Palladium end-capped polyynes via oxidative addition of 1-haloalkynes to $Pd(PPh_3)_4$.

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Streszczenie

Reported here is the use of 1-haloacetylenes and 1-halopolyynes as synthons for the preparation of new palladium(II) end-capped polyynes. The 1-haloalkynes were obtained in a series of transformations from *para*-substituted bromoarenes that included Sonogashira coupling followed by halogenation and chain elongation via Cadiot–Chodkiewicz protocol. The key step for the synthesis of metal complexes was oxidative addition of 1-haloalkynes to $Pd(PPh_3)_4$, which allowed obtaining a series of metal compounds **1**–**5**-C_nX with carbon chains up to hexatriyne in 75–100% yield. All the compounds were characterized by NMR and HRMS or elemental analysis. The ^{13}C spectra of the 1-haloalkynes showed interesting, although expected, shifts of the carbon chain atoms close to the halogen termini. X-ray crystal structures were obtained for three polyynes—two butadiynes (**2**-C_4[Pd]Br and **3**-C_4[Pd]Br) and one hexatriyne (**1**-C_6[Pd]Br)—and the latter is the first reported X-ray crystal structure of palladium end-capped hexatriyne.

Adres publiczny

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https://www.acs.org/content/acs/en.html