

DOCTORAL THESIS

Synthesis and characterization of naphthodithiophene based copolymers for bulk heterojunction solar cells

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Abstract

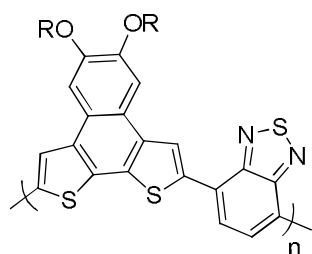
Naphthonaphtho[2,1-*b*:3,4-*b'*]dithiophene is a good electron-rich building block for p-type semiconducting materials and has been extensively studied in our group. Various donor-acceptor type copolymers based on naphtho[2,1-*b*:3,4-*b'*]dithiophene were designed and synthesized for high-performance bulk heterojunction solar cell applications. The structure-property relationship of these copolymers with respect to the influence of alkyl side-chain position and chain length, fluorination substitution effect as well as acceptor group effect with different electron withdrawing ability were also investigated.

The results of the PV device performance based on these copolymers indicated that the device efficiency was sensitive to the position of the alkyl side-chains attached, which could cause non-planarity of polymer backbone. The resulting naphthodithiophene-based copolymer with shorter side-chains afforded higher device efficiency. The incorporation of fluorine atoms into the copolymers leading to the poor solubility caused a decrease in the device performance compared to the non-fluorinated counterparts. The copolymer with thiadiazol[3,4-*c*]pyridine as an electron-deficient unit also showed promising device performance with efficiency up to 5.10%.

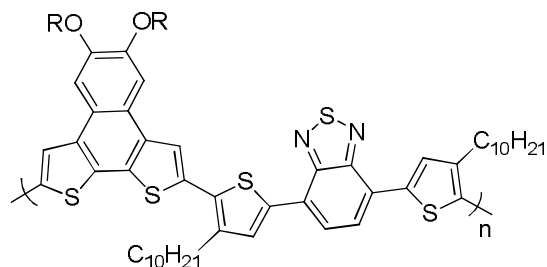
Among all the copolymers designed and synthesized, three copolymers namely **PNB-4**, **PNB-C2,6** and **PNTF** exhibited excellent preliminary device performance with a PCE more than 5.0% showing potential for further device optimization and

development. And the molecular structure of all the copolymers synthesized are shown

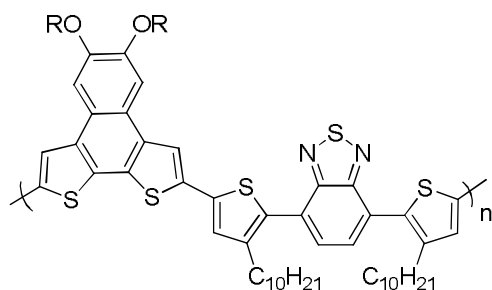
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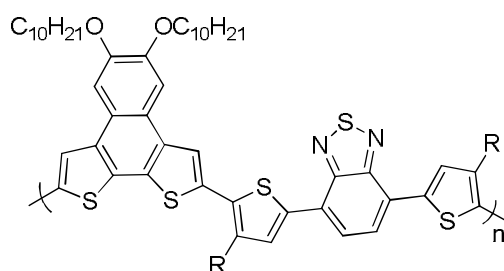
PNB-3 R = 2-ethylhexyl



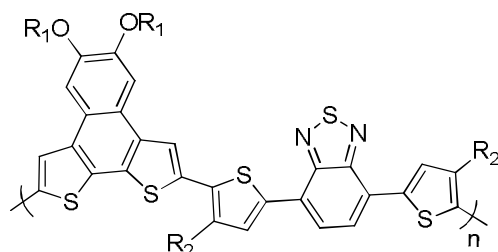
PNB-4 R = 2-ethylhexyl



PNB-5 R = 2-ethylhexyl



PNB-6 R = 2-ethylhexyl

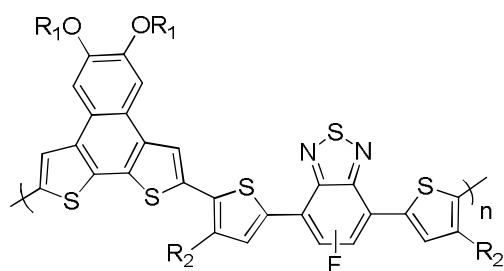


PNB-C2,6 R₁ = 2-ethylhexyl, R₂ = 2-ethylhexyl

PNB-C12 R₁ = 2-ethylhexyl, R₂ = *n*-C₁₂H₂₅

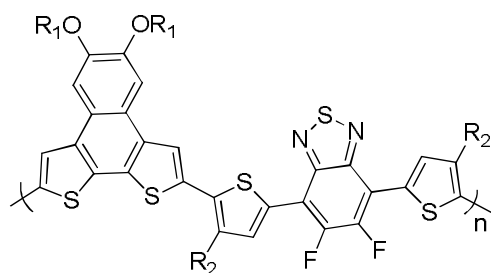
PNB-C14 R₁ = 2-ethylhexyl, R₂ = *n*-C₁₄H₂₉

PNB-C16 R₁ = 2-ethylhexyl, R₂ = *n*-C₁₆H₃₃



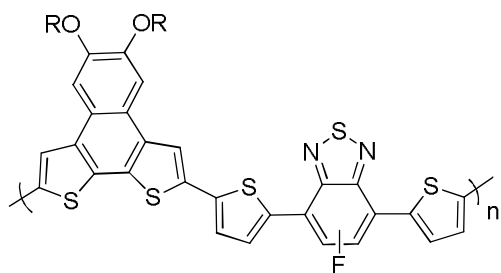
PNFtB-C2,6;C10 R₁ = 2-ethylhexyl, R₂ = *n*-C₁₀H₂₁

PNFtB-C2,6;C2,6 R₁ = R₂ = 2-ethylhexyl

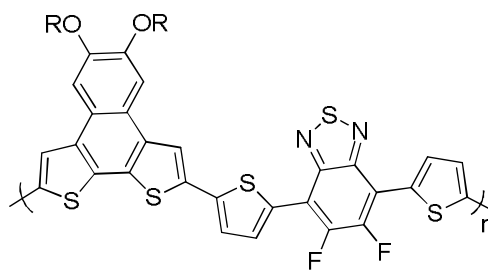


PNFftB-C2,6;C10 R₁ = 2-ethylhexyl, R₂ = *n*-C₁₀H₂₁

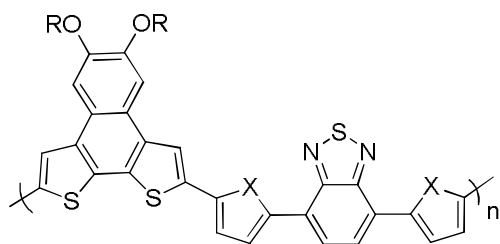
PNFftB-C2,6;C2,6 R₁ = R₂ = 2-ethylhexyl



PNfTB-C10,C14 R = 2-decyltetradecyl

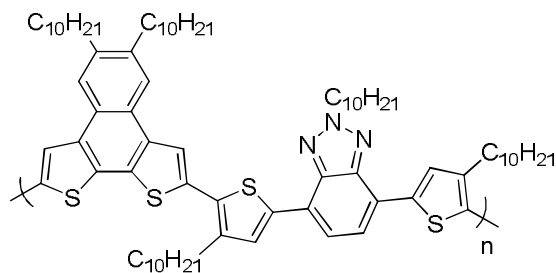


PNffTB-C10,C14 R = 2-decyltetradecyl

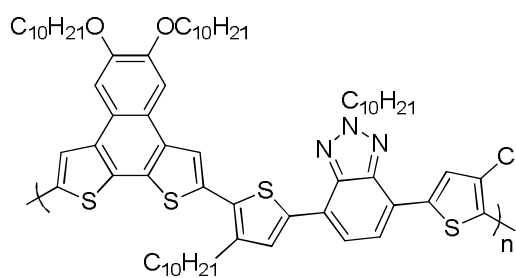


PNTB-C10,C14 X = S, R = 2-decyltetradecyl

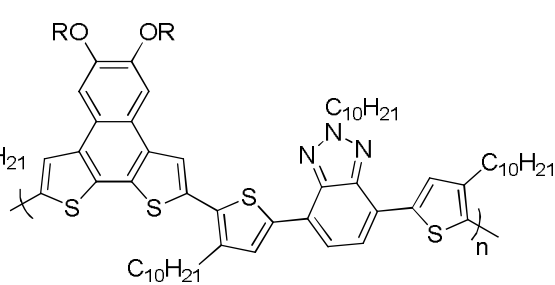
PNSeB-C10,C14 X = Se, R = 2-decyltetradecyl



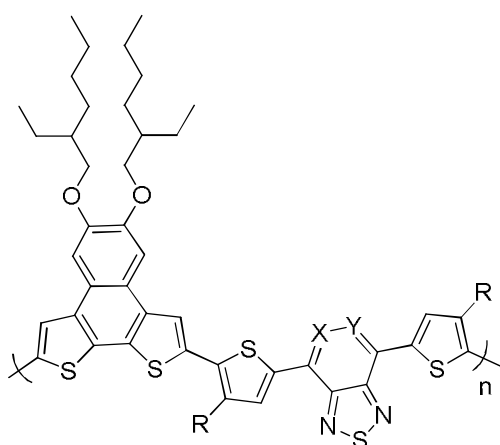
PNBTA-1



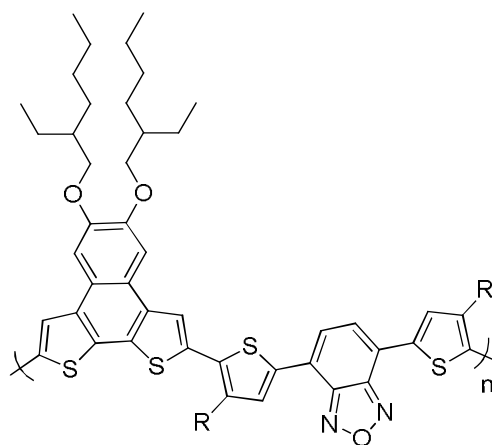
PNBTA-2



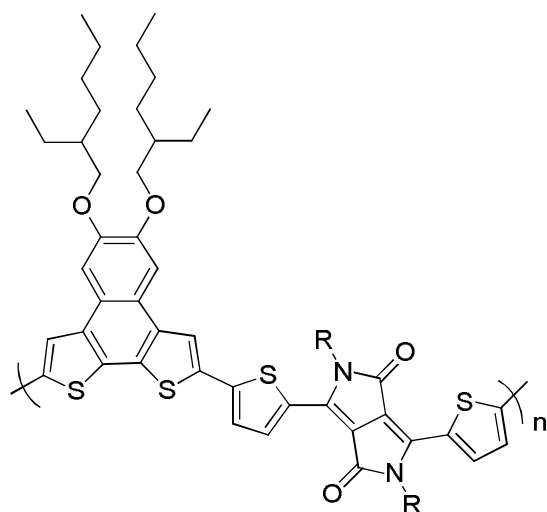
PNBTA-3 R = 2-ethylhexyl



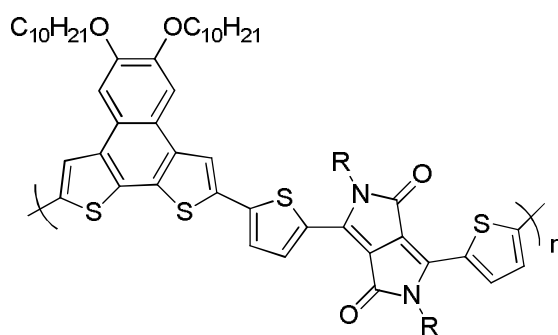
PNTP X = C, Y = N. or X = N, Y = C R = 2-ethylhexyl



PNBO R = 2-ethylhexyl



PNDPP-1 R = 2-decyltetradecyl



PNDPP-2 R = 2-decyltetradecyl

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