Preparation and properties of substituted acenes for organic electronics: pentacene through heptacene

JOHN ANTHONY, Univ. of Kentucky, Dept. of Chemistry — Acenes (such as pentacene and tetracene) and functionalized acenes (such as rubrene) have demonstrated remarkable electronic properties in thin film devices and in single crystals. Our research effort is directed toward the synthesis of new classes of acene-based compounds that are stable, soluble, and that can be used to probe the relationships between solid-state order and electronic properties. Careful consideration of the relationship between molecular substituent and crystal packing has led to the development of new, soluble materials with thin-film properties comparable to their unfunctionalized counterparts. Functionalization of the central ring of pentacene can lead to a change in solid-state order from the classic herringbone arrangement to the less-common face-to-face interactions, while functionalization of the outermost rings of pentacene leads to subtle variations in the herringbone arrangement. Similar approaches can be taken with heteroacenes, again leading to solid-state interactions that favor strong interactions between the aromatic pi-clouds. Furthermore, the added stability gained through functionalization has allowed for the first time the preparation and study of derivatives of higher acenes such as hexacene and heptacene. The detailed study of the optical and electronic properties of a variety of functionalized acenes has led to the development of new materials for use in photovoltaics, light-emitting diodes and thin-film transistors. We are grateful to the Office of Naval Research for support of this research.

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