ = SMe
6: R₁ = OH; R₂, R₂ = SCH₂CH₂S



- 7:** R = SMe
8: R = SC₆H₁₃
9: R = SC₁₀H₂₁
10: R, R = SCH₂CH₂S