Push-pull chromophores with different heterocyclic donor moieties synthesized by [2+2] cycloaddition-retroelectrocyclization reaction

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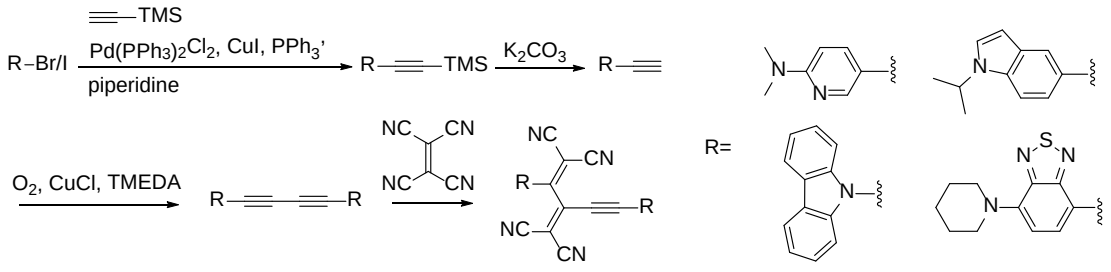
The [2+2] cycloaddition-retroelectrocyclization (CA-RE) reaction is an effective method for synthesizing push-pull chromophores with the advantages of the click reaction.[1] 2-[4-(Dimethylamino)phenyl]-3-([4(dimethylamino)phenyl]-ethynyl)-buta-1,3-diene-1,1,4,4-tetracarbonitrile (DDMEBT), obtained by the [2+2] CA-RE reaction, is a promising nonlinear optical (NLO) material.[2] DDMEBT can form a homogenous film with high-optical quality due to the nonplanar structure, leading to further advanced applications in all-optical switching.[3]

NLO properties of organic molecules can be tuned by molecular design. In this study, we designed and synthesized various donor-substituted 1,1,4,4-tetracyanobutadienes (TCBDs), in which the donor moiety is substituted with different heterocyclic substituents, including pyridine, carbazole, indole, and benzothiadiazole, referring to the structure of DDMEBT. These new TCBDs were characterized by ^{1}H-NMR, ^{13}C-NMR, FT-IR, and MALDI-TOF MS. Optical properties, electrochemical properties, and thermal stability of these chromophores were investigated by UV-Vis spectroscopy, cyclic voltammetry, TGA and DSC. Single crystal XRD data were employed to estimate the bond length alternation of the donor cyclic unit, which is a good indication of the efficiency of intramolecular charge transfer from donor to acceptor moieties.



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